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Using the Foldy-Wouthuysen Transformation to Derive Acoustic Parabolic Equations that Properly "Dress" Discontinuities

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14. ABSTRACT

This effort develops a firm theoretical foundation for the acoustic parabolic equation (PE) used in the presence of penetrable rough interfaces. As the interface roughness extends through the wavelength scale, it induces Bragg scattering (i.e., behaves like a diffraction grating). This is a nontrivial, phase-sensitive problem that involves theoretical and computational challenges that go beyond those found in problems to which the PE is most typically applied. A satisfactory formalism that addresses Bragg scattering should fully integrate the PE with field and rough surface scattering theories. In this report, the Foldy-Wouthuysen (FW) transformation is used to design a PE formalism that addresses this challenge. Along an interface where the density jumps, the full-wave problem predicts a jump in the downrange flux, but the PE generated by the FW transformation buffers this discontinuity by absorbing it into the higher-order boundary conditions. The new formalism is free of the ad hoc fixes that have characterized the PE methods currently used in the vicinity of a jump in the density, and it is ideally suited for the modeling of (forward) scattering from multiscale rough surfaces. The formalism can also be used to generate stochastic equations in circumstances where it has been impossible until now to do so.

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EXECUTIVE SUMMARY

OVERVIEW

The goal of this effort is to develop a firm theoretical foundation for the acoustic parabolic equation (PE) used in the presence of penetrable rough interfaces. As the interface roughness extends through the wavelength scale, it induces Bragg scattering (i.e., it behaves like a diffraction grating). This is a nontrivial, phase-sensitive problem that involves theoretical and computational challenges that go beyond those found in problems to which the PE is most typically applied. A satisfactory formalism that addresses Bragg scattering should fully integrate the parabolic equation with field and rough surface scattering theories. Such a formalism is available for impenetrable rough surfaces (i.e., infinite density jumps), but the traditional PE formalism for a finite density jump is based on ad hoc arguments rather than on a formal development grounded in these theories. In this report, the Foldy-Wouthuysen transformation is used to design a parabolic equation formalism that addresses this challenge. The associated parabolic equations predict phenomena not previously noted, and two of these are examined in detail:

1. the classical equivalent of vacuum polarization
2. the buffering of jumps in the downrange flux at a density jump.

The former involves interesting physics, but it is a modest effect and there are no immediate applications related to underwater sonar. The study of the classical "vacuum polarization" is primarily significant for the insights it provides about the nature of the parabolic equations generated by our formal approach. The second topic of this study, on the other hand, leads to significant practical applications. Along an interface where the density jumps, the full-wave problem predicts a jump in the downrange flux, but the parabolic equation generated by the Foldy-Wouthuysen transformation buffers this discontinuity by absorbing it into the higher-order boundary conditions. The new formalism is free of the ad hoc fixes that have characterized the parabolic equation methods currently used in the vicinity of a jump in the density. This is significant because the techniques used to adapt the PE to rough impenetrable interfaces ultimately rely on conformal mappings, a local method of images, perturbation theory, or some similar distortion of the range-independent problem, while the ad hoc fixes currently employed at a density jump prevent the use of such distortions. The new PE, on the other hand, allows interfaces where the density jumps (such as the ocean bottom) to be distorted into rough ones, and so it is ideally suited for the modeling of (forward) scattering from multiscale rough surfaces. The formalism can also be used to generate stochastic equations in circumstances where it has been impossible until now to do so.

TECHNICAL APPROACH

The parabolic equation (PE) is widely used to model the propagation of classical fields in ducted environments. This equation is essentially the Schrödinger equation for a classical field, where the range plays the role of the time. One of the principal challenges in constructing this type of 1-way stepping algorithm is the incorporation of multiscale stochastic range-dependent fluctuations of the environment near interfaces where the environmental parameters or their gradients are discontinuous. Atomic physics suggests a technique for doing so. As the hydrogen atom is advected by vacuum fluctuations, the electron field encounters a turbulent environment similar to that encountered, for example, by an underwater acoustic field. In Welton's semi-classical model, the atomic Lamb shift is generated by a contact potential

that is a direct consequence of time-averaging the interaction of the electron field with these fluctuations. This contact potential at the nucleus of the atom is connected to a singularity in the gradient of the potential that is step-like in the sense that its divergence is a δ-function. This contact potential shifts the energy levels (i.e., eigenvalues) for the stochastic coherent (i.e., average) field. A Schrödinger equation derived using the Foldy-Wouthuysen transformation introduces an aspect of this phenomenon that is often missed by semi-classical treatments. Although the fluctuations in 3-dimensional physical space are imposed by hand, the resultant time-dependent potential also induces virtual fluctuations in the time domain, and this effect appears in the form of new terms that appear in the Schrödinger equation derived using the Foldy-Wouthuysen transformation. *Even before time averaging*, the fluctuating singularity at the nucleus has been buffered by a cloud of virtual particle pairs. Using the terminology of field theory, "vacuum polarization" has "dressed" the bare singularity. The "vacuum polarization" effect also induces a δ-function, and it provides a correction to the basic Lamb shift effect.

This provides a context for using the parabolic equation to explore acoustic effects directly analogous to the Lamb shift. Consider a sound speed profile that contains singularities such as jumps in the sound speed and/or its gradient. Take a stochastic average, and consider the coherent (i.e., average) field. The averaging process leaves us with contact potentials along the range-*in*dependent *average* of the interfaces, where the sound speed profile contains singularities. By taking transverse integrals, we see that the contact potentials modify the boundary conditions on the wave function at the interface. We can decompose the coherent field solutions into modes (i.e., eigenfunctions). In the acoustic Lamb shift, the downrange components of the wavevectors characterizing the modes are the eigenvalues, and so these take the place of the energy in the atomic problem, and so it is shifted by the changes in the boundary conditions. In a realistic shallow-water scenario, this in turn shifts the features of the transmission loss curve. While this can be "significant" in a formal sense (10 dB or more at a fixed location if we also go on to include for this particular effect the contribution from a density jump at the ocean bottom), given the nature of field experiments and current sonar implementations, the data are rarely taken in a way that would readily lend itself to an examination of this phenomenon. Therefore currently, the primary significance of the classical Lamb shift lies in what in tells us about the nature of the parabolic equations generated by our formal approach. The dominant contribution to the Lamb shift results from the smearing of a stochastic rough surface, but the Foldy-Wouthuysen transformation applied to the acoustic wave equation also generates a classical manifestation of the "vacuum polarization" correction to the Lamb shift. As with the quantum problem, this effect provides only a modest contribution to the classical Lamb shift, but it is significant because it is intrinsic to the parabolic approximation and so the smearing already occurs in the deterministic problem. While this is the first example in acoustics of the Foldy-Wouthuysen transformation "dressing" a bare singularity, the formalism similarly addresses other singularities that are apparently unique to classical fields. Most importantly, it "dresses" the jump in downrange flux associated with a density discontinuity, thus eliminating the need for the ad hoc fixes usually employed whenever the parabolic equation is used to model an acoustic field near a 2-fluid interface (such as a penetrable rough ocean bottom). The formalism reproduces as special cases the most successful methods currently in use, and puts them on a firm theoretical foundation. It also suggests higher-order corrections to these results. Most significantly, by buffering the singularity, the new formalism imposes well-behaved boundary conditions along the interface that can be incorporated naturally into a stepping algorithm – even along a sloping interface. In this way, the formalism is uniquely applicable to multiscale deterministic rough interfaces. he second-order deterministic theory is specifically examined in this report. The formalism moreover allows consideration of stochastic rough ocean bottoms in realistic scenarios, where it has not been previously possible to do so.

Similar issues appear with electromagnetic and elastodynamic fields, and this technique can be applied to these problems as well. Here, the creative insights needed to adapt the formalism to these cases are addressed.

USING THE FOLDY-WOUTHUYSEN TRANSFORMATION TO DERIVE ACOUSTIC PARABOLIC EQUATIONS THAT PROPERLY "DRESS" DISCONTINUITIES

1. INTRODUCTION AND ROADMAP

A new systematic technique for deriving the parabolic equation (PE) for classical fields has been developed over the last several years. This effort began with a novel derivation of the acoustic PE that introduced a new physical effect into the context of long-range propagation in the underwater sound channel [1]. Over the ensuing years, this line of research has spawned a wide range of new developments. Preliminary reports of aspects of this long-term effort have been presented orally [2-6], while in two recent articles by the author [7, 8] the result of this effort that is of most immediate practical concern was discussed: an acoustic PE that inherently buffers density discontinuities in a manner dictated by a precise physical theory. The practical relevance of this result lies in the fact that it addresses a key challenge confronting the PE technique: the need to model scattering from and propagation through penetrable rough interfaces characterized by a density jump (such as are found at the ocean bottom).

This NRL report provides a comprehensive treatment covering the entire body of work performed on this topic during the last seven years. It provides a new formal development of the physical and mathematical theory associated with the range-dependent PE. The narrative below is structured in a way that provides insight into the evolution of the formalism. It involves both a deeper look at topics introduced in previous papers [1, 7-8] and a look at new topics.

After the effort motivation is described in Section 2, Section 3 develops the tools that lie at the core of the new approach. Section 4 introduces jumps in the sound speed, and looks at a comparatively straightforward phenomenon associated with such jumps: the classical Lamb shift, including a small correction term that is very significant for what it reveals about the basic nature of the PE. Section 5 introduces the density jump, and expands the analysis of Section 4 to include the density jump. Section 6 leverages the insights gained in Sections 3 through 5 to develop a full understanding of the issues related to the PE in the vicinity of a density jump, while Section 7 extends the basic technique to electromagnetic and elastodynamic fields. The discussion is summarized by Section 8.

The rest of this section provides a detailed roadmap of the report.

Section 2. This section aims to establish the need for designing a PE adapted for use near a penetrable rough surface, and to explore its potential significance to underwater acoustics. Section 2.1 provides an overview of the relevant aspects of the PE formalism, while Section 2.2 discusses the basic approaches used to adapt this formalism to an interface where the density jumps. Section 2.3 examines previous adaptations of the PE formalism specifically tailored to the very tricky problem of Bragg scattering[a] from a rough interface associated with a density jump, and then identifies the shortcomings that have limited the utility of these approaches. This state of affairs has resulted in a dearth of adequate PE models for the

[a] Bragg scattering occurs when the surface has wavelength-scale roughness, and consequently scatters the field like a diffraction grating.

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very important problem of roughness-induced acoustic penetration into the ocean bottom. The primary goal of this work is, therefore, to design a new PE that is well-suited for this problem.

Figure 1 provides a more detailed schematic overview of Section 2. The basic PE in the water column essentially corresponds to a factorization of the Helmholtz equation. However, when range dependence is added, the PE actually propagates an auxiliary field that roughly corresponds to the square root of the downrange flux. Many common ocean bottoms consist of sand and mud, which are typically modeled as fluids. Then, the associated density jump is treated using one of two formal approaches. The first involves a global change of variables, and then replaces the interface with a gradual transition. The second approach breaks the interface into stair steps, and once again, an auxiliary field corresponding roughly to the square root of the downrange flux is conserved at the vertical interfaces. Because of its success in matching benchmark solutions, the second method is now usually used to model standard problems in underwater acoustics. However, when the interface is rough through the wavelength scale, the physics of the problem changes. The standard approach ceases to be practicable, and it is consequently preempted by a host of alternate approaches. None of these alternatives is entirely satisfactory. This report, therefore, provides a new approach that is designed for the rough interface problem and solves the shortcomings of both the stair step approach and the alternatives that have been used for the rough interface problem.

Section 3. The formal approach used to develop the new PE theory is examined here. The development begins with the introduction of the Foldy-Wouthuysen (FW) transformation in Section 3.1. This transformation was originally developed in order to connect the full relativistic theory of the hydrogen atom to the widely used non-relativistic theory based on the Schrödinger equation, and here it is adapted to the similar problem of connecting the Helmholtz equation for an acoustic field with the corresponding PE. Section 3.2 discusses the direct acoustic equivalent of the atomic Lamb shift, which occurs when a cusp in the sound speed (i.e., a discontinuity in the sound speed gradient) is advected by a stochastic rough surface. The dominant component of the classical Lamb shift is associated with roughness-induced smearing of the interface in the transverse direction, but it is also shown that the new terms generated by the FW transformation produce a correction to the Lamb shift associated with uprange/downrange smearing. These assertions are backed up by the development of a "toy model" of the atomic Lamb shift that shows the connection between the classical and the quantum mechanical Lamb shift. Our consideration of the sound speed cusp along a stochastic rough surface is unique in that it both has a clear precedent and also involves the new contact potentials imposed by the FW transformation along a penetrable rough surface. Subsequently in Section 3.3, the systematic construction of a new downrange stepping procedure begins with an examination of the mechanics of discretizing a PE in order to create a downrange stepping algorithm near a sloped penetrable interface. (This issue of interface slope was sidestepped by the approaches discussed in Section 2.3). Section 3.3.1 discusses the discrete form of the PE, while Section 3.3.2 addresses the crucial problem of evaluating the Hamiltonian at the interface in the discrete problem. It is shown that higher-order boundary conditions are a key ingredient of this stepping procedure. The existence of such conditions has occasionally been noted in the past, but no procedure for determining (let alone exploiting) them has met with wide acceptance. Section 3.3.3 outlines the way that the FW transformation imposes boundary conditions at an interface. These boundary conditions are generated by contact potentials, which emerge from the FW procedure. The examination in Section 3.2 of the contact potentials generated by the classical Lamb shift serves to lay the groundwork for the expanded role that contact potentials play in the context of Section 3.3.3.

Section 4. This section examines the issue of an interface, where the sound speed itself (and not just its gradient) is discontinuous. At the core of this study once again lie the two ways in which interface roughness buffers the singularity at a sound speed cusp–uprange/downrange and transverse smearing (i.e., the classical Lamb shift)–and examines these phenomena in the context of the sound speed jump. Our study of these phenomena will provide a vehicle allowing us to further develop various aspects of the formal structure that were introduced in Section 3. In Section 4.1, a "quasi-first-order" theory

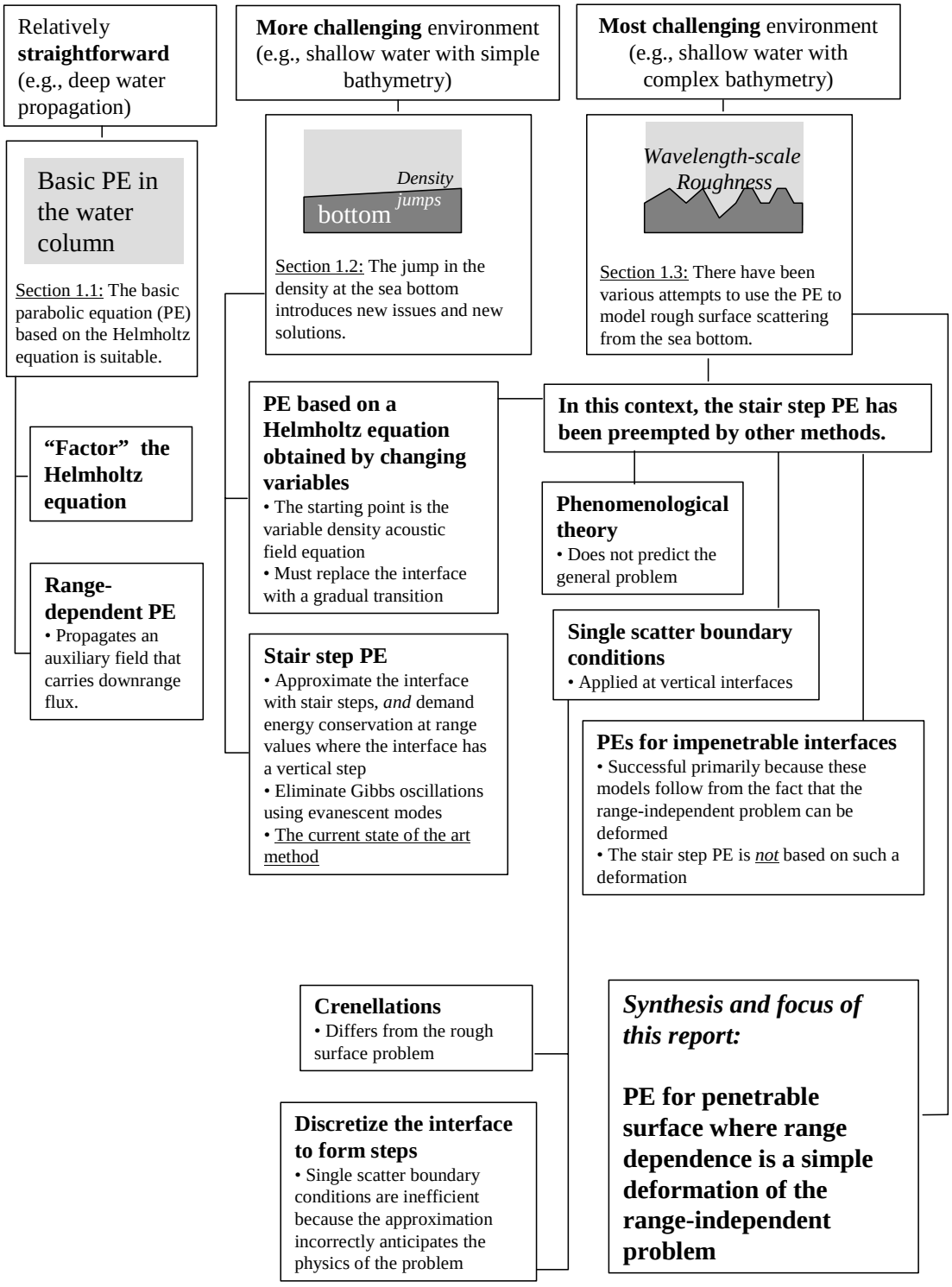

Fig. 1 — A schematic of the context of the results of this report in the development of underwater acoustics

is considered. The term from the FW transformation that is known to be responsible for uprange/ downrange smearing is paired with the basic lowest order Hamiltonian. The result is a hybrid between first- and third-order PE theory, but the two extra orders in the FW term come from downrange derivatives, which are in this context excluded from the power counting. Next, in Section 4.2, the resultant boundary conditions along a deterministic interface are examined in detail. In order to interpret these conditions, it is necessary to consider how boundary conditions "migrate" as the lead order in the Hamiltonian changes. Indeed, we find that the relationships between some of the boundary conditions that appear in the PE and their corresponding manifestations in the full wave problem are often the most apparent for a PE of specific order, and that the connections can become quite obscure at other orders. This finding will play a pivotal role later in Section 6.1. Section 4.3 includes stochastic effects, most notably the classical Lamb shift induced by a sound speed jump. This time, uprange/downrange smearing cancels out in the stochastic problem, leaving only transverse smearing to contribute to the Lamb shift associated with a sound speed jump. In Section 4.4, the various physical phenomena examined in this effort are placed into a broader context.

Section 5. The density jump is introduced here. In Section 5.1, the basic components of the FW procedure are adapted to the case where the density jumps, and then Section 5.2 discusses δ-function bifurcation, an important new tool needed for adapting the results to interfaces where the density jumps. In Section 5.3, the interface where the density jumps is examined for the first time. Once again, deterministic "quasi-first-order" theory is used to examine the smearing induced by the new FW term. Then, the stochastic problem is considered and the classical Lamb shift associated with a density and sound speed jump is obtained. Transverse smearing induced by averaging the rough interface once again dominates, but now with a density jump present, the smearing induced by the FW term survives the averaging process. The examination of the classical Lamb shift concludes with a discussion of its possible relevance to underwater acoustics.

Sections 4 and 5 juxtapose the dominant component of the Lamb shift, transverse smearing in the stochastic problem, with tilt-induced smearing in the deterministic problem in order to demonstrate that the PE buffers (i.e., smears out) singularities in the deterministic problem in a way that closely mimics the buffering imposed by the stochastic problem.

Section 6. With the conclusion of our discussion of the classical Lamb shift, we finally have developed the formal wherewithal to pursue the primary goal of this report: the construction of a PE suitable for a rough interface characterized by a density jump. This issue, which is the most pressing one from a practical point of view, is addressed in Section 6. In Section 6.1, a new effect associated with a density jump is identified, named (as Bragg-scale vorticity), and then incorporated into the PE formalism. Bragg-scale vorticity occurs because along a density jump, the fluid picks up an oscillating twist at the wavelength scale. Although Bragg-scale vorticity enters the acoustic problem in a way that evokes no direct analogies from atomic physics, the mathematical formalism built up to this point imposes a specific procedure for incorporating this effect. It emerges naturally from the high-order PE at an interface, where the density jumps. A full second-order PE at the interface is derived and analyzed. The subtle mechanics associated with the formalism is discussed as well. Once again, we find that the singularity (in this case the density jump) has been buffered. This type of buffering is more subtle than the ones studied in Sections 3.2, 4, and 5.3, and these previous results provide a conceptual groundwork for recognizing and understanding this phenomenon. The new result is then placed into the context of current PE techniques in Section 6.2.

Section 7. This section adapts the formal approach developed for the acoustic field with varying density to the electromagnetic (Section 7.1) and elastodynamic (Section 7.2) problems. The discussion sets up the problem by deriving the state space equation and by taking a brief look at the transformations connecting the familiar full-wave fields with the associated auxiliary fields that are propagated by the PE. It turns out that jumps in electric and magnetic permeability (in electromagnetic theory) and in the second

Lamé parameter (in the theory of elastic waves) involve issues that are similar to those associated with jumps in the density in the acoustic problem (i.e., the issues associated with Bragg-scale vorticity).

Section 8. This wraps up the current discussion. The results are summarized in Section 8.1, and finally future developments are discussed in Section 8.2.

2. BACKGROUND AND MOTIVATION

This section examines the context of this work. Section 2.1 establishes the basic PE formalism to be used in this report, while in Section 2.2 examines the implications of an interface where the density jumps. Section 2.3 reviews previous adaptations of the PE formalism to Bragg scattering from a rough interface associated with a density jump, and then identifies the shortcomings that have limited the utility of these approaches.

2.1 The Parabolic Equation (PE)

2.1.1 The Significance of the Parabolic Equation

The salient features of the PE are that it inherently selects out a preferred direction designated as the range and then further stipulates that the range dependence of the environmental parameters is modest and that the propagation is mostly in the downrange direction. A more precise definition of these conditions will emerge as we examine the formalism below. For the moment, note that this scenario is most typical of ducted propagation – in other words, it occurs in environments where the propagation is by and large constrained to the vicinity of the downrange direction for a broad range of initial conditions. Two examples commonly found are long-range propagation in the deep-water sound channel and shallow water propagation (for current purposes, the shallow water problem is characterized by depths on the order of 30 to 100 m and ranges in the 1 to 40 km range). The latter is currently of more interest from a practical point of view, and it also involves the more challenging issues from a modeling perspective. In this context the PE is typically applied to the 50 to 5000 Hz frequency range, but the results developed in the discussion that follows are not a priori restricted to this range. The theoretical work developed here therefore aims to broaden the techniques that are available for modeling the propagation of acoustic waves in a ducted underwater environment.

If the features of the ducted environment are all significantly larger than a wavelength, then the geometrical acoustics limit applies, and the propagation can be modeled by tracing rays. This method is attractive because it is fast. This advantage is particularly significant in time-dependent problems. The time imposes an extra dimension, and one must either discretize the time domain or use Fourier decomposition. This complicates the problem and slows the numerical algorithms used to model the field, but ray tracing bypasses this need. The widespread use of ray tracing is further guaranteed by the fact that it is a very effective way to model signal spread due to multipathing, which is of particular interest to those that evaluate a field's utility as a signal carrier.

The utility of ray tracing is, however, limited by several factors. In complex environments, rays proliferate dramatically, and the bookkeeping associated with this technique can become prohibitive. In fact, in environments with significant range dependence, a ducted environment can exhibit chaos-like ray proliferation, and the breakdown of ray-tracing method occurs on a fundamental level [9,10]. On an equally fundamental level, ray tracing cannot model full-wave effects associated with physical acoustics. These are present when the environmental parameters vary on the wavelength-scale (as often occurs in acoustics). For these reasons, in underwater acoustics, ray-tracing will often have to be abandoned in favor of full-wave techniques.

In principle, ducted propagation problems can be solved using full-wave techniques such as numerical inversion or coupled modes. In such approaches, all points are causally connected in the sense that the field at any given point is influenced by what happens to the field at every other point. In one manner or another, the formalism is ultimately forced to calculate all these mutual relationships. In many realistically complex environments, these techniques become so numerically intensive that they often fall beyond the practical range of even the fastest computers. Furthermore, brute force calculations of this type are so divorced from physical insight that their utility as diagnostic tools is limited, and it is often difficult to separate numerical artifact from bona fide physical effect.

The PE is a one-way stepping algorithm based on the physical insight that in ducted propagation the value of the field at a given point in space can be by and large determined without knowledge of what subsequently happens to the field downrange from that point[b]. The scaled-back causal structure significantly streamlines numerical calculations based on the PE. Furthermore, in range-dependent environments, the PE correctly models mode coupling, and strong mode-coupling is precisely the phenomenon that leads to the breakdown of the coupled-mode and ray-tracing approaches[c]. The PE thus expresses the wave equation in a representation that is ideally suited for the computer modeling of classical wave propagation in a ducted environment[d].

2.1.2 The Underlying Physical Problem

This section establishes a basic notation for our study of the PE and then uses it to outline the physical problem that is to be approximated by the PE.

2.1.2.1 The Basic Geometry of the Environment

Assume a Cartesian coordinate system with the positive *x*-axis pointing in the downrange direction and *z* the depth coordinate (the convention in this report has the *z*-axis point upward, for example, away from the ocean bottom and towards the air-sea interface). Denote the two-dimensional vector transverse to the range by $\underline{R}_T = (y, z)$[e]. The geometry of the ducted environment is shown in Fig. 2.

[b] To see this, note that Huygens' principle recovers all the geometrical and physical optics (or acoustics) associated with forward propagation, is valid in the physical three-dimensional space, and only depends on the same one-way causality inherent in the PE.

[c] The former breaks down because solutions constantly need to be glued together, and the latter because of ray proliferation.

[d] It should also be noted that the PE often provides more physical intuition than do "brute-force" simulations based on full-wave theory. That is ultimately the reason why the Schrödinger equation is still widely taught and used to study the hydrogen atom, even though simulations based on numerical solutions to relativistic quantum mechanics are in principle available.

[e] This coordinate system is preferable for the formal work pursued in this report, although cylindrical coordinates are more appropriate for many physical applications. The result in cylindrical coordinates is mathematically identical to that obtained when the Cartesian coordinate system is used, provided that the radial coordinate *r* is substituted for *x*, the wave function is rescaled by a factor $1/\sqrt{r}$, and nonpropagating terms proportional to $1/r$ are dropped.

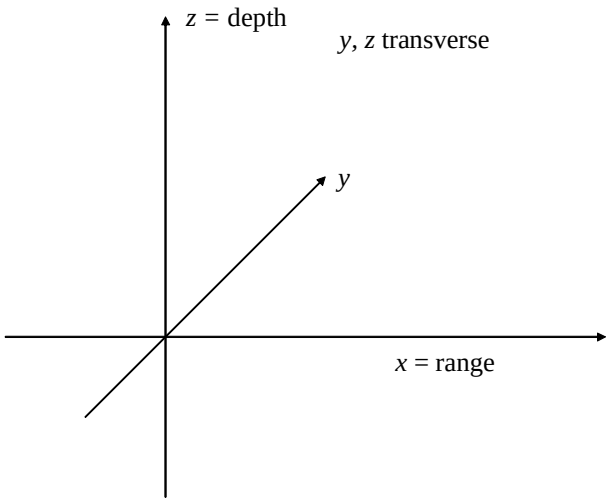

Fig. 2 — The geometry of a typical ducted environment

2.1.2.2 The Related Full-Wave Equation

The acoustic pressure field $P(x,\underline{R}_T,t)$ is assumed to propagate according to the acoustic wave equation (see Ref. 11)

$$\rho\vec{\nabla}\cdot\left(\frac{1}{\rho}\vec{\nabla}P\right)-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}P=0$$

through a time-independent environment. The three-dimensional gradient is given by $\vec{\nabla}\equiv(\partial/\partial x,\underline{\nabla}_T)$, where $\underline{\nabla}_T=(\partial/\partial y,\partial/\partial z)$ is the two-dimensional gradient in the transverse direction. In general, the density ρ and the sound speed c can depend on the coordinates $(x,\underline{R}_T)$. Since the problem is time-independent, each frequency ω can be considered separately, and so the pressure is given by the integral over ω of $P_\omega(x,\underline{R}_T,t)=\mathrm{Re}\left[A(x,\underline{R}_T)e^{-i\omega t}\right]$, where A is a complex field obeying the equation

$$\rho\vec{\nabla}\cdot\left(\frac{1}{\rho}\vec{\nabla}A\right)+\frac{\omega^2}{c^2}A=0\,. \tag{1}$$

By time averaging over the period of the wave, observable physical quantities such as the downrange energy flux and the scattering cross-section can be calculated directly from the complex field *A*.

Note that *c* and ρ depend on the two-dimensional transverse coordinate $\underline{R}_T$. In many instances below, we consider the two-dimensional problem where the *y*-coordinate falls out and the depth *z* is the only transverse coordinate. To be specific, general formal development will apply both to the full three-dimensional $x-y-z$-space and to two-dimensional $x-z$ space. However, in the current report, once interfaces are explicitly introduced into the formalism, only one-dimensional interfaces $z=f(x)$ embedded in two-dimensional $x-z$ space are considered. The generalization to the full three-dimensional space is very briefly examined at the end of Section 3.3.1 and again in Section 3.3.3. Although this treatment is supplemented by Appendix G, the full development of a formalism good for

two-dimensional surfaces $z = f(x,y)$ embedded in three-dimensional $x-y-z$ space is deferred to future work. Currently available applications of the PE formalism also typically apply to the two-dimensional problem ($x-z$ -space).

2.1.3 A First Look at the PE

Let us now introduce the PE with an intuitive and frequently used derivation of its most basic form and then briefly examine how the result is used by modelers. The effects of range-dependence are examined next, and this is followed by a discussion of the fundamental limits inherent to the kinds of PEs developed by the approaches pursued in this report.

2.1.3.1 A "Quick And Dirty" Derivation

For the moment assuming that the density is constant, A obeys the Helmholtz equation:

$$\frac{\partial^2 A}{\partial x^2} + \nabla_T^2 A + k^2(x, \underline{R}_T)A = 0\,. \tag{2}$$

The wave number *k* is the frequency ω divided by the sound speed *c*. In the traditional derivation of the PE, the range dependence of the sound speed profile is assumed to be sufficiently modest that it can be ignored (i.e., temporarily assume that $k \equiv \omega/c(\underline{R}_T) = k(\underline{R}_T)$). It is then possible to unambiguously factor the Helmholtz equation:

$$\left(-i\frac{\partial}{\partial x} + \sqrt{\nabla_T^2 + k^2}\right)\left(i\frac{\partial}{\partial x} + \sqrt{\nabla_T^2 + k^2}\right)A = 0\,. \tag{3}$$

Since *k* is range-independent, $i\partial/\partial x$ and $\sqrt{\nabla_T^2 + k^2}$ commute[f] and the cross-terms cancel so that the product above indeed reproduces the Helmholtz operator. Furthermore, the order of the factors in the product does not matter, and thus *A* is a solution to the Helmholtz equation whenever either factor operating on *A* is zero. Typically, the branch that corresponds to downrange propagation is chosen, and the terms are reorganized to create an operator "$2\lambda/k_0$" that is small in some sense[g]:

$$-i\frac{\partial A}{\partial x} = \sqrt{\nabla_T^2 + k^2}\,A = \sqrt{\nabla_T^2 - (1-n^2)k_0^2 + k_0^2}\,A = k_0\sqrt{1 + \frac{2\lambda}{k_0}}\,A\,, \tag{4}$$

where

$$\begin{aligned} &k = nk_0 \text{ for reference } k_0\,, \\ &\lambda \equiv \frac{\nabla_T^2}{2k_0} - \mu k_0\,, \\ &\text{and} \\ &\mu \equiv \frac{1-n^2}{2}. \end{aligned} \tag{5}$$

Complying with usage standard in Quantum Mechanics, differential operators (such as λ) embedded inside functions are understood to be the Taylor series expansions of the function with the operator acting

[f] Two operators α and β commute if $[\alpha,\beta] \equiv \alpha\beta - \beta\alpha = 0$. $[\alpha,\beta]$ is called the commutator of α and β . We will also make frequency use of the anti-commutator $\{\alpha,\beta\} \equiv \alpha\beta + \beta\alpha$. If $\{\alpha,\beta\} = 0$, then the two operators are said to anti-commute.

[g] Typically small means "corresponds to small (dimensionless) eigenvalues in the range independent case," but this has to be generalized when the density varies.

as the expansion parameter[h]. Specifically, the operator $\sqrt{1+2\lambda/k_0}$ will always be understood to be synonymous with the Taylor series expansion obtained by treating $2\lambda/k_0$ as an expansion parameter. The finite expansion of $k_0\sqrt{1+2\lambda/k_0}$ is known as the Hamiltonian *H*. For example, in Section 6.2.2, it will be convenient and illuminating to use the shorthand whereby functions of the operator $k_0\sqrt{1+2\lambda/k_0}$ are written as functions of $-i\partial/\partial x$ (following Eq. (4)).

The PE derived from the Helmholtz equation closely parallels the Schrödinger equation derived from the Klein-Gordon equation[i]. The first-order version of the PE was applied to electromagnetic fields by Leontovitch and Fock [12], and it was later applied to problems in geophysics by Claerbout [13]. Claerbout introduced the full square root operator to the classical problem in 1971 [14]. Tappert brought the PE formalism to underwater acoustics in 1977 [15].

2.1.3.2 The Numerical Implementation

When the PE is used in numerical calculations, it is discretized and transformed into a stepping algorithm as follows. Consider some field χ that obeys a generic PE $-i\,\partial\chi/\partial x = H\chi$. The Hamiltonian *H* is a function of the transverse derivative ∇_T. The leading order term is proportional to $\nabla_T^m\chi$. The equation is discretized to first-order in the step size Δx using the Mean Value Theorem. This constitutes the basic stepping algorithm. In a practical application, a pair of additional manipulations would typically be superimposed on top of this basic algorithm. The Crank-Nicholson procedure is usually used to make the algorithm manifestly unitary (even for finite step size) [16], and often (for a variety of technical reasons, including most notably to speed convergence), *H* would also be broken into fractions using a Padé approximation (pioneered by M. Collins – see, for example, Refs. 17 or 18; more precise terminology would be to call this a rational function approximation)[j]. Since these operations are imposed in separate formal steps after the basic stepping algorithm has been fully specified, it is not appropriate to consider them in the formal development being pursued in this report. Only the basic stepping algorithm is therefore discussed here. Subsequent imposition of the Crank-Nicholson algorithm should be fairly straightforward since it involves the same Hamiltonian, but adaptation of the Padé approximation to the new basic formalism will be a nontrivial topic for future research.

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[h] Differential operators embedded inside functions are more generally called pseudo-differential operators, but this terminology also incorporates circumstances where the Taylor series expansion does not converge.

[i] In this case, (using units where the Planck's constant $\hbar$ and the speed of light are set equal to one) the reference wave number k_0 becomes the rest mass, time takes the place of the range x, the transverse space is physical $x-y-z$-space, and the Minkowski metric of four-dimensional space time imposes an extra minus sign in front of the transverse gradient: $\nabla_T^2 = \underline{\nabla}_T\cdot\underline{\nabla}_T \Rightarrow -\vec{\nabla}\cdot\vec{\nabla} = -\nabla^2$. Second and higher orders in $2\lambda/k_0$ provide relativistic corrections. Usually, μ (now some dimensionless measure of a scalar potential) is set to 0 in this case. Scalar potentials affecting bosons are not typically introduced directly into the scalar Klein-Gordon equation. In fact, the physically realistic version of that problem would involve subtleties not relevant to the discussion here.

[j] The Crank-Nicholson procedure is necessary because we have discretized with finite steps: $-i\Delta A = (HA)\Delta x + \mathrm{O}\left((\Delta x)^2\right)$. At finite order in Δx, this operation is unitary only in the limit as $\Delta x \to 0$. The Crank-Nicholson procedure replaces this with a stepping prescription that is the same to $\mathrm{O}\left((\Delta x)^2\right)$, but preserves unitarity exactly (even for finite Δx). For example: $A_{\mathrm{new}} = (1+i(\Delta x)H)A_{\mathrm{old}} \to A_{\mathrm{new}} = [(1+i(\Delta x)H/2]/(1-i(\Delta x)H/2)]A_{\mathrm{old}}$ or $\left(1-i\left(\Delta x\right)H/2\right)A_{\mathrm{new}} = \left(1+i\left(\Delta x\right)H/2\right)A_{\mathrm{old}}$. When the problem is formulated in this form, it is possible to solve for A_{new} using standard techniques in numerical analysis. The Padé approximation represents yet another step beyond this. Now $H = p/q$ and we have $\left(q-i\left(\Delta x\right)p/2\right)A_{\mathrm{new}} = \left(q+i\left(\Delta x\right)p/2\right)A_{\mathrm{old}}$. This is a convenient way to obtain *H* to high orders in $2\lambda/k_0$.

2.1.3.3 Range Dependence

The formalism related to the PE can be upgraded to incorporate the effects of range dependence[k] via a two-step process. The first step is intuitively straightforward, while the second step is subtler[l].

The procedure begins with the observation that in a range-dependent environment, a factorization of the type given in Eq. (3) generates an unwanted commutator term in addition to the terms in the Helmholtz Eq. (2). The first step for incorporating this artifact of range dependence into the PE formalism occurs when we introduce order-by-order correction terms into the Hamiltonian to cancel the unwanted commutator terms (maintaining the symmetry between the uprange and downrange classes of solutions). Note that every time we add a new term to the Hamiltonian, we end up generating a new unwanted commutator term of higher order, so the procedure is iterative. A term proportional to $i\dot{\mu}$ ($= i\,\partial\mu/\partial x = \left[i\partial/\partial x, \mu\right] \propto \left[i\partial/\partial x, k_0 + \lambda\right]$; in this report the dot above a variable always denotes the downrange derivative $\partial/\partial x$) is added to perform the first iteration on the O(λ) Hamiltonian. To O($\lambda\dot{\lambda}$) this term indeed cancels the commutator term produced by a factorization of the type given in Eq. (3) above. A lucid and well-developed examination of the effects of such a term is given in Schurman et al. [19]. Some interesting results are obtained, for example, for the case of fronts, but there is a potential problem with this formulation that can cause trouble if this procedure is applied to the general range-dependent problem. The additional term induced by the range dependence is non-Hermitian, so the integral over transverse space of the magnitude of the field $\int d\underline{R}_T \left|A\right|^2$ is no longer conserved. Lacking a conservation law, there is nothing to enforce stability in numerical calculations.

The second step of the procedure for incorporating the effects of range dependence sidesteps this problem by noting that the non-Hermitian terms in the Hamiltonian do not accumulate with downrange propagation, but only operate at the endpoints. Taking a cue from earlier work by Bremmer [20], Tappert had already by 1977 incorporated this insight to form an optimal range-dependent formalism for the PE [15, 21-22] (in Ref. 15, see especially pp. 278-279, and in Ref. 21, note the discussion following Eq. (11)). This formalism can be derived from the first step described above using the following logic. Since $i\dot{\mu}$ is a perfect range-derivative in the sense that

$$i\dot{\mu} = i\frac{\partial\lambda}{\partial x} = i\dot{\lambda} + \left[H, \lambda\right] = i\frac{d\lambda}{dx},$$

(where recall that H is the expansion in $2\lambda/k_0$ of $k_0\sqrt{1+\frac{2\lambda}{k_0}}$), we can immediately recognize that this term only operates at the endpoints, and so it is not an inherent part of the propagation itself. It can therefore be removed from the propagation equation, and applied as a transformation at the endpoints. Generalizing to include higher orders, this class of effects can be incorporated into the theory using the following prescription: take out the WKB amplitude at the initial range to form the auxiliary field $\chi = \left(1+\left[2\lambda/k_0\right]\right)^{1/4} A$, propagate the field χ, and put the WKB amplitude back in after propagation is completed $A = \left(1+\left[2\lambda/k_0\right]\right)^{-1/4}\chi$. (A nice derivation of this result for the one-dimensional string displacement problem can be found in Ref. 23.) The Hamiltonian used to propagate this auxiliary field is Hermitian, which implies that the integral across transverse space of the magnitude squared of the field

[k] This means that the sound speed now depends on the range: $c = c\left(x, \underline{R}_T\right)$, and so $\omega/c \equiv k = k\left(x, \underline{R}_T\right)$, but for the moment the density ρ still remains everywhere the same.

[l] The two-step argument outlined here is provided primarily for historical context. While the basic results that emerge from this process will in one way or another reemerge from all the techniques we will subsequently be examining, they will be the product of very different lines of reasoning.

χ is conserved. Since $|\chi|^2$ is to within an integration by parts the downrange flux (see Appendix A), this conservation rule also guarantees energy conservation. Note that Hermiticity of the Hamiltonian also produces a propagation equation that is numerically stable. Since energy conservation is so intimately connected to numerical stability, it is a very desirable attribute to find in a PE.

2.1.3.4 Phenomena Not Addressed by this Formalism

It is important to bear in mind that this formalism is designed to model downrange propagation. It ignores coupling between downrange and uprange propagation (backscatter). Furthermore, by considering $2\lambda/k_0$ as a small parameter, we exclude an entire class of solutions to the Helmholtz equation associated with purely transverse energy flow (evanescent solutions; for more on this phenomenon, see the recent work by Fishman and collaborators [24, 25] and a brief discussion in the next to last paragraph of Appendix A). Both backscatter and evanescent modes are coupled to the downrange propagating solutions by terms that go to zero faster than any finite order of the PE expansion in the limit as the range dependence goes to zero. Specifically, this type of coupling comes from a physical process known as "pair-production" and the probability of pair-production occurring in a given unit volume goes to zero as $\exp\left(-\text{constant}/\sqrt{\mu}\right)$ (see Appendix B for more on this topic). The coupling is quite weak in many typical underwater propagation problems, and in such cases it can safely be ignored.

2.2 The Ocean Bottom: Introducing a Density Jump

2.2.1 The Change of Variable Technique

A premier example of an effort based on the PE to model shallow water ducted propagation is given in a recent article by Rouseff and Ewart [26]. A series of simulations are conducted. At first, the bottom, air-sea interface and depth-dependent sound speed profile are all smooth — in other words, they are not functions of the range. Then random roughness is added to the air-sea interface and bottom (e.g., see Figs. 1 and 3 of the reference). There is also a gentle slope to the bottom (a slope of roughly 4 m/km or an angle of about 0.2°), but this range dependence is very small compared with stochastic roughness and it is neglected for the purposes at hand (both in Ref. 26 and below in this report). The simulation by Rouseff and Ewart confirms the intuitive result that in the absence of significant range dependence, mode stripping eliminates bottom-penetrating modes, and the field is confined to the water column. The numerical simulation also plausibly predicts that with the introduction of multiscale range dependence, energy is pumped back into bottom-penetrating modes, and there is enhanced bottom penetration. This kind of bottom penetration is currently the focus of active research [27-30] and it has potential relevance to practical applications. For example, an acoustic field that penetrates the bottom can scatter from buried objects, and so it can in principle be exploited to remotely image these objects. However, in order to extract such information from the field, it is necessary to accurately model its behavior as it traverses the range-dependent environment on the way to and from the object being imaged. This accuracy must not only be qualitatively correct, but also quantitatively accurate.

As the field propagates downrange, three multiscale stochastic processes continuously pump energy back into the bottom-penetrating modes (i.e., modes such that for one reason or another the grazing angle is effectively greater than the critical angle):

- Roughness of the air-sea interface.
- Advection of the water column by internal waves and turbulence (Rousseff and Ewart do not pursue this in the referenced paper, but the phenomenon exists in the real ocean, and could be added to such a simulation as well.)
- Roughness of the ocean bottom.

The interaction of the field with the impenetrable rough air-sea interface is well described using a theory by Tappert and Nghiem-Phu [31], and advection of the layers in the water column by internal waves and turbulence can be adequately modeled using the basic PE described above.

The treatment of the rough bottom, however, requires further scrutiny. This problem is challenging because the density jumps at the ocean bottom. The classic PE technique outlined in Section 2.1 assumes that the density is everywhere uniform, but at the ocean bottom the density jump is significant. The density may jump by as much as a factor of 2, while the sound speed jump is typically much more modest (often just a few percent). Furthermore, we know from rough surface scattering theory that at a two-fluid interface, the density ρ formally plays just as prominent a role in the formulas for the reflected and transmitted scattering amplitudes as does the sound speed (e.g., see Appendix C of Ref. 32). Therefore, to properly model scattering from the ocean bottom, the PE technique must be modified to allow the density to change.

Reference 26 employs a technique by Tappert (see pp. 262 through 264 of Ref. 15) to incorporate density variation into the PE formalism. The auxiliary field defined by $u = A/\sqrt{\rho}$ obeys a Helmholtz equation with an effective index of refraction, and this Helmholtz equation can be converted to a PE (ρ is the density as a function of the coordinates). However, in the limit as the density dependence acquires a step, the effective index of refraction acquires δ-functions, and the following ad hoc fix must be imposed: the step is replaced with a gradual transition. The PE that is produced by this technique will henceforth be referred to as the Change of Variable (COV) PE.

2.2.2 The "Stair Step" PE

As attested to by Ref. 26, the COV PE is still used for specialized problems such as scattering from rough surfaces, but for most standard problems in underwater acoustics, it has been supplemented by an alternate technique by Collins and Westwood [18]. In this approach, the interface is approximated by stair steps in order to the exploit the fact that it is possible to directly take the square root of the range-independent problem (even when the density varies as a function of a transverse coordinate such as the depth). When the interface steps vertically, energy conservation is explicitly forced (by demanding continuity of the downrange energy flux). This much of the procedure was concurrently proposed by Porter et al. [33], but Ref. 18 perfects the technique with an additional ingredient. Forcing energy conservation at a vertical interface leads to a discontinuity of the pressure field, while the boundary conditions along the horizontal interface demand pressure continuity. This leads to an unphysical discontinuity in the pressure at the corners of the stair step, which in turn spawns Gibbs oscillations. These are eliminated using *complex* Padé coefficients[m]. The imaginary parts of the Padé coefficients effectively introduce (in this case unphysical) evanescent modes that restore field continuity without introducing a superfluous downrange flux. Below in this report, the approach by Collins and Westwood is referred to as the Stair Step PE.

The current prominence of the Stair Step PE dates back to its record of accuracy established during the late stages of a program that during the late 1980's and early 1990's systematically benchmarked various PE methods [34-36]. The Stair Step PE generally produced the most accurate results [36], and it has been dominant ever since.

[m] Strictly speaking, these coefficients actually appear in *rational function* approximations to the Hamiltonian generated by the PE. These rational functions are not designed to formally match the Taylor series expansion order by order (a type of least squares fit is generally used to generate the optimal coefficients in the rational functions). As Frank Henyey has pointed out that (personal communication), these rational functions are thus not strictly speaking true Padé approximations, but the terminology has become so ubiquitous in this context that we will use it here as well.

2.3 Adapting the PE to the Rough Surface Scattering Problem

2.3.1 Previous Efforts to Design a PE Optimized for Rough Surface Scattering

2.3.1.1 Bragg Scattering Taxes the Stair Step PE

The Stair Step PE can become somewhat unwieldy if the imposition of the energy conservation condition and the accompanying introduction of evanescent waves have to be done very often. As a consequence, although the state-of-the-art PE (Stair Step PE) has been used to model a wide range of problems, the issue of Bragg scattering from penetrable interfaces has typically been explored using alternate techniques.

In fact, while PE techniques that apply to rough surface scattering from *impenetrable* boundaries have been adequately benchmarked [37, 38], the first effort to benchmark the Stair Step PE applied to rough *penetrable* boundaries is only now being pursued by Thorsos (APL-UW). This is significant for several reasons:

1. Bragg scattering is phase sensitive in a way that typical benchmark problems are not. The typical benchmark problem involves a wedge with a tilted interface separating two media that have different sound speed and density. Since the slope and curvature are the same along the entire interface, the effects of introducing an overall phase shift would be invisible. On the other hand, the Bragg scattering that is so characteristic of scattering from multiscale rough surfaces depends on a delicate interplay of the relative phases of the field scattered from nearby points on the interface. Without accurate information about the relative phase of the different components of the field, it is impossible to model Bragg scatter. Furthermore, in ducted propagation, errors accumulate with the range. For this reason, we need a rigorous theory that unambiguously imposes a unique phase.
2. The Stair Step PE implicitly makes a number of ad hoc choices, and so one cannot a priori assume that it will produce the one uniquely correct value of the phase for the field generated at a given point on an interface. Let us consider several arbitrary choices made by the Stair Step PE. The energy conservation condition coupled with behavior of the field along horizontal interfaces forces the use of evanescent waves to eliminate Gibbs oscillations. There is some arbitrariness in how the Gibbs oscillations are removed, and the actual choice constitutes one ad hoc imposition that can only be validated by benchmarking. Similarily, the stair steps are artificial, and energy need not be independently conserved on the treads and risers. The assumption that it is constitutes another ad hoc imposition.
3. The Stair Step PE leaves out parts of both the physics and mathematical requirements related to the PE problem. For example, as discussed in Section 3.3.3, the full PE has higher-order derivatives right up to the interface, and these carry extra boundary conditions that are not specified by the Stair Step PE in its present form. Furthermore, although the Stair Step PE, like all PE methods, is sensitive to physical acoustics effects like diffraction, which in turn depend on the curvature of the surface over an extended distance, it does not allow for effects that are sensitive to the intrinsic local curvature (cf. polaritons in electromagnetic theory).

All these factors can play an important role in Bragg scattering, particularly within a ducted environment, where errors accumulate, even though the same factors are insignificant in the benchmark problems that have given the Stair Step PE its current dominance.

Thus, it is premature to assume that the success of the Stair Step PE in less challenging problems is a reliable indication of the approach's capabilities regarding the Bragg scattering problem. The Stair Step PE cannot be used with confidence to model Bragg scattering until Eric Thorsos' benchmarking is complete, and its validity is fully established in this context.

2.3.1.2 Existing Alternatives More Appropriate to Rough Surfaces than the Stair Step PE

Ideally, an alternate formulation that does not rely on ad hoc arguments in its development would improve on the Stair Step PE in two ways:

1. Being a systematic theory, it would be improvable by adding higher orders until its predictions benchmark to the required tolerance.
2. It is also reasonable to hope that a theory constructed from fundamental principles will pose the problem in its irreducible form, and consequently be easier to implement.

For the purpose of examining scattering from penetrable rough surfaces, Collins (with collaborators) has developed two approaches that are alternatives to the Stair Step PE. Both of these represent progress toward the goals listed above. The first is designed so that its predictions can be made to agree with a given result to a required tolerance, and is fairly easy to implement. The second approach returns to the fundamental assumptions behind the Stair Step PE, and recasts the problem so that ad hoc mathematical patches are no longer necessary.

The first approach, developed by Collins and Chin-Bing, actually predates the Stair Step PE [39]. It consists of a phenomenological theory applicable to the stochastic problem. Along the flat average surface, roughness-induced changes in the phase and amplitude of the field are modeled by effective boundary conditions that correspond to angle-dependent complex transmission and reflection coefficients. As with all phenomenological methods, previously obtained results are reliably reproduced, but the technique is not designed to accurately predict the general problem.

In the second alternative to Stair Step PE, Collins and Evans replace the rough surface with a crenellated surface (resembling battlements on a medieval castle) [40]. These features are a little bigger than a wavelength. A PE is used to step whenever the interface is locally flat. At vertical interfaces, the full Helmholtz boundary conditions including backscatter are imposed. (These boundary conditions are called the “single-scatter” boundary conditions.) Although the problem chosen is modeled accurately, this scenario is quite different from the rough surface scattering scenario. The most important difference is that a rough surface typically involves tilted interfaces (with slope $< 45°$) that produce only subtle curvature-induced backscatter, while the vertical interfaces found on a crenellated surface naturally tend to backscatter strongly.

This distinction is so fundamental that it continues to cause trouble even if more sophisticated implementations of the single-scatter technique are constructed. In principle, the basic approach could be applied to interfaces that are continuous functions of the range. The surface would then be broken into stair steps, and the PE would be used to step downrange when the surface is horizontal, while the single-scatter boundary conditions would be applied at the vertical interfaces. The problem begins to appear when we note that it is possible to design scenarios where even a correct solution to the full Helmholtz equation does not backscatter. For example, consider a field incident on a surface with tilt but no curvature, and assume that the grazing angles of the incoming spectral components of the field and the surface tilt are all sufficiently small that the reflected and transmitted wavevectors all point downrange. There is obviously no backscattering in this case. On the other hand, a calculation that discretizes a surface to form stair steps and additionally imposes the full Helmholtz-equation boundary conditions on the vertical interfaces, will continue to predict backscattering from these vertical interfaces deep into the physical acoustics limit. It would be necessary to discretize the interface to a very fine (much smaller than one wavelength) resolution before backscatter would finally fade away. A numerical solution based on this formalism would be much more resource-intensive than necessary, and it would involve one-way

stepping without a built-in conservation law and so it could be numerically unstable (recalling the relationship between energy conservation and stability discussed in Section 2.1)[n].

2.3.2 Towards A New Approach

2.3.2.1 The Physical Significance of Conserving Energy in Downrange Propagation

Scattering from penetrable quasi-planar rough interfaces typically involves tilts, grazing angles, and environmental parameters that are compatible with the scenario examined in the previous paragraph (aside from surface curvature, which induces a relatively weak type of backscatter). Thus, for the purpose of calculating the scattering from a typical rough surface, an energy-conserving PE would have an important advantage over the PE based on the single scattering boundary conditions. Since the energy-conserving PE a priori assumes small departures from range independence, it correctly anticipates the no-backscatter result, and consequently closely reflects the physics of the problem. As a result, its numerical implementation is more efficient and robust.

The thought experiment above also assures us that a better energy-conserving PE must exist. Once again, consider the tilted interface without curvature. Since there is no backscatter, it should be possible to construct a downrange stepping algorithm that generates a field that can be made arbitrarily close to the full-wave solution. In other words, there is nothing inherently special about a variable density that would preclude the existence of a systematic expansion of the field equation. An ad hoc procedure that reaches a limit beyond which improvement is impossible cannot be the final word.

Now that we have a better idea of what we are looking for, we can proceed to find it. Collins' and Evans' decision (in Ref. 40) to construct a new formalism directly from the underlying field equation was a sound one. In fact, we have just seen that the basic approach they specifically used to describe a crenellated interface could in principle be applied to any interface to obtain an answer that is accurate to any given precision. However, such an approach turns out to be poorly suited for the broad class of scattering problems where the incident grazing angle and interface slope are modest. On the other hand, the approach developed in this report begins with the same starting point, but then it employs a strategy more closely attuned to the physics and the modeling requirements of the problem: begin with the original field equation, and then perform a series of canonical transformations to systematically generate the PE. (These transformations are known as FW transformations, and they are discussed in Section 3.1.) In this way, an energy-conserving PE that is accurate to any given precision is constructed.

2.3.2.2 The Practical Utility of the New Energy-Conserving PE

There is a very real need for such a robust energy-conserving PE, particularly if it also turns out to be efficient when applied to the penetrable rough interface. The general utility of the PE is underscored by the fact that in the past, as soon as the technique was adapted to a new context, it rapidly gained wide acceptance. The examples that are particularly relevant to our discussion here concern the application of PE techniques to model rough surface scattering from impenetrable rough surfaces. Particularly useful results were obtained when various techniques were employed to introduce the Dirichlet (air-sea

[n] Similarly, one could impose one-way stepping on the *full* Helmholtz equation (e.g., see J.A. DeSanto, J.S. Perkins, and R.N. Baer, "A Correction to the PE," *J. Acoust. Soc. Am.* **64**, 1664-1666, 1978). In this case, one would have to start with the field specified on two range grid points rather than one and subsequently use the second downrange derivative to generate downrange stepping. Once again, in the absence of energy conservation, such a procedure runs into problems with numerical stability. These can be solved by *artificially enforcing* energy conservation, but this introduces ad hoc changes to the problem with unknown consequences. To consider a final permutation of the examples in this footnote and in the paragraph that references it, one could of course use the ordinary PE to step downrange and impose the single-scatter boundary conditions for a truly tilted (i.e., not stepped) interface. Again, this will lead to stability problems associated with the absence of a stabilizing conservation law.

interface) and sometimes also the Neumann (ideal infinitely hard bottom) boundary conditions directly into the stepping algorithm, which was then used to propagate a field adjacent to the rough impenetrable interface [31, 37-38, 41-46]. A hybrid Green's function/PE technique for calculating acoustic scattering from rough impenetrable boundaries is also available [47-52]. The PE technique has even been successfully applied to obtain good models of electromagnetic scattering from rough interfaces bordering conducting materials [53-55]. In this case, impedance boundary conditions[o] were imposed along the interface with the conducting surface. Strikingly, there has been virtually no analogous work employing the PE to model the general problem of scattering from and propagation through realistic rough penetrable surfaces (as opposed to artificially smoothed ones or crenellations). This is significant in light of the facts that, as we have seen, the problem is relevant to the important issue of roughness-induced penetration into the ocean bottom [26-30], and that the PE is generally the preferred method for modeling underwater acoustics.

We are now in a good position to better understand why the modeling community has been so reluctant to use the current state of the art PE formalism for the penetrable interface (the Stair Step PE) to model the rough interface problem. The key difference between this formalism and those for impenetrable interfaces is that in the latter case, a flat (range-independent) interface can easily be distorted into a rough one, while in the former case it cannot. This is significant because the techniques that allow us to adapt the PE to rough impenetrable interfaces ultimately rely on conformal mappings, a local method of images, or some similar distortion of the range-independent problem. On the other hand, as alluded to in Section 2.2 and as will be further elaborated in Section 6.2.2, the current state of the art theory for a flat penetrable interface cannot be distorted in this way. The stair step method treats the vertical interface in a way that is fundamentally different from the way it treats the horizontal interface — hence the superfluous Gibbs oscillations that then need to be eliminated by the ad hoc introduction of evanescent waves. This procedure is so unwieldy and therefore so ill suited to the rough surface scattering problem precisely because surface roughness cannot be imposed as a straightforward distortion of the range-independent problem. Seen in this light, the objective here is to develop a PE for the penetrable interface such that a flat surface can naturally be distorted into a rough one. This is a basic property of any good field theory, and we can therefore expect it to emerge from a PE that is produced by a systematic expansion of the field equation.

2.3.2.3 A Concrete Strategy for Replacing the Current Techniques

Such a PE will be developed below by adapting and extending a technique that was developed previously for a similar problem. Underlying this approach is the recognition (alluded to above in Section 2.1) that the Schrödinger equation is the PE that corresponds to the Klein-Gordon equation of relativistic quantum mechanics. Once the relationship between the quantum and acoustic problems is recognized, then the method used to systematically derive the Schrödinger equation from the Klein-Gordon equation can be applied to acoustics. (This method is constructed around the FW transformation mentioned a few paragraphs above.) Then the recognition that the semi-classical (i.e., non-relativistic) theory of the atomic Lamb shift essentially involves a rough-surface scattering problem will be leveraged to establish the validity of the PE based on our technique to the acoustic rough surface scattering problem.

[o] The impedance boundary conditions involve constants of proportionality that are imposed a priori and do not directly depend on the value of the field. They are not to be confused with impedance *matching* conditions of the sort found, for example, at two-fluid interfaces. The PEs for the Neumann and Dirichlet boundary conditions typically conserve energy, but these impedance conditions may violate this conservation rule. As noted earlier, energy conservation is a desirable attribute for a PE since it helps ensure numerical stability.

3. THE FORMAL APPROACH

Section 3 establishes the basic formal approach that will be used to construct a new PE for classical fields (initially the acoustic field, but in Section 4.3 the approach will also be applied to two classical vector fields). At the core of this approach is the FW transformation. The FW transformation was developed in the late 1940s for use in quantum mechanics [56], and it has recently been applied to the acoustic problem [1]. The latter treatment is based on Chapter 4 and Section 9.7 of the text by Bjorken and Drell [57]. Section 3.1 provides an overview of the resulting formal structure, while the rest of Section 3 begins to probe the behavior of this formalism near range-dependent discontinuities of the environmental parameters or their derivatives. (As discussed in Section 2.2, such singularities do in fact occur in a realistic ocean environment.) In Section 3.2, we examine the effects of range dependence, and then concentrate on the way that a cusp in the sound speed profile (i.e., a discontinuity of the sound speed gradient) induces a classical Lamb shift when it is advected by stochastic range-dependent fluctuations. We also examine a "toy model" of the atomic Lamb shift, and thus provide a justification for our identification of the acoustic field effect with the atomic Lamb shift. Finally in Section 3.3, we will move from the stochastically advected cusp to the numerical evaluation (in a discretized space) of an acoustic field propagating through deterministic interfaces that have slope and curvature. This will prepare us for our consideration in Section 4 of the classical Lamb shift associated with a rough interface where the environmental parameters themselves jump, and then in Section 6 of the main result of this work: a PE that incorporates Bragg-scale vorticity (i.e., a jump in the flux transverse to an interface where the density jumps). Thus, the results of Section 3 are in Section 4, and the understanding gained in these two sections will be used to mount a broad-based assault on the core problem associated with a rough interface where the density jumps.

3.1 The Foldy-Wouthuysen Transformation

The FW transformation is a canonical transformation that can be used to convert the full-wave equation into a PE. Here in Section 3.1, the related procedure is introduced and formally applied to the basic (i.e., fixed density) acoustic problem, and later (in Section 7) the technique will be used to develop PEs for other classical fields as well.

3.1.1 The Conceptual Framework

This subtle procedure is best introduced by briefly reviewing its origins, and then examining its broad outlines.

3.1.1.1 Exploiting Similarities Between Quantum Mechanics and Acoustics

The well-developed formalism from the quantum mechanical description of hydrogen's atomic spectrum will be exploited to derive a new acoustic PE. This effort is built upon the well-known observation that the PE has the same form as the Schrödinger equation of quantum mechanics (e.g., see Refs.15 (pp. 282-283), 58 (pp. 286-289)), and, consequently, that it approximates the Helmholtz equation for an acoustic field in much the same way that the non-relativistic Schrödinger equation approximates the relativistic Klein-Gordon equation[p]. The basis of the analogy is summarized in Table 1. Time development of the quantum mechanical field corresponds to down-range propagation of the acoustic field. The solutions to the forward- propagating PE of the acoustic problem correspond to the components of the quantum field, which propagate forward in time. The latter are commonly referred to as "particles" in contrast to "antiparticles," which, mathematically speaking, propagate backwards in time and are

[p] Note that the Klein-Gordon equation describes bosons (such as mesons) and not fermions (such as the electron and proton in the hydrogen atom), so the direct analogy being drawn is between a classical scalar field and a mesonic atom, and not exactly with the hydrogen atom.

Table 1 – The nature of the analogy between the Schrödinger equation for a relativistic quantum wave function obeying the Klein-Gordon equation and the PE for a scalar classical field obeying the Helmholtz equation. (For a more detailed discussion of the nonrelativistic limit and the shallow grazing angle condition, see Appendix C2.3.1.)

QUANTUM FIELD	**CLASSICAL FIELD**
Klein-Gordon equation	Helmholtz equation ($k_0 = m$)
Schrödinger equation	Parabolic equation (PE)
time	range
rest mass m	reference wave number k_0
4-dimensional space-time	3-dimensional space
Minkowski metric [1,-1,-1,-1]	Euclidean metric [1,1,1]
non-relativistic limit	shallow grazing angle
antiparticles	backscatter

analogous to the backscattered acoustic wave. In this report, we complete the analogy by introducing a scalar time-dependent external potential into the quantum mechanical problem. This is the direct analog to range dependence of the environment in the acoustic problem, but as discussed below, it is really a "toy model" and not an accurate physical description of an atom made up of bosons (e.g., a mesonic atom).

A number of important insights emerge from the analogy between quantum mechanics and acoustics. Most significantly, quantum field theory suggests a systematic technique for generating PEs. The Schrödinger equation, complete with relativistic corrections, can be derived using the FW transformation [56, 57, 59]. This transformation provides an order-by-order prescription for decoupling the forward- and backward-propagating solutions of the Klein-Gordon equation. The iterative procedure superficially resembles renormalization in the narrow sense that, with each iteration, terms with an undesirable characteristic (in this case coupling between forward and backward propagation) are shifted to higher and higher order.

3.1.1.2 A General Overview of the Foldy-Wouthuysen Procedure

The FW procedure consists of several steps. In the ansatz, a second-order differential equation is converted to a first-order equation by adding a degree of freedom. A vector is formed, and its components are linear combinations of the pressure field and its first derivative. The linear combinations are chosen so that the two components of the vector are carriers of the downrange and uprange flux. This two-dimensional vector obeys a PE where the Hamiltonian is a 2×2 matrix. A series of canonical transformations are employed to uncouple the fluxes order by order in the PE expansion parameter(s). In other words, the off-diagonal terms in the *matrix* Hamiltonian $\mathcal{H}$ are removed, and each flux now propagates independently using a scalar PE (containing a *scalar* Hamiltonian H). The now uncoupled fluxes differ from the field by an operator that corresponds to a WKB amplitude. Typically, the scalar PE is used to propagate the carrier of the downrange flux, while the uprange flux is zero. The WKB amplitude is applied at the endpoint of the downrange propagation to recover the acoustic pressure field. When the range dependence is weak, the WKB amplitude involves a near-eigenoperator, and the transformation from the pressure field to the carrier of flux (before propagation) and the transformation back from the carrier of flux to the pressure field (after propagation) nearly cancel. Under these circumstances, the distinction between propagating the auxiliary field and the actual acoustic field can be ignored. Finally, we note that the PE derived using the FW transformation contains unique new terms.

Thus, the PE of motion propagates an auxiliary field χ, which is related to the pressure field A, but not identical to it. To further familiarize ourselves with the fundamental attributes of the procedure, let us fix the density and review the treatment given in Ref. 1. The details from Ref. 1 are reproduced in Appendix C for completeness. (Since we are not yet explicitly introducing interfaces, the rest of this subsection will apply to both two-dimensional *x*-*z* and three-dimensional *x*-*y*-*z* spaces.)

3.1.2 Implementing the Procedure

Now the broad outline presented above is converted into a specific procedure**.**

3.1.2.1 The Ansatz for Acoustics

Given the Helmholtz equation

$$\frac{\partial^2 A}{\partial x^2} + \nabla_T^2 A + k_0^2 n^2 A = 0, \tag{6}$$

the FW ansatz becomes

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix} \equiv \frac{1}{2} \begin{pmatrix} A + \dfrac{i}{k_0}\dfrac{\partial A}{\partial x} \\ A - \dfrac{i}{k_0}\dfrac{\partial A}{\partial x} \end{pmatrix}. \tag{7}$$

Φ is a two-dimensional vector. Taking the inner product of Φ with itself under the metric Φ

$$\eta \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{8}$$

we have

$$\Phi^\dagger \eta \Phi = |\theta|^2 - |\chi|^2 = \frac{-1}{k_0} \mathrm{Im}\left[A^* \frac{\partial A}{\partial x} \right] \propto S_x = \text{ uprange/downrange flux}.$$

Thus, θ and χ are indeed carriers of the uprange and downrange flux, respectively.

3.1.2.2 Using Canonical Transformations to Decouple Uprange and Downrange Solutions

As shown in Appendix C.1.1 (and in Section I.A of Ref. 1), the definitions in Eq. (7) combined with the Helmholtz equation (Eq. (6)) generate the state space equation:

$$i\frac{\partial \Phi}{\partial x} = \mathcal{H}\Phi,$$

where

$$\mathcal{H} \equiv \mathcal{O} + \mathcal{E} + k_0 \eta. \tag{9}$$

η is defined in Eq. (8) above, and the odd operator $\mathcal{O}$ and the even operator $\mathcal{E}$ are given by

$$\begin{aligned} \mathcal{O} &= \lambda \xi \\ \mathcal{E} &= \lambda \eta \end{aligned}, \tag{10}$$

λ is as in Eq. (5) and ξ is a 2×2 matrix that is "odd" in the sense that it anti-commutes with η:

$$\xi \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{11}$$

Note that η is "even" in the sense that it anti-commutes with itself.

As described in Refs. 1 and 57 and in Appendix C.2.3.2, the FW transformation consists of a transformation

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix} \to \tilde{\Phi} = \begin{pmatrix} \tilde{\theta} \\ \tilde{\chi} \end{pmatrix}$$

such that

$$\tilde{\Phi} = e^{iS}\Phi \quad \text{with} \quad S \equiv \frac{i\eta\mathcal{O}}{2k_0}, \tag{12}$$

and the transformation $\mathcal{H} \to \tilde{\mathcal{H}}$

$$\tilde{\mathcal{H}} = e^{iS}\mathcal{H}e^{-iS} + [\text{terms generated by the range dependence}]. \tag{13}$$

This transformation is canonical in the sense that the basic form of the equation is unchanged:

$$i\frac{\partial\tilde{\Phi}}{\partial x} = \tilde{\mathcal{H}}\tilde{\Phi}.$$

It is iterative in that it is used over and over again to eliminate odd terms that couple uprange and downrange propagation. The order of the remaining odd terms increases with each iteration of the procedure.

The Hamiltonian diagonalized (denoted by a tilde) to fourth order (denoted by the Roman numeral IV) is given by

$$\tilde{\mathcal{H}}^{IV} = k_0\eta + \mathcal{E}^{II}, \tag{14}$$

where

$$\begin{aligned}\mathcal{E}^{II} = {} & \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\left[\mathcal{O},[\mathcal{O},\mathcal{E}]\right] - \frac{i}{8k_0^2}\left[\mathcal{O},\dot{\mathcal{O}}\right] \\ & + \frac{\eta}{8k_0^3}\left(-[\mathcal{O},\mathcal{E}]^2 - i\left\{\dot{\mathcal{O}},[\mathcal{O},\mathcal{E}]\right\} + \dot{\mathcal{O}}^2\right) + 5^{\text{th}}\text{ order}\end{aligned}. \tag{15}$$

As always, the dot denotes the downrange derivative $\partial/\partial x$. Orders are denoted by powers of the original odd and even operators $\mathcal{O}$ and $\mathcal{E}$, as well as powers of the downrange derivative $\partial/\partial x$. (The commutator $[,]$ and anti-commutator $\{,\}$ are defined in footnote f.) Equation (15) is a result taken from the treatment of the FW transformation in Ref. 57 extended up an order in Ref. 1. The calculation is reproduced in Appendix C.2.4, where Eqs. (14) and (15) are simply Eq. (C.28) and (C.29).

Equation (15) is quite general. It is a direct consequence of the fact that the initial odd operator $\mathcal{O}$ is a sum of operators[q] multiplied by ξ or $\eta\xi$, and the initial even operator $\mathcal{E}$ is a linear combination of

[q] These operators are Hermitian or anti-Hermitian depending of whether they are coefficients to ξ (which is anti-Hermitian); or of either $\eta\xi$, η or **1** (which are all Hermitian); and whether the overall Hamiltonian $\mathcal{H}$ is Hermitian or pseudo-Hermitian.

operators[q] multiplied by η or $\mathbf{1}$. Since these four matrices span the space of 2×2 matrices, it is always possible to break a given 2×2 matrix Hamiltonian $\mathcal{H}$ into such $\mathcal{O}$ and $\mathcal{E}$ operators. As discussed at the end of Appendix C.2.3.2, the result shown in Eq. (15) depends on the fact that $\pm\eta$, $\pm\xi$, $\pm\eta\xi$, and $\pm\mathbf{1}$ (the 2×2 matrices that operate on state space vectors) are closed under multiplication. (In fact, they form a group. Again, this is no surprise since the four matrices span the space of all 2×2 matrices). This means that at all iterations of the procedure, the odd operator $\mathcal{O}$ continues to be a sum of operators[q] multiplied by ξ or $\eta\xi$, and the even operator $\mathcal{E}$ continues to be a sum of operators[q] multiplied by η or $\mathbf{1}$. The matrices ξ and $\eta\xi$ are called odd, because they anti-commute with η, and the matrices η and $\mathbf{1}$ are called even because they commute with η. The anti-commutation relation implies that $\{\mathcal{O},\eta\}=0$. This condition, along with the basic form of the definition of *S* given in Eq. (12) and the basic form of the Hamiltonian given in Eq. (9), are all that is needed so that the FW transformation works properly.

Thus, the procedure developed by Foldy and Wouthuysen applies whenever the field equation can be written in the form of the state space equation (Eq. (9)), where in some sense the initial odd operator $\mathcal{O}$ is a linear combination of ξ and $\eta\xi$, and the corresponding even operator $\mathcal{E}$ is a linear combination of η and $\mathbf{1}$. It turns out that this will trivially be the case when we consider the variable-density acoustic equation (here, $\mathcal{H}$ is still a basic 2×2 matrix), and it will also hold in some broader sense when we consider vector fields (e.g., electromagnetic and elastodynamic fields). For the vector fields, the situation will be similar to that in the quantum mechanical problem. In the quantum problem, $\mathcal{O}$ is constructed of matrices that are outer products of the form $\sigma_i\otimes(\eta\xi)$ (σ_i are Pauli spin matrices), and both $\mathcal{E}$ and the term corresponding to $k_0\eta$ are proportional to $\mathbf{1}\otimes\eta$. The closed multiplicative structure and commutation rules needed for the FW transformation are again generated by the group of 2×2 matrices made up of ξ, $\eta\xi$, η, $\mathbf{1}$, and their negatives. As the FW procedure is implemented, these will cycle through in the right-hand slot of the outer product. (As discussed in Appendix C.2.3.1, the quantum mechanical problem also follows a slightly different set of power-counting rules, and as we see at various points throughout the treatment below, it subtly differs in various other respects.) We see in Section 7 that the Hamiltonians $\mathcal{H}$ for electromagnetic and elastodynamic fields are also constructed from matrices that involve outer products between submatrices related to the detailed properties of the field, and the usual group of 2×2 matrices associated with state space.

3.1.2.3 The Decoupled State Space Equation for Acoustics

Substituting for the values of $\mathcal{O}$ and $\mathcal{E}$ specific to the acoustic constant-density problem and performing two extra FW transformations to generate manifest range-reversal symmetry (denoted by the superscript 2), this leads to

$$\tilde{\mathcal{H}}^{IV.2}=\eta k_0\left(\sqrt{1+\frac{2\lambda}{k_0}}-\frac{\ddot{\lambda}}{8k_0^3}+\frac{\dot{\lambda}^2}{4k_0^4}+\frac{3\{\lambda,\ddot{\lambda}\}}{16k_0^4}\right)+\text{5th order}\,. \tag{16}$$

This is Eq. (51b) of Ref. 1 and Eq. (C.345) in Appendix C.2.5. Here, orders are obtained by counting the powers of λ, and the number of times the downrange derivative $\partial/\partial x$ operates on a λ. For example, $\ddot{\lambda}$ is third order, and $\dot{\lambda}^2$ is fourth order. The significance of range-reversal symmetry is discussed briefly in Section 3.1.3.3 and Appendix C.2.5.

Defining the scalar Hamiltonian H:

$$H = k_0\left(\sqrt{1+\frac{2\lambda}{k_0}} - \frac{\ddot{\lambda}}{8k_0^3} + ...\right), \tag{17}$$

(where the square root operator *must* be expanded to finite order in $2\lambda/k_0$), we have the result $\tilde{\mathcal{H}} = \eta H$. Note that

$$i\frac{\partial\tilde{\Phi}}{\partial x} = \tilde{\mathcal{H}}\tilde{\Phi} \quad \text{where} \quad \tilde{\Phi} = \begin{pmatrix}\tilde{\theta}\\ \tilde{\chi}\end{pmatrix}.$$

We will generally be interested in one-way (downrange) propagation (i.e., $\tilde{\theta} = 0$). In such propagation, we drop the tilde on $\tilde{\chi}$, and from now on just use χ. Thus, the scalar Hamiltonian H generates downrange propagation via the PE:

$$-i\frac{\partial\chi}{\partial x} = H\chi. \tag{18}$$

We notice that the Hamiltonian associated with this PE involves the familiar expansion of the square root operator, and new terms that involve downrange derivatives. These additional terms are strictly associated with the range dependence.

3.1.2.4 The Auxiliary Field χ

Note that Eq. (18), the PE obtained using the FW transformation, actually propagates an auxiliary field χ. In Appendix D.1, we show that, ignoring the range dependence locally (but not necessarily at more distant values of the range or the transverse coordinates), the field χ is related to the physical pressure field by the equation

$$\chi = \left(1+\frac{2\lambda}{k_0}\right)^{1/4} A = \sqrt{H/k_0}\cdot A. \tag{19}$$

In other words, the FW transformation indeed recovers the result so that the PE actually propagates an auxiliary field where the WKB amplitude has been removed from the pressure field.

3.1.2.5 How Energy Conservation is Built into the Formalism

As discussed in Ref. 1, the FW procedure is designed to maintain certain conservation laws. In Section I.B of this reference (or equivalently Appendix C.2.1 below), it is demonstrated that conservation of the total downrange energy flux forces the matrix Hamiltonian $\mathcal{H}$ originally generated by the FW ansatz to obey a property called pseudo-Hermiticity. (Pseudo-Hermiticity means that $(\eta\mathcal{H})^\dagger = \eta\mathcal{H}$, where η is, as always, the matrix defined in Eq. (8) above and the dagger † denotes Hermitian conjugation.) As shown in Section II.A of Ref. 1 (or equivalently in Appendix C.2.1 below), the FW transformation is designed to be pseudo-unitary so that pseudo-Hermiticity of the matrix Hamiltonian $\mathcal{H}$ is maintained as it is diagonalized by the FW procedure. (Some of the formal issues discussed just above are also briefly revisited at the beginning of Appendix I below.) Pseudo-Hermiticity of the diagnonalized matrix Hamiltonian in turn forces the scalar Hamiltonian H defined in Eq. (17) to be Hermitian (i.e., $H^\dagger = H$ since the diagonalized matrix Hamiltonian is ηH and $\eta^2 = 1$). The Hermiticity of H is also confirmed

by direct inspection of Eq. (17) (provided, of course, that the square root is understood to be a placeholder for its finite series expansion). If we take a range derivative of the integral over transverse space of the magnitude squared of χ (i.e., $\int d\underline{R}_T \left|\chi\right|^2$), use the parabolic Eq. (18) to replace downrange derivatives of χ with the Hamiltonian operating on χ, and apply Hermiticity of the Hamiltonian H, it follows that $\int d\underline{R}_T \left|\chi\right|^2$ is conserved during downrange propagation. The line of reasoning just completed ties the conservation rule for $\left|\chi\right|^2$ to the conservation of the downrange flux, and so to the conservation of energy. As discussed in Appendix A, the connection between the auxiliary field χ and the energy flux serves to illuminate the relationship between χ and the pressure field A as given by Eq. (19).

An important related point is also discussed in Appendix A. If there is no range dependence, there is no mode coupling, and the endpoint transformations from A to χ at the beginning and χ back to A at the end precisely cancel. If the coupling is weak in the sense that most of the coupling is between nearby eigenfunctions—nearby means the eigenvalues are close, the endpoint transformations nearly cancel. In such typical cases, reasonably accurate answers can be obtained using the PE to directly propagate *A*. Although this is often done, it is good practice to keep in mind that this is an approximation, and that the PE really propagates an auxiliary field χ.

3.1.3 Comments and Implications

Recall that in this section interfaces were not explicitly introduced, and so the discussion here applies to both three-dimensional and two-dimensional spaces. In Section 3.3.3, we return to the interface problem, and once again restrict ourselves to two-dimensional space and one-dimensional interfaces.

Thus, here in Section 3.1, the FW transformation has been borrowed from quantum mechanics and applied to derive the basic acoustics PE (i.e., constant density, but the sound speed can vary). The treatment in this section is similar to the derivation of the Schrödinger equation from the Klein-Gordon equation given in the classic relativistic quantum mechanics text by Bjöken and Drell (Ref. 57; Section 9.7). Two aspects of the problem known previously to the acoustic community from other considerations have been brought into the FW formulation for the first time. These are the explicit relationship between the PE field and the full-wave field, and the introduction of a true scalar potential into the PE formalism. New ideas also flowed in the other direction as the FW transformation for the first time introduced into the acoustic PE terms, which are related to range dependence, and which, as we will see in the next section, generate the classical equivalent of an often-overlooked component of the atomic Lamb shift (known as "vacuum polarization"). Finally, an entirely new innovation to the FW procedure was introduced as an extra FW transformation was performed to make the scalar Hamiltonian H (and so $\tilde{\mathcal{H}} = \eta H$) manifestly range-reciprocal. Let us examine these features more closely.

3.1.3.1 Insights Brought from Acoustics into the Foldy-Wouthuysen Procedure

The first insight brought from acoustics into the FW formal structure is the relationship between the auxiliary field χ propagated by the PE and the acoustic pressure field A propagated by the Helmholtz equation. As shown in Eq. (19), the two fields differ by a quarter-power operator sometimes known as a WKB amplitude (because the same operator shows up as an amplitude term in the WKB approximation). This was never a consideration in the quantum problem as described in Ref. 57, Section 9.7, because in that problem one is only concerned with expectation values. These are integrals over transverse (in this case, three-dimensional physical) space of the inner product $\Phi^\dagger \eta \Phi$, where Φ is as always the field in state space. The operator transforming the original field Φ to $\tilde{\Phi}$, the field propagated by the diagonal Hamiltonian, is pseudo-unitary, and so the transverse integral of the inner product $\tilde{\Phi}^\dagger \eta \tilde{\Phi}$ is the same as

that of $\Phi^{\dagger}\eta\Phi$, and so it automatically yields the desired expectation value, and there is no need to directly calculate the original field Φ. In the acoustic problem, on the other hand, we can observe and therefore need to recover the actual acoustic field A, and so in this case we need to be able to explicitly transform back and forth between the PE field χ and A.

The second innovation brought from the acoustic formalism into the FW formal structure is the concept of the true scalar potential. The acoustic scalar potential was introduced directly into the Helmholtz equation (as a spatial dependence on the sound speed). It shows up in the odd operator $\mathcal{O} = \lambda\xi$, since the operator λ incorporates both a "kinetic energy" part $\underline{\nabla}_T \cdot \underline{\nabla}_T / 2k_0$ and a potential $-k_0\mu$. On the other hand, for a quantum field obeying the Klein-Gordon equation (e.g., a pionic atom), the operator corresponding to λ only includes a kinetic energy term $\vec{\pi}\cdot\vec{\pi}/2m$, where $\vec{\pi}$ is a generalized momentum $\vec{\pi} = \vec{p} - \vec{A}$ (here $\vec{A}$ is a vector potential). In Ref. 57 (Section 9.7), the scalar potential is introduced directly into the state space equation as a scalar times the unit matrix. Since it has intrinsic matrix properties, it only shows up in the even operator $\mathcal{E}$, but not in the odd operator $\mathcal{O}$. The true scalar potential is therefore new to the blend of the FW approach and acoustics.

3.1.3.2 Insight that the Foldy-Wouthuysen Procedure Brings to Acoustics

The approach based on the FW transformation introduces something new into the basic acoustic PE. These are new terms that are generated by range dependence – for example, the term $-\ddot{\lambda}/8k_0^3$ in Eq. (17). We will examine these in detail shortly and discover that these terms are connected to the classical equivalent of the atomic Lamb shift.

3.1.3.3 What is Completely New in the Approach Developed Here?

Finally, there is something entirely new to the treatment of the FW transformation outlined above. Following a suggestion by Dashen, an extra FW transformation is used so that the new range-dependent terms introduced by the basic FW transformation exhibit range-reversal symmetry (i.e., $\tilde{\mathcal{H}}(-x) = \tilde{\mathcal{H}}(x)$). This is a symmetry exhibited by the Helmholtz equation, and it is therefore expected that an optimal parabolic approximation to it obeys it as well. In the deterministic problem, the term $-\ddot{\lambda}/8k_0^2$, for example, replaces the term $\frac{i}{8k_0^2}\left[\lambda, \dot{\lambda}\right]$. In the stochastic problem, this change will effectively move incoherent terms like $\left\langle \left(\nabla_T^2 \dot{\mu}\right)\delta\chi \right\rangle$ and $\left\langle \left(\nabla_T \dot{\mu}\right)\nabla_T \delta\chi \right\rangle$ to the purely coherent term $\langle\ddot{\mu}\rangle\langle\chi\rangle$ ($\delta\chi$ is the incoherent part and $\langle\chi\rangle$ the coherent part of the field: $\chi = \langle\chi\rangle + \delta\chi$). This will be very important so that we will be able to correctly recognize the Lamb shift as a purely coherent effect. Thus, the range-reversal-invariant formulation transparently leads to correct physical interpretations that would otherwise be obscured. This version of the result also happens to be easier to evaluate, again because it exploits a key symmetry of the problem. However, we need to note that the Dirac equation exhibits a symmetry that is a little more subtle than pure time reversal, and so this particular operation is not appropriate for the atomic problem.

3.1.3.4 Summing up the Flow of Ideas

An accounting of what has been brought from acoustics into the FW formalism, what has come from the FW formalism into acoustics, and what is unique to the new synthesis is given in Table 2. From here on, the material is generally unique to the effort developed here.

Table 2 – This table summarizes the six paragraphs above. It catalogues what is new to the approach here, what has come from the existing knowledge base in acoustics, and what has come from the existing formal structure developed for the FW transformation in the context of quantum mechanics.

	The FW Transformation as used for Scalar Quantum Fields (Bjöken-Drell [57], Section 9.7)	PE Developed by the Acoustics Community Using Traditional Methods	New Treatment of the Acoustics PE Using the FW Transformation
Known relationship between PE field χ and full wave field (φ or A)	No	Yes	Yes
True *scalar* potential	No	Yes	Yes
Unique range-dependent terms (ultimately connected to a new type of Lamb-shift effect)	Yes	No	Yes
Extra FW transformations so that the new terms exhibit range/time-reversal symmetry	No	No	Yes

3.2 The Classical Lamb Shift for a Cusp and a "Toy Model" for the Atomic Lamb Shift

3.2.1 The Physical Implications of a Singularity

When there is a jump in μ or in the derivative of μ, then the "new" term in the FW transformation $-\ddot{\lambda}/8k_0^3 = \ddot{\mu}/8k_0^2$ generates δ'- or δ-functions, respectively. The appearance of such δ-function potentials in a PE has interesting precedents in the Schrödinger equation for the hydrogen atom. These so-called contact potentials are associated, for example, with the fine and hyperfine structure of the spectrum of the atom. One of these contact potentials has particular relevance to the present discussion. It emerges when the FW transformation is used to obtain a semirelativistic picture of the atomic Lamb shift [60, 61]. In these calculations, vacuum fluctuations are imposed by hand as a kind of incident radiation, or alternately as a time dependence of the scalar and/or vector potentials. The calculations presented in Refs. 60 and 61 are sophisticated extrapolations of Welton's qualitative description of the Lamb shift [62], which is nicely described in Ref. 57.

From Eq. (4.5) in Ref. 61 and the discussion that follows, we learn that the Lamb shift occurs when the Coulomb (i.e., the electrostatic) potential, which is singular at the origin, is averaged as the electron vibrates under the influence of vacuum fluctuations. The averaging process generates a distribution (we also need to make use of the general result $\nabla^2(1/r) = -4\pi\delta(\vec{r})$). Cohn-Tanoudji et al. note elsewhere that "the average potential differs from the value of the potential at the average position only inside the source of the Coulomb potential, hence the function $\delta(r)$" [63]. Immediately below, they note "...the

Lamb shift is a quantum effect, just like the vacuum fluctuations that give rise to it. Nevertheless, once the existence of these fluctuations is acknowledged, their effect is the same as the one which would be produced by a random classical field characterized by a spectral density corresponding to an energy $\hbar\omega/2$ per mode" [63].

Significantly, the very same singularities that are responsible for the traditional Lamb shift discussed in the previous paragraph also cause the new FW terms associated with vacuum fluctuations to include distributions (e.g., δ-functions). These δ-functions (and sometimes also other distributions such as some of those proportional to δ'-functions) are immune to cancellations during averaging, and they provide correction terms to the standard Lamb shift.

Moving to the classical problem, range dependence takes the place of time dependence, and a stochastic range dependence in the environmental parameters replaces the vacuum fluctuations. This analogy exploits the fact that vacuum fluctuations can be interpreted as a stochastic time dependence of the potentials in the atomic problem. For example, we can imagine vacuum fluctuations advecting the nucleus of an atom. As the source of the scalar potential (for example) moves back and forth, a time dependence of this potential is induced. The world line of the nucleus (embedded in four-dimensional space-time) forms a rough surface along which the potential is singular. Similarly, in the classical problem, a quasiplanar interface along which an environmental parameter or its gradient is singular forms a rough surface in three-dimensional space.

Building on the analogy to atomic physics, the classical Lamb shift occurs when the second derivative in transverse space becomes a distribution. This, in turn, means that when the singularity is advected by stochastic fluctuations, it will average to a distribution at the origin. The new terms from the FW transformation involve the fluctuations in the uprange/downrange direction, and these terms are associated with a comparatively obscure contribution to the Lamb shift. The better-known and larger part of the Lamb shift effect involves fluctuations in transverse space. The semiclassical theories that deal with the Lamb shift often involve only the latter. We consider both below, but concentrate particularly on the part associated with fluctuations in the downrange direction (i.e., the new terms that only appear when the FW transformation is used to generate the PE), since these are completely new to acoustics. Eventually, we recognize that the acoustic effect induced by these terms is analogous to the vacuum polarization contribution to the atomic Lamb shift.

Specifically in the constant-density acoustic problem, a discontinuity in the sound speed or in its first derivative will force the second derivative with respect to the variable(s) of transverse space, and so also the lowest order FW term (involving a second range derivative of $\mu = \frac{1}{2}\left(1-n^2\right)$), to pick up a δ'- and/or a δ-function, respectively[r]. Types of the sound speed profiles that will lead to these contact potentials are illustrated in Fig. 3. After stochastic averaging, a δ-function survives along the average plane of a cusp of the sound speed, but the FW term associated with a sound speed *jump* will average to zero. Furthermore, it turns out that stochastically averaging the sound speed jump or cusp as it fluctuates in transverse space will lead to a δ'- and/or a δ-function, respectively, along the average plane. The effects associated with downrange and transverse fluctuations combine to form the acoustic Lamb shift,

[r] As discussed in Section 3.3.3, these contact potentials modify the boundary conditions of the field at the surface along which μ or its derivative jumps. This will be examined in much more detail throughout Section 4, where it is shown that these contact potentials, coupled with the lowest-order part of the basic range-independent Hamiltonian, $H = k_0 + \lambda$, lead to new boundary conditions on the field and/or its first derivative.

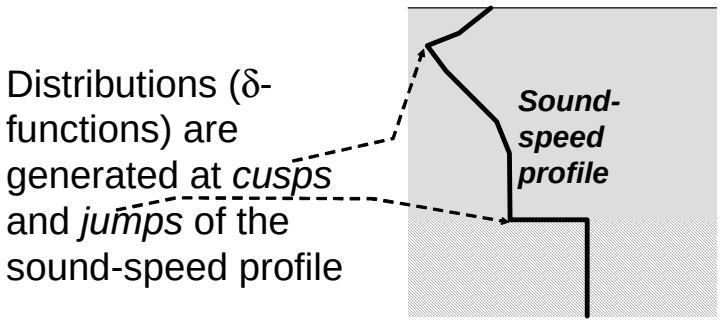

Fig. 3 — The traditional Lamb shift emerges as a fluctuating singularity, such as a sound speed cusp or jump, is averaged. The new terms introduced by the FW transformation will in the context of acoustics generate contact potentials at jumps in the sound speed or its gradient. These contact potentials very closely resemble the true Lamb shift effects. In fact, at a sound speed cusp and apparently also at a density jump (but not a sound speed jump), the new FW term survives averaging to contribute to the stochastic problem, and so contribute to the true Lamb shift. The contribution from the FW term will be called a downrange Lamb shift, as opposed to the traditional Lamb shift (also called here a transverse Lamb shift). The meaning of this terminology will become clearer below.

with the discontinuity in the first derivative of the sound speed forming the direct analogy to the quantum Lamb shift. The assertions in this section are summarized in Fig. 4.

3.2.2 A Range-dependent Environment Generated by Stochastic Fluctuations

3.2.2.1 Parameterizing a Range-dependent Environment as a Perturbation of a Range-independent Environment

Now, let us examine the specifics. For the current context, assume two-dimensional space where x is the range and z is the depth. To begin with, consider a sound speed profile without discontinuities in either the sound speed or its gradient (or equivalently, in either $\mu = \frac{1}{2}\left(1 - c_0^2/c^2\right)$ or its gradient). We have $\mu(x,z)\big|_{\text{undistorted}} = [\mu](z)$. Now distort it by a function of the range: $\mu(x,z)\big|_{\text{undistorted}} = [\mu](z) \Rightarrow \mu(x,z) = [\mu](z - f(x))$ (Fig. 5).

More generally, we should consider a distortion that varies with the depth: $f(x,z)$. This problem is similar, but there is one extra tricky issue. As long as the scalar Hamiltonian H is a simple function, then we can fix z and Taylor series expand in $f(x,z)$. However, higher-order Hamiltonians contain cross-terms, proportional to $\partial^n \mu / \partial z^n$, and these will also pull down extra terms proportional to $\partial^n f / \partial z^n$. This can add considerable complexity to our calculation, without adding anything new conceptually.

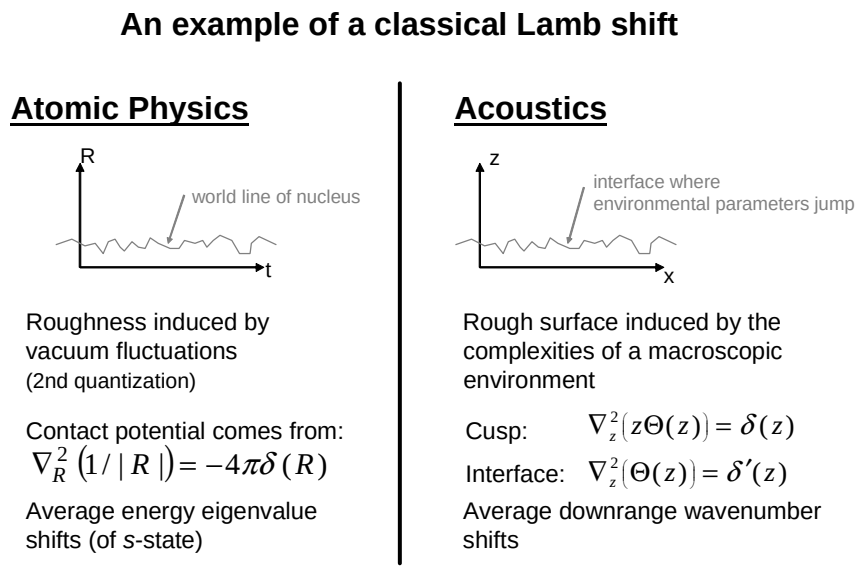

Fig. 4 — The new terms predicted by the FW transformation are related to time- (or range-) dependence. In atomic physics, vacuum fluctuations induce a time-dependence, while for classical fields the complex environment involves a range-dependence. The FW transformation predicts new terms, which lead to contact potentials either at the source of field acting on a electron, or alternately when the sound speed or its gradient is discontinuous. In the stochastic problem, an averaged rough surface essentially generates similar terms, which directly modify the coherent field. As discussed in greater detail in Section 4.4, these terms modify eigenvalues of the coherent field rather than coupling its modal components. The connection between the new terms induced by the FW transformation and the stochastic problem suggests that the FW transformation effectively induces a kind of averaging, which buffers the singularity.

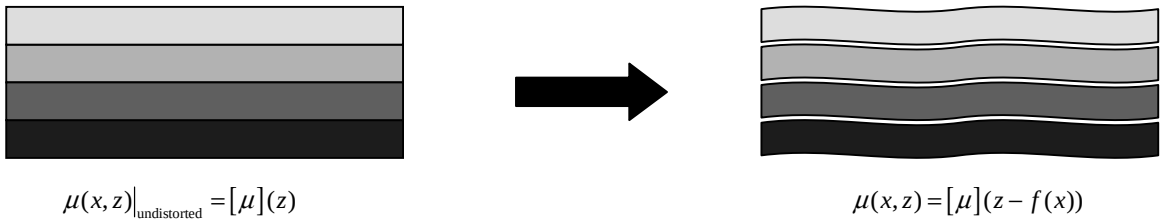

Fig. 5 — A range-dependent sound speed profile is generated by distorting a range-independent sound speed profile by a function $f(x)$

Since this is a side issue in the current context, and these terms are generally small anyway, we will ignore them here. What is of particular interest to the current investigation is the lowest-order of the new terms introduced by the FW transformation: $-\ddot{\lambda}/8k_0^3 = \ddot{\mu}/8k_0^2$, and for this term, we explicitly evaluate the contribution to this term from volume scattering and show for the stochastic problem that the z-dependence in f does not change the result at all (see Appendix E).

3.2.2.2 Stochastically Averaging the Perturbative Range-Dependence

Recall the Hamiltonian (Eq. (17)). For the time being, let us include only powers of λ and not downrange derivatives in the power counting. This allows us to examine the lowest-order FW term in a workable and familiar environment – as a modification to the familiar first-order PE. We now have a "quasi-first order" Hamiltonian:

$$H(x,z) = k_0 + \lambda - \frac{\ddot{\lambda}}{8k_0^2} = [H](z-f) + \frac{\ddot{\mu}}{8k_0}, \tag{20}$$

where $[H](z)$ is the undistorted range-independent Hamiltonian (i.e., $H(x,z) = [H](z - f(x))$). Now, average the equation

$$\left\langle -i\frac{\partial \chi}{\partial x} = H\chi \right\rangle$$

and expand

$$H(x,z) = [H](z) + \frac{\ddot{\mu}}{8k_0} + \boxed{f\frac{\partial [H]}{\partial z} + \frac{f^2}{2}\frac{\partial^2 [H]}{\partial z^2}} + O(f^3).$$

As we will see shortly, the terms in the box are related to previously known types of scattering. Break the field into coherent $\langle\chi\rangle$ and incoherent $\delta\chi$ components:

$$\chi(x,z) = \langle\chi\rangle(x,z) + \delta\chi$$

and make use of the fact that

$$\begin{matrix} \langle\delta\chi\rangle, \langle f\rangle = 0 \\ \langle f\,\delta\chi\rangle, \langle f^2\rangle \neq 0 \end{matrix}.$$

This leads to

$$-i\frac{\partial\langle\chi\rangle}{\partial x} = ([H](z))\langle\chi\rangle + \frac{\langle\ddot{\mu}\rangle}{8k_0}\langle\chi\rangle + \frac{\partial[H]}{\partial z}\langle f\cdot\delta\chi\rangle + \frac{\langle f^2\rangle}{2}\frac{\partial^2[H]}{\partial z^2}\langle\chi\rangle + \ldots. \tag{21}$$

The first term on the right-hand side of Eq. (21) is the right-hand side of the unperturbed (range-independent) problem. The second term is the averaged "FW term." We evaluate this term in Section 3.2.2.3.

The third term, $\langle f\cdot\delta\chi\rangle\partial[H]/\partial z$, is the well-known diffuse-scattering term. This non-Hermitian term measures the losses to the coherent wave as some of it is scattered into the incoherent field[s]. One

[s] This use here of the term "diffuse scattering" is quite broad. It subsumes several types of coherent-incoherent coupling, including Bragg scattering, mode coupling and, as is noted in Section 4.4, the transition probabilities in time-dependent perturbation theory in quantum mechanics. When *f* encompasses wavelength scales, the contribution from this term is dominated by Bragg scattering, and for this reason diffuse scattering is often associated with this phenomenon. Bragg scattering emerges naturally from perturbation theory (both in the context of the PE and in full-wave theory). For this effect, the inhomogeneities in the volume (or similarly the rough surface) look like a collection of diffraction gratings, which in higher-order perturbation theory become modulated by diffraction effects induced by scales larger than the Bragg wavelength (i.e., the size of the effective diffraction grating). As used here, diffuse scattering also includes weak mode-coupling induced by large scales acting alone in the absence of Bragg-scale roughness. The latter effect is very similar to the coupling between atomic levels induced by slow time dependence. Vacuum fluctuations are multiscale and can in principle induce a kind of mode coupling between electron states in the hydrogen atom that is quite similar to Bragg scattering (including modulation by larger scales).

can use the WKB approximation and the assumption that this is a Markov process to show the incoherent wave is proportional to the coherent wave:

$$\delta\chi \propto if\langle\chi\rangle$$

and so incorporate this term into an equation of motion involving the coherent field alone [64, 65]. This class of scattering events is relatively well understood[t] (at least in the present context where the density never changes), and the related term is from time to time dropped from our discussion below with the understanding that the coherent field calculated neglecting this term (crudely speaking) has to be multiplied by an exponentially decaying envelope[u].

The ellipsis in Eq. (21) subsumes a new cross-term between the incoherent field $\delta\chi$ and the new term $\ddot{\mu}/8k_0$. This provides a modest correction to the Bragg scattering loss term, and it will also be neglected. Also subsumed in the ellipsis are fourth-order and higher terms, and these are also dropped from the present discussion.

The fourth term in Eq. (21),

$$\frac{\langle f^2\rangle}{2}\frac{\partial^2[H]}{\partial z^2}\langle\chi\rangle,$$

involves a kind of "smearing out" to the rough interface as far as the coherent wave is concerned. This is the term that produces the well-known form of the Lamb shift effect when the second derivative is a δ-function – as opposed to the more obscure aspect of the Lamb shift effect that emerges from the term $\left(\langle\ddot{\mu}\rangle/8k_0\right)\langle\chi\rangle$, which is examined next in Section 3.2.3.3.

3.2.2.3 Stochastically Averaging the New Term Introduced by the Foldy-Wouthuysen Transformation

Having examined the incoherent scattering and the smearing terms in Eq. (21), we still need to evaluate the new term $\langle\ddot{\mu}/8k_0\rangle\langle\chi\rangle$. Assuming that the range dependence $f(x)$ is independent of the depth, this is easy to do. We start with

$$\mu(x,z)=[\mu]\left(z-f(x)\right).$$

The new term is proportional to

$$\ddot{\mu}\big|_{z=z_0} = \dot{f}^2\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=z_0-f} - \ddot{f}\left.\frac{\partial[\mu]}{\partial z}\right|_{z=z_0-f}. \tag{22}$$

[t] For a good discussion of the parabolic equation and diffuse scattering induced by volume inhomogeneities, see the classic text by Ishimaru [64]. A discussion similar to the one being pursued here, but for rough surfaces in the context of normal mode theory, is presented in a classic paper by Kuperman [65].

[u] By no means is it being claimed here that diffuse scattering is small, or that it would be trivial to graft it to a solution later. However, the goal below will be to examine the newly introduced physics in isolation so that its potential impact in the context of underwater acoustics can be determined. This is not unlike atomic physics, where the set of hydrogen eigenstates (including the Lamb shift) is examined independently of any consideration of transition probabilities, induced for example by the same vacuum fluctuations as those that cause the Lamb shift and similar in nature to the diffuse scattering found in acoustics.

Since $\partial[\mu]/\partial z$ is here assumed to be continuous, we can Taylor expand it:

$$\left.\frac{\partial[\mu]}{\partial z}\right|_{z_0-f} = \left.\frac{\partial[\mu]}{\partial z}\right|_{z_0} - f\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z_0} + \mathrm{O}(f^2) \tag{23}$$

to get

$$\left.\ddot{\mu}\right|_{z=z_0} = \dot{f}^2\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=z_0-f(x)} - \ddot{f}\left(\left.\frac{\partial[\mu]}{\partial z}\right|_{z_0} - f\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z_0}\right) + \mathrm{O}(f^3)\,. \tag{24}$$

Similarly,

$$\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=z_0-f(x)} = \left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=z_0} + \mathrm{O}(f)\,.$$

Substituting this in Eq. (24) and averaging yields

$$\left\langle\ddot{\mu}\right\rangle\Big|_{z=z_0} = \left\langle\dot{f}^2\right\rangle\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=z_0} - \left\langle\ddot{f}\right\rangle\left.\frac{\partial[\mu]}{\partial z}\right|_{z_0} + \left\langle f\cdot\ddot{f}\right\rangle\left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z_0} + O(f^3)\,. \tag{25}$$

By construction, $\left\langle\ddot{f}\right\rangle = 0$ (the distortion is assumed to be symmetric). Furthermore, writing $\left\langle f(x_1)\,f(x_2)\right\rangle = \int dk\left[S(k)e^{ik(x_1-x_2)}\right]$ (this form follows from the assumption that the statistics of the distortion are range-invariant), and taking derivatives, it is easy to show that $\left\langle f\cdot\ddot{f}\right\rangle = -\left\langle\dot{f}^2\right\rangle$. It follows that there is a cancellation to force $\left\langle\ddot{\mu}\right\rangle\Big|_{z=z_0} = 0$. When we allow the range dependence to vary with the depth ($f = f(x,z)$), then the calculation is a bit trickier, but once again we find that as long as the sound speed and its gradient are continuous, the average $\left\langle\ddot{\mu}\right\rangle$ is zero. The details are provided in Appendix E.

Finally, note that if $\partial[\mu]/\partial z$ or $[\mu]$ have jumps (i.e., there is a singularity in transverse space), it is still possible to perform a Taylor series expansion everywhere except at the discontinuity. Rather obviously, it is however not legitimate to use a Taylor series to generate δ-functions that were not in the function to begin with (effectively, the Taylor series generates the principal value of the derivatives). Thus, the bona fide δ-functions generated by $\ddot{\mu}$ do not cancel (recall that the FW transformation is not an expansion based on the Mean Value Theorem, but rather a canonical transformation of the wave equation), and we are left with δ-functions (or δ'-functions) at the discontinuity, even after performing the stochastic averaging procedure outlined above. Later in Sections 4.1 to 4.4, when we examine the case of $[\mu]$ discontinuous, we take a much more detailed look at what happens when we distort the world line of a singularity in transverse space to create a rough surface. For the time being, let us familiarize ourselves with the concepts involved by taking a rudimentary look at the milder singularity where the derivative $\partial[\mu]/\partial z$ is discontinuous (i.e., a cusp in the sound speed profile). Then to illustrate this result, and in the process further justify the line of argument that led to it, the deep connection between this phenomenon and the quantum Lamb shift will be explored by examining a "toy model" of the atomic

Lamb shift that essentially extends the sound speed cusp in two-dimensional depth-range space so that it can be embedded into four-dimensional space-time.

3.2.3 A Cusp in the Sound Speed Profile

This section considers the cusp in the sound speed profile. The boundary conditions are evaluated in Section 3.2.3.1 and then in Section 3.2.3.2 they are projected down to the line $z = 0$ in preparation for the stochastic averaging performed in Section 3.2.3.3. The step in $\ddot{\mu}$ is averaged in Section 3.2.3.4 and the smearing term is simplified to a familiar form in Section 3.2.3.5. Finally in Section 3.2.3.6 the boundary conditions are converted to contact potentials. This calculation forms the prototype for many that follow, and so it is considered explicitly here rather than being relegated to an appendix as are some comparable calculations later in this study.

3.2.3.1 The Boundary Conditions Along a Cusp

Figure 6 below illustrates a profile $[\mu](z)$ that has a cusp at the origin $z = 0$.

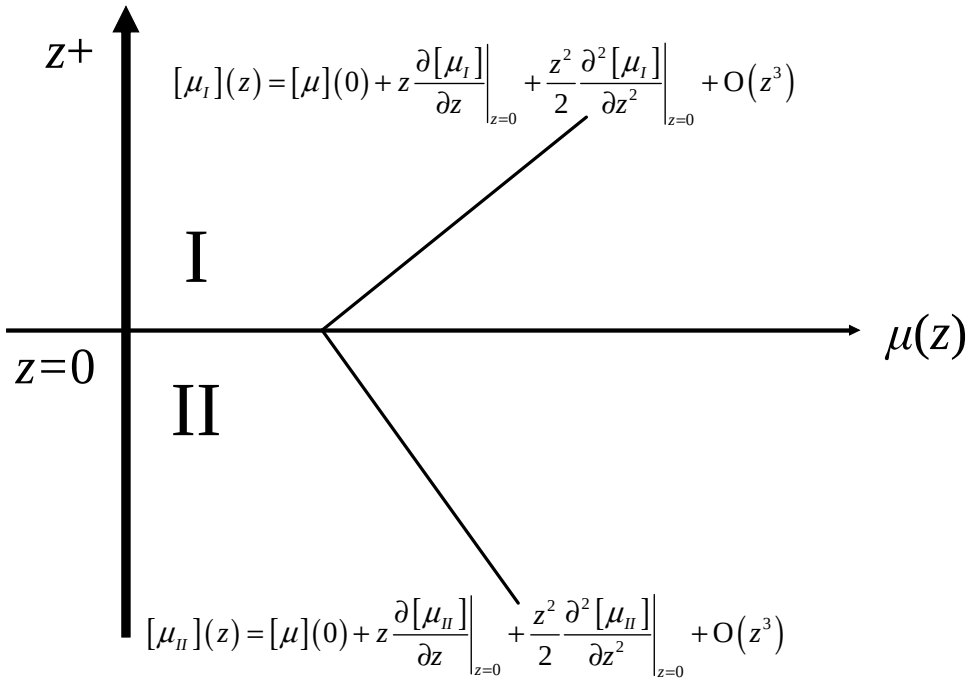

Fig. 6 — The basic cusp at $z = 0$. We expand in a Taylor series to keep track of the discontinuities of derivatives of the sound speed function $[\mu]$. In this report the two sides of an interface are labeled II and I, with the positive z-axis pointing from II into I.

We use a Taylor series expansion to $\mathrm{O}\left(z^2\right)$ to break $[\mu]$ into a part that will induce discontinuities and a δ-function in $\ddot{\mu}$, and a part that contributes to the continuous part of $\ddot{\mu}$ (which as we have just seen averages to zero). Therefore, we begin with

$$\begin{aligned}[\mu](z) = [\mu](0) &+ z\Theta(z)\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} + z\Theta(-z)\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0} \\ &+ \frac{z^2}{2}\Theta(z)\left.\frac{\partial^2[\mu_I]}{\partial z^2}\right|_{z=0} + \frac{z^2}{2}\Theta(-z)\left.\frac{\partial^2[\mu_{II}]}{\partial z^2}\right|_{z=0} + \mathrm{O}\left(z^3\right)\end{aligned}, \tag{26}$$

where $\Theta(z)$ is the Heaviside step function

$$\Theta(z) = \begin{cases} 1 & z \geq 1 \\ 0 & z = 0 \end{cases}. \tag{27}$$

Note that

$$\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0}, \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}, \left.\frac{\partial^2[\mu_I]}{\partial z^2}\right|_{z=0} \text{ and } \left.\frac{\partial^2[\mu_{II}]}{\partial z^2}\right|_{z=0}$$

are now treated as constants.

Using the fact that $z\delta(z) = 0; z^2\delta(z) = 0$, we have

$$\begin{aligned}\left.\frac{\partial[\mu]}{\partial z}\right|_{z=\tilde{z}} &= \Theta(\tilde{z})\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} + \Theta(-\tilde{z})\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0} \\ &\quad + \tilde{z}\Theta(\tilde{z})\left.\frac{\partial^2[\mu_I]}{\partial z^2}\right|_{z=0} + \tilde{z}\Theta(-\tilde{z})\left.\frac{\partial^2[\mu_{II}]}{\partial z^2}\right|_{z=0} \\ \left.\frac{\partial^2[\mu]}{\partial z^2}\right|_{z=\tilde{z}} &= \delta(\tilde{z})\left(\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right) \\ &\quad + \Theta(\tilde{z})\left.\frac{\partial^2[\mu_I]}{\partial z^2}\right|_{z=0} + \Theta(-\tilde{z})\left.\frac{\partial^2[\mu_{II}]}{\partial z^2}\right|_{z=0}\end{aligned}. \tag{28}$$

Now, setting $\tilde{z} = z_0 - f$ and substituting into Eq. (22), we have

$$\begin{aligned}\ddot{\mu}\big|_{z_0} &= \dot{f}^2\delta(z_0 - f)\left(\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right) \\ &\quad + \dot{f}^2\left(\Theta(z_0 - f)\left.\frac{\partial^2[\mu_I]}{\partial z^2}\right|_{z=0} + \Theta(-z_0 + f)\left.\frac{\partial^2[\mu_{II}]}{\partial z^2}\right|_{z=0}\right). \\ &\quad - \ddot{f}\left(\Theta(z_0 - f)\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} + \Theta(z_0 - f)\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right) \\ &\quad + \text{ a part that is continuous}\end{aligned} \tag{29}$$

Substituting into the "quasi-first order" Hamiltonian $H = k_0 + \lambda - \ddot{\lambda}/8k_0^2$ given by Eq. (20), and dropping the "0" in z_0, the basic PE $-i\partial\chi/\partial x = H\chi$ (Eq. (18)) gives us

$$\frac{\nabla_T^2\chi}{2k_0} + \frac{\dot{f}^2}{8k_0}\left(\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right)\delta(z-f)\chi + \begin{array}{c}\text{terms that are continuous}\\ \text{or (at worst)}\\ \text{proportional to a step function}\end{array}. \tag{30}$$

Here we find a δ-function "potential" in the PE much like that found in the Kronig-Penney model known from quantum mechanics (e.g., see Ref. 66). Let us follow the precedent from that context and evaluate this contact potential by taking an infinitesimal integral in the transverse space $\int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$ (we take a much closer look and generalize the result in Section 3.3.3). The terms that are continuous or proportional to the step function potential do not contribute to the infinitesimal integration and so they drop out. Following the conventions in Fig. 7, this leaves us with the boundary conditions[v]

$$\begin{aligned}&\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} = \left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \frac{\dot{f}^2}{4}\left[\frac{\partial[\mu_I]}{\partial z} - \frac{\partial[\mu_{II}]}{\partial z}\right]\chi(f)\\ &\chi_{II}(f) = \chi_I(f) = \chi(f)\end{aligned}. \tag{31}$$

Fig. 7 — By convention, in this report, the z-axis always points from side II into side I. Integration is also from side II to side I. Note that here the horizontal axis is in the downrange direction, while in Fig. 6, the horizontal axis measures the sound speed parameter $\mu(z)$.

3.2.3.2 Effective Boundary Conditions Aong the Line $z = 0$

Now, convert the boundary conditions on χ and $\partial\chi/\partial z$ at $z = f$ to effective boundary conditions down at $z = 0$ by performing, independently on each of the two sides of the interface, Taylor series expansions of the function χ and $\partial\chi/\partial z$, respectively. Beginning with χ, we have

$$\chi_I(0) = \chi_I(f-f) = \chi_I(f) - f\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \frac{f^2}{2}\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} + \mathrm{O}(f^3),$$

[v] Note that continuity of χ guarantees that it and $\partial\chi/\partial x$ are free from δ-functions. This in turn guarantees that the related terms in Eq. (30) are indeed free from δ-functions as asserted.

and exactly the same for χ_{II}. Subtracting the equations for χ_I and χ_{II} gives us

$$\begin{aligned}\chi_I(0)-\chi_{II}(0) &= -f\left(\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f}-\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f}\right)+\frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f}-\left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right)+\mathrm{O}\left(f^3\right)\\ &= \frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f}-\left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right)+\mathrm{O}\left(f^3\right)\end{aligned}. \tag{32}$$

Here we have used the fact that $\partial\chi/\partial z$ is continuous to $\mathrm{O}\left(\dot{f}^2\right)$. Similarly, we see that χ is continuous on the surface $z=f$, so the tangential derivative

$$\hat{t}\cdot\vec{\nabla}\chi \propto \frac{\partial\chi}{\partial x}+\dot{f}\,\frac{\partial\chi}{\partial z}$$

is continuous. Since $\partial\chi/\partial z$ is continuous to $\mathrm{O}\left(\dot{f}^2\right)$, $\partial\chi/\partial x$ at the surface is continuous to $\mathrm{O}\left(\dot{f}^3\right)$, and from the PE so must $H\chi$. Evaluating $H_I\chi_I - H_{II}\chi_{II}=0$, and noting that χ and μ are continuous at the interface $z=f$, we have

$$\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f}-\left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}=0, \tag{33}$$

and so Eq. (32) gives us

$$\chi_I(0)-\chi_{II}(0)=0+\mathrm{O}\left(f^3\right). \tag{34}$$

Similarly, taking a Taylor series expansion of the first derivative of χ,

$$\begin{aligned}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=0}-\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=0} &= \left.\frac{\partial\chi_I}{\partial z}\right|_{z=f}-\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f}-f\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f}-\left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right)\\ &\quad+\frac{f^2}{2}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f}-\left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right)+\mathrm{O}\left(f^3\right)\\ &= \frac{\dot{f}^2}{4}\left[\frac{\partial[\mu_{II}]}{\partial z}-\frac{\partial[\mu_I]}{\partial z}\right]\chi(0)+\frac{f^2}{2}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=0}-\left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=0}\right)+\mathrm{O}\left(f^3\right).\end{aligned} \tag{35}$$

3.2.3.3 Averaging the Effective Boundary Conditions

Now adapt a technique originally developed by Kuperman for the slightly different context of rough surfaces in normal mode theory [65]. In Eqs. (32) and (35), once again break the wave function into coherent and incoherent parts: $\chi|_{z=0}=\langle\chi\rangle(0)+\delta\chi$, and average these boundary conditions. This gives us

$$\begin{aligned}
&\langle \chi_I \rangle(0) - \langle \chi_{II} \rangle(0) = 0 + \mathrm{O}\left(f^3\right) \\
&\left.\frac{\partial \langle \chi_I \rangle}{\partial z}\right|_{z=0} - \left.\frac{\partial \langle \chi_{II} \rangle}{\partial z}\right|_{z=0} = \frac{\langle \dot{f}^2 \rangle}{4}\left[\frac{\partial [\mu_{II}]}{\partial z} - \frac{\partial [\mu_I]}{\partial z}\right]\langle \chi \rangle(0) \\
&\qquad + \frac{\langle f^2 \rangle}{2}\left(\left.\frac{\partial^3 \langle \chi_I \rangle}{\partial z^3}\right|_{z=0} - \left.\frac{\partial^3 \langle \chi_{II} \rangle}{\partial z^3}\right|_{z=0}\right) + \mathrm{O}\left(f^3\right)
\end{aligned} \quad . \tag{36}$$

Note that we have effectively replaced the actual boundary condition at $z = f$ with an effective boundary condition at $z = 0$. Thus, we have effectively moved the δ-function in Eq. (29) down to the $z = 0$ line. As described in Appendix E, to ensemble average *away from the interface*, we must similarly express the (in this case very well-behaved) environmental parameter $\ddot{\mu}$ in terms of a Taylor series that measures its departure from its unperturbed values. Obviously, the same applies to the part of $\ddot{\mu}$ that is continuous at the interface.

3.2.3.4 Averaging the Step Functions in $\ddot{\mu}$

It only remains to do the same for the step functions $\Theta\left(\pm\left(z - f\right)\right)$ found in Eq. (29). To move such a step function back to the $z = 0$ line, use a Taylor series to project the coefficients of the step $\Theta\left(\pm\left(z - f\right)\right)$ down a distance $-f$. This effectively extends the half-spaces down to the $z = 0$ line, with the Taylor series analytically extending the coefficients of the step $\Theta\left(\pm\left(z - f\right)\right)$ as necessary. This changes the location of the step without affecting the function outside the interval $z \in [0, f]$. For the step functions in Eq. (29), this gives us

$$\begin{aligned}
\ddot{\mu}\big|_{\text{step}} &= +\dot{f}^2\left(\Theta(z_0)\left.\frac{\partial^2 [\mu_I]}{\partial z^2}\right|_{z=-f} + \Theta(-z_0)\left.\frac{\partial^2 [\mu_{II}]}{\partial z^2}\right|_{z=-f}\right) \\
&\quad -\ddot{f}\left(\Theta(z_0)\left.\frac{\partial [\mu_I]}{\partial z}\right|_{z=-f} + \Theta(z_0)\left.\frac{\partial [\mu_{II}]}{\partial z}\right|_{z=-f}\right) \\
&= \dot{f}^2\left(\Theta(z)\left.\frac{\partial^2 [\mu_I]}{\partial z^2}\right|_{z=0} + \Theta(-z)\left.\frac{\partial^2 [\mu_{II}]}{\partial z^2}\right|_{z=0}\right) \\
&\quad -\ddot{f}\left(\Theta(z)\left(\left.\frac{\partial [\mu_I]}{\partial z}\right|_{z=0} - f\left.\frac{\partial^2 [\mu_I]}{\partial z^2}\right|_{z=0}\right) + \Theta(-z)\left(\left.\frac{\partial [\mu_{II}]}{\partial z}\right|_{z=0} - f\left.\frac{\partial^2 [\mu_{II}]}{\partial z^2}\right|_{z=0}\right)\right) \\
&\quad +\mathrm{O}\left(f^3\right).
\end{aligned} \tag{37}$$

Note that like the continuous part of $\ddot{\mu}$, this averages to zero: $\left\langle \ddot{\mu}\big|_{\text{step}} \right\rangle = 0$.

3.2.3.5 Simplifying the Smearing Term

Now, let us look at the smearing term in the boundary condition for $\partial\langle\chi\rangle/\partial x$ given by the second part of Eq. (36). This term involves the boundary condition for the third derivative $\partial^3\langle\chi\rangle/\partial x^3$. To obtain this, consider Eq. (21),

$$-i\frac{\partial\langle\chi\rangle}{\partial x}=[H](z)\langle\chi\rangle+\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle,\langle\ddot{f}\delta\chi\rangle,\langle\dot{f}^2\rangle\right),$$

and take the transverse derivative $\nabla_T=\partial/\partial z$ of this stochastic Helmholtz equation on either side of the interface:

$$\begin{aligned}&\nabla_T\cdot\left[-i\frac{\partial\langle\chi\rangle}{\partial x}=[H](z)\langle\chi\rangle+\cdots=\frac{\nabla_T^2\langle\chi\rangle}{2k_0}-k_0[\mu](z)\langle\chi\rangle+\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle\ldots\right)\right]\Rightarrow\\&-i\frac{\partial\nabla_T\langle\chi\rangle}{\partial x}=\frac{\nabla_T^3\langle\chi\rangle}{2k_0}-k_0\left(\nabla_T[\mu](z)\right)\langle\chi\rangle-k_0\left([\mu](z)\right)\nabla_T\langle\chi\rangle+\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle\cdots\right),\end{aligned}\tag{38}$$

and evaluate the second equation on both sides of the interface and subtract. Note that $\langle\chi\rangle$, $\nabla_T\langle\chi\rangle$ and consequently its transverse $\partial\nabla_T\langle\chi\rangle/\partial x$ only violate continuity at $\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle\right)$ or higher. Therefore subtracting Eq. (38) evaluated just inside the two regions gives us

$$\begin{aligned}0&=\frac{\nabla_T^3\langle\chi_I\rangle\big|_{z=0}-\nabla_T^3\langle\chi_{II}\rangle\big|_{z=0}}{2k_0}-k_0\left(\nabla_T[\mu_I]\big|_{z=0}-\nabla_T[\mu_{II}]\big|_{z=0}\right)\langle\chi\rangle+\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle\right)\\\nabla_T^3\langle\chi_I\rangle\big|_{z=0}-\nabla_T^3\langle\chi_{II}\rangle\big|_{z=0}&=2k_0^2\left(\nabla_T[\mu_I]\big|_{z=0}-\nabla_T[\mu_{II}]\big|_{z=0}\right)\langle\chi\rangle+\mathrm{O}\left(\langle f\delta\chi\rangle,\langle f^2\rangle\right),\end{aligned}\tag{39}$$

and Eq. (36) becomes[w]

$$\begin{aligned}&\langle\chi_I\rangle(0)-\langle\chi_{II}\rangle(0)=0+\mathrm{O}\left(f^3\right)\\&\left.\frac{\partial\langle\chi_I\rangle}{\partial z}\right|_{z=0}-\left.\frac{\partial\langle\chi_{II}\rangle}{\partial z}\right|_{z=0}=-\frac{\langle\dot{f}^2\rangle}{4}\left[\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0}-\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right]\langle\chi\rangle\big|_{z=0}\\&\qquad\qquad+k_0^2\langle f^2\rangle\left[\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0}-\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right]\langle\chi\rangle\big|_{z=0}+\mathrm{O}\left(f^3\right)\end{aligned}\quad.\tag{40}$$

[w] Note that we have demonstrated that here in in quasi-first order (i.e., $\mathrm{O}(\lambda,\ddot{\lambda})$) theory – or for that matter in ordinary first order $\mathrm{O}(\lambda)$ theory – jumps in the third derivative $\partial^3\langle\chi\rangle/\partial z^3$ are generated by jumps in the gradient of $[\mu]$ (i.e., $\partial[\mu]/\partial z$). Later, when we relax the condition that $[\mu]$ be continuous, then will see that jumps in the sound speed $[\mu]$ similarly lead to jumps in the second derivative of the field $\partial^2\langle\chi\rangle/\partial z^2$. Ultimately, these jumps in the higher-order derivatives of the field provide the underlying physics behind the contact potentials that appear in perturbation theory. Interestingly, in the context of first order $\mathrm{O}(\lambda)$ and quasi-first order (i.e., $\mathrm{O}(\lambda,\ddot{\lambda})$) theories, these contact potentials in turn spawn effective boundary conditions on $\partial\langle\chi\rangle/\partial z$ and later also in $\langle\chi\rangle$. This kind of transference of discontinuity from higher-order down to lower-order derivatives is examined further in Section 4.2.2.

Note that there are no Bragg scattering terms (i.e., proportional to $\delta\chi$) in the boundary conditions (Eq. (40)). If we assume Gaussian statistics, then the expectation values of odd powers of the surface displacement function f and its derivatives are zero, and consequently the error terms in the boundary conditions (Eq. (40)) are in fact fourth-order.

3.2.3.6 The Effective Boundary Conditions as a Contact Potential

In the quasi-first order (i.e., $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$) theory currently being used, the lead-order derivative in the kinetic term is $\nabla_T^2\langle\chi\rangle/2k_0$. This allows us to replace boundary conditions (Eq. (40)) by adding a contact potential to the unperturbed sound speed function $[\mu]\to[\mu]+[\mu]_{\text{contact}}$, where

$$[\mu]_{\text{contact}}=\delta(z)\left(-\frac{\langle\dot{f}^2\rangle}{8k_0^2}\left[\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0}-\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right]+\frac{\langle f^2\rangle}{2}\left[\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0}-\left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0}\right]\right). \tag{41}$$

The $\langle f^2\rangle$ contribution to this δ-function happens to be the same as if we added

$$\frac{\langle f^2\rangle}{2}\frac{\partial^2[\mu]}{\partial z^2}$$

to μ, so we can interpret this term as representing the smearing of the sound speed profile in the transverse direction by a root mean distance $\sqrt{\langle f^2\rangle}$ and average displacement $\langle f\rangle=0$. The $\langle\dot{f}^2\rangle$ part of the δ-function came from the new term contributed by FW transformation, and it can be written as

$$\left\langle-\frac{\ddot{\mu}}{8k_0^2}\right\rangle=\frac{1}{2}\left(\frac{i}{2k_0}\right)^2\left\langle\frac{\partial^2\mu}{\partial x^2}\right\rangle.$$

As discussed in Appendix A, this implies that the new term contributed by the FW transformation corresponds to the smearing of the potential in range-domain by virtual fluctuation of size $i/2k_0$. The imaginary factor occurs because the phenomenon is evanescent in the downrange direction.

Returning to the very important result (Eq. (41)), note that we could have obtained the part proportional to $\langle\dot{f}^2\rangle$ immediately by

- taking Eq. (22), and
- treating the term proportional to $\dot{f}^2$ as a principal value *plus* a bona fide δ-function, which to this order can simply be translated down to the origin,
- taking the term that is merely discontinuous, but free of δ-functions (i.e., the one proportional to $\ddot{f}$), and expanding it in a Taylor series, being sure to keep only the principal values of any derivatives generated by the Taylor series,
- and finally taking an ensemble average and noting that $\langle\dot{f}^2\rangle+\langle\ddot{f}\cdot f\rangle=0$.

Also note that we could have immediately obtained the transverse smearing term proportional to $\left\langle f^2 \right\rangle$ by adding $\left\langle f^2 \right\rangle / 2 \cdot \partial^2[\mu] / \partial z^2$ and this time accepting any δ-functions generated (this particular shortcut will work until we introduce a density jump in Section 4). For our next example, we will exploit some of these shortcuts.

3.2.4 A "Toy Model" of the Atomic Lamb Shift

3.2.4.1 Transferring the Results for a Cusp in Two Dimensions to a Central "1/*r*" Potential in Four-dimensional Space-time

Now, let us illustrate the connection between the cusp in a sound speed profile and the quantum Lamb shift. To do so, we will consider a crude "toy model" of the atomic Lamb shift that will not only reproduce a well known non-relativistic model of the atomic Lamb shift but also add some very interesting new physics to it. Begin with a Klein-Gordon equation with a scalar potential:

$$\left[\frac{\partial^2}{\partial t^2} - c^2\vec{\nabla}^2 + \omega_0^2\left(1+U(\vec{r},t)\right)\right]\phi = 0\,. \tag{42}$$

Now, compare Eq. (42) to the Helmholtz (Eq. (2)):

$$\left(\frac{\partial^2}{\partial x^2} + \nabla_T^2 + k_0^2 n^2(x,\underline{R}_T)\right)A = 0 \tag{43}$$

and make the identifications

$$\omega_0^2 \Leftrightarrow k_0^2 \quad t \Leftrightarrow x \quad \nabla_T^2 \Leftrightarrow -c^2\vec{\nabla}^2 \quad n^2 \Leftrightarrow 1+U\left(\vec{r},t\right). \tag{44}$$

Note that $\hbar\omega_0 = \text{Rest energy} = m_0c^2$. The fourth identification in Eq. (44) implies

$$\mu = \frac{1-n^2}{2} \Rightarrow \mu_{\text{effective}} = \frac{1-\left(1+U\right)}{2} = -\frac{U}{2}.$$

Now, the expansion parameter for the FW transformation goes as

$$\lambda = \frac{\nabla_T^2}{2k_0} - k_0\mu \Rightarrow \lambda_{\text{new}} = \frac{-c^2\vec{\nabla}^2}{2\omega_0} - \omega_0\mu_{\text{effective}} = \frac{-c^2\vec{\nabla}^2}{2\omega_0} + \omega_0\frac{U}{2} \tag{45}$$

and the corresponding PE (in this case, a Schrödinger equation) is

$$\begin{aligned} \pm i\frac{\partial\tilde{\varphi}}{\partial t} &= \left(\omega_0 + \lambda_{\text{new}} + \frac{\ddot{\mu}_{\text{effective}}}{8\omega_0} + \cdots\right)\tilde{\varphi} \\ &= \left(\omega_0 + \frac{-c^2\vec{\nabla}^2}{2\omega_0} + \omega_0\frac{U}{2} + \frac{\ddot{\mu}_{\text{effective}}}{8\omega_0} + \cdots\right)\tilde{\varphi} \end{aligned}. \tag{46}$$

Now, make the replacement $\tilde{\varphi} = e^{\mp i\omega_0 t}\varphi$ to remove the rest energy ω_0. Also, multiply through by $\hbar$ and use $c^2/\omega_0 = \hbar/m_0$ to get

$$\pm i\frac{\partial\varphi}{\partial t} = \left(\frac{-\hbar^2\vec{\nabla}^2}{2m_0} + \hbar\omega_0\frac{U}{2} + \frac{\hbar\ddot{\mu}_{effective}}{8\omega_0} + \cdots\right)\varphi,$$

and this time choose the top branch to match conventions in quantum mechanics. Make the identification

$$V \equiv \hbar\omega_0\frac{U}{2} = -\hbar\omega_0\mu_{\text{effective}}$$

to get

$$i\hbar\frac{\partial\varphi}{\partial t} = \left(\frac{-\hbar^2\vec{\nabla}^2}{2m_0} + V - \frac{1}{8\omega_0^2}\frac{\partial^2 V}{\partial t^2}\right)\varphi + \cdots. \tag{47}$$

Now, let us consider the standard radial potential corresponding to an electric field around a point source (typically the nucleus of an atom):

$$V(\vec{r}) = \frac{V_0}{r}$$

(where $r = |\vec{r}|$). Impose second quantization (vacuum fluctuations) by perturbing the spatial coordinate[x]:

$$\vec{r} \to \vec{r} + \delta\vec{r}(t) \quad \text{so that} \quad V(\vec{r}) \to V\left(\vec{r} + \delta\vec{r}(t)\right).$$

Now the world line of the nucleus is a rough interface (Fig. 8)[y].

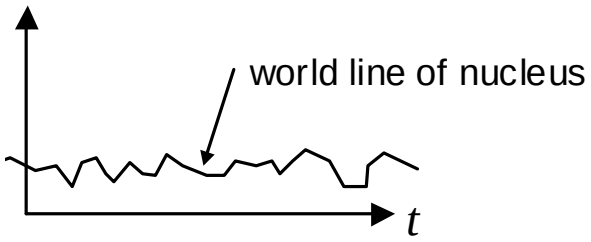

Fig. 8 — The world line of the nucleus is a rough surface

[x] We could have used the more general $\delta\vec{r}(\vec{r},t)$, and applied the basic derivation given in Appendix E to evaluate this problem. We would once again determine that adding the spatial dependence in $\delta\vec{r}$ adds a great deal of complexity to the calculation without adding much new to the problem or changing the result.

[y] Incidentally, it is primarily the very light electron that is advected by the fluctuations, and not really the very heavy nucleus. However, in the current context it does not really matter which is moving, since only the relative position is relevant.

Taking derivatives, we have

$$\begin{aligned}\frac{\partial V}{\partial t} &= \delta\dot{\vec{r}}\cdot\vec{\nabla}V\left(\vec{r}+\delta\vec{r}\right)\\ \frac{\partial^2 V}{\partial t^2} &= \delta\ddot{\vec{r}}\cdot\vec{\nabla}V\left(\vec{r}+\delta\vec{r}\right)+\delta\dot{\vec{r}}\cdot\vec{\nabla}\frac{\partial V\left(\vec{r}+\delta\vec{r}\right)}{\partial t}\\ &= \delta\ddot{\vec{r}}\cdot\vec{\nabla}V\left(\vec{r}+\delta\vec{r}\right)+\delta\dot{\vec{r}}\delta\dot{\vec{r}}:\vec{\nabla}\vec{\nabla}V\left(\vec{r}+\delta\vec{r}\right)\end{aligned}.$$

Now expand in $\delta\vec{r}$ to $\mathrm{O}\left(\delta\vec{r}^{\,2}\right)$ using the shortcuts we just developed by examining the cusp (PV = principal value)

$$\frac{\partial^2 V}{\partial t^2} = \delta\ddot{\vec{r}}\cdot\vec{\nabla}V\left(\vec{r}\right)+\delta\ddot{\vec{r}}\delta\vec{r}:\mathrm{PV}\left[\vec{\nabla}\vec{\nabla}V\left(\vec{r}\right)\right]+\delta\dot{\vec{r}}\delta\dot{\vec{r}}:\vec{\nabla}\vec{\nabla}V\left(\vec{r}\right),$$

and average (noting that $\left\langle\delta\ddot{\vec{r}}\right\rangle=0$)

$$\left\langle\frac{\partial^2 V}{\partial t^2}\right\rangle = \left\langle\delta\ddot{\vec{r}}\delta\vec{r}\right\rangle:\mathrm{PV}\left[\vec{\nabla}\vec{\nabla}V\left(\vec{r}\right)\right]+\left\langle\delta\dot{\vec{r}}\delta\dot{\vec{r}}\right\rangle:\vec{\nabla}\vec{\nabla}V\left(\vec{r}\right).$$

Now $-\left\langle\delta\ddot{\vec{r}}\delta\vec{r}\right\rangle=\left\langle\delta\dot{\vec{r}}\delta\dot{\vec{r}}\right\rangle=\left\langle\vec{\mathrm{v}}\vec{\mathrm{v}}\right\rangle$, where $\delta\dot{\vec{r}}=\vec{\mathrm{v}}$ is the velocity of the displacement. Furthermore, assume the displacement follows Gaussian statistics; specifically, that the motions in the x, y, z directions are not correlated to obtain

$$\left\langle\vec{\mathrm{v}}\vec{\mathrm{v}}\right\rangle=\frac{\mathrm{v}^2}{3}\delta_{ij}.$$

(To see where the factor of 3 came from, take the trace of both sides.) This leads to

$$\left\langle\frac{\partial^2 V}{\partial t^2}\right\rangle=-\frac{\left\langle\mathrm{v}^2\right\rangle}{3}\mathrm{PV}\left[\vec{\nabla}^2V\left(\vec{r}\right)\right]+\frac{\left\langle\mathrm{v}^2\right\rangle}{3}\vec{\nabla}^2V\left(\vec{r}\right). \tag{48}$$

From the basic identity

$$\vec{\nabla}^2\left(\frac{1}{r}\right)=-4\pi\delta\left(\vec{r}\right), \tag{49}$$

we have $\mathrm{PV}\left[\vec{\nabla}^2V\left(\vec{r}\right)\right]=0$ and $\vec{\nabla}^2V\left(\vec{r}\right)=V_0\left[-4\pi\delta\left(\vec{r}\right)\right]$. Thus, substituting Eq. (49) into Eq. (48) and then the result into Eq. (47), we find that the new term introduced by the FW procedure is

$$-\frac{1}{8\omega_0^2}\frac{\left\langle\mathrm{v}^2\right\rangle}{3}\vec{\nabla}^2V\left(\vec{r}\right)=-\frac{1}{8\omega_0^2}\frac{\left\langle\mathrm{v}^2\right\rangle}{3}V_0\left(-4\pi\delta\left(\vec{r}\right)\right). \tag{50}$$

Via the uncertainty principle, we have that the lifetime t_0 of the virtual particle pair (or equivalently fluctuation) is given by

$$\Delta t_{\max} = t_0 = \frac{1}{2\omega_0},$$

and so the new term becomes

$$-\frac{t_0^2}{6}\left\langle \mathrm{v}^2 \right\rangle \vec{\nabla}^2 V = -\frac{\left\langle \left(\Delta r_{\text{time fluctuation}}\right)^2 \right\rangle}{6}\vec{\nabla}^2 V \,. \tag{51}$$

To within a sign, this is just the smearing out of the Coulomb potential due to virtual fluctuations (i.e., particles) in the time domain that travel an average distance $\sqrt{\left\langle \left(\Delta r_{\text{time fluctuation}}\right)^2 \right\rangle}$ during their lifetime. The negative sign occurs because time-domain fluctuations are evanescent. Since the frequency $2\omega_0$ corresponds to the rest mass of the "electron-positron"[z] pair, it is very large. There is no reason to expect the velocities of the virtual particles to be relativistic, and so we would not a priori expect Eq. (50) (or equivalently Eq. (51)) to be very large in this context. The precise nature of the fluctuations is determined by quantum field theory, which is outside the scope of this report.

Now, let us add the smearing term. We could just replace $\left\langle f^2 \right\rangle / 2 \cdot \partial^2[\mu] / \partial z^2$ with $\left\langle \delta r^2 \right\rangle / 6 \cdot \vec{\nabla}^2 V$, and use the shortcut describe above. However, adapting the relevant term from Eq. (41) directly provides an opportunity to further explore the relationship between the atomic problem and the classical field. In the $\mathbb{R}^3$ radial transverse space with a point singularity, the infinitesimal integral

$$\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0} = \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} dz \frac{\partial^2 \mu}{\partial z^2}$$

gets replaced as follows:

$$\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0} = \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} dz \frac{\partial^2 \mu}{\partial z^2} \Rightarrow \lim_{\varepsilon\to 0} \oint_{\substack{\text{Sphere}\\ \text{of radius } \varepsilon\\ \text{centered at } 0}} d^3 r \vec{\nabla}^2 V \,. \tag{52}$$

Now, use Stokes' theorem to evaluate this infinitesimal integral[aa]:

$$\begin{aligned} \lim_{\varepsilon\to 0} \oint_{\substack{\text{Sphere}\\ \text{of radius } \varepsilon\\ \text{centered at } 0}} d^3 r \vec{\nabla}^2 V &= \lim_{\varepsilon\to 0} \oint_{\substack{\text{Surface of Sphere}\\ \text{of radius } \varepsilon\\ \text{centered at } 0}} dS \left(\hat{n}\cdot\vec{\nabla} V\right) \\ &= \oint_{\substack{\text{all}\\ \text{directions}}} d\Omega \;\; V_0 \left[r^2 \left(-\hat{r}\cdot\frac{\hat{r}}{r^2}\right)\right]_{r=\varepsilon} = -4\pi V_0 \end{aligned} \,. \tag{53}$$

[z] The term is, of course, used very loosely here since these objects are spinless in our toy model.

[aa] The differential element of solid angle $d\Omega$ can be parameterized, for example, by $d\Omega = \sin(\theta)\, d\theta d\varphi$, where θ is the azimuth angle and φ the polar angle.

This leaves us with the identification

$$\left.\frac{\partial[\mu_I]}{\partial z}\right|_{z=0} - \left.\frac{\partial[\mu_{II}]}{\partial z}\right|_{z=0} \Rightarrow -4\pi V_0 ,$$

and replacing $\left\langle f^2 \right\rangle$ with $\left\langle \delta r^2 \right\rangle / 3$, we have from the second term on the right-hand side of Eq. (41)

$$\delta V_{\text{transverse smear}} = \delta(z)\left(\frac{\left\langle \delta r^2 \right\rangle}{6}\left[-4\pi V_0\right] \right) = \frac{\left\langle \delta r^2 \right\rangle}{6}\vec{\nabla}^2 V , \tag{54}$$

which precisely agrees with Welton's qualitative description of the Lamb shift [62] (see also Ref. 57, page 59 for a clear exposition of Welton's theory). Note that overall, we have generalized Welton's model by adding time-domain smearing – Eq. (51) – to his smearing in the transverse-domain (three-dimensional space) – Eq. (54). This is the contribution of the Foldy-Wouthuysen transformation in this context.

3.2.4.2 Insights Concerning the Two Contributions to the Lamb Shift

Thus, the "toy model" used here nicely confirms the identification of the acoustic phenomenon given in Eqs. (40) and (41) as a classical-field Lamb shift. We have also discovered that there are two types of Lamb shift: a downrange Lamb shift and a transverse Lamb shift. Welton's model of the Lamb shift only includes the latter effect. The [time/range]-domain smearing (or downrange Lamb shift) is new here. Note that it occurs because the transverse space oscillations, which are imposed by hand, automatically induce secondary oscillations in the time/range-domain, and that our field theory automatically generates this effect.

An interesting distinction between the downrange Lamb shift and the traditional Lamb shift emerges when we consider the volume scattering problem. As noted in the discussion following Eq. (25), for volume scattering (i.e., when the potential does not contain singularities), the downrange Lamb shift invariably disappears[bb]. (Equation (25) addresses the acoustic problem, but it is trivial to transfer the result over to the "toy" atomic problem.) This is not necessarily true of the traditional or transverse Lamb shift. For the radial potential V_0/r in $\mathbb{R}^3$, $\vec{\nabla}^2 V$ is invariably 0, except at the origin, so there is no smearing of the potential away from the origin. Thus, in the atomic problem, there is also no volume-induced transverse Lamb shift (at least at lowest order). On the other hand, for an arbitrary sound speed function $[\mu]$, it is perfectly possible for the term $\partial^2\mu/\partial z^2$ to be nonzero, and so we can see from Eq. (21) that we can have a nonzero transverse smearing term, even in the absence of any singularities. The transverse (or traditional) Lamb shift comes from this term, and so it follows that fluctuations in a volume can in general generate a transverse (or traditional) Lamb shift effect in the acoustic problem.

Whether the downrange Lamb shift or the transverse Lamb shift dominates depends on whether the interface is slowly oscillating while eventually achieving a fairly large amplitude (on the scale of a wavelength), or rapidly oscillating with a more modest amplitude. If the fluctuations fall into the second category, then the downrange Lamb shift will dominate. It is in principle possible that in some classical environments, fluctuations at the Bragg wavelength may fall into the second category. However, a typical scenario in underwater acoustics is assessed in Section 5.4, and there the transverse Lamb shift still turns out to be the dominant effect.

[bb] However, recall that the new FW term also induces a small correction to diffuse scattering, which was relegated to the ellipsis in Eq. (21). This effect need not disappear in the volume scattering problem.

If the fluctuations fall into the first category, then we would expect the transverse Lamb shift to dominate. As alluded to above, this is the case for the atomic Lamb shift. The reason is that imposed fluctuations δr are caused by vacuum fluctuations of the electromagnetic field (i.e., virtual photons), and not by virtual electron-positron pairs[y]. The lifetime of a massless virtual photon can be much longer than t_0, the lifetime determined by the uncertainty principle for a virtual electron-positron pair with rest mass $2m_0$. Thus, $\delta r \sim t_{\text{photon}}\vec{\text{v}}$ can be much larger than $\Delta r_{\text{time fluctuation}} = t_0\vec{\text{v}}$. (Note that the electron-positron pair is stationary aside from the velocity of the field fluctuations on which it (along with the nucleus) is advected[y].) Indeed, Welton's model of the Lamb shift falls a little short of the correct answer, and the time-domain Lamb shift has the wrong sign to narrow the difference[cc]. Therefore, the time-domain Lamb shift must be pretty small.

3.2.4.3 Limitations of the "Toy" Model for the Hydrogen Atom

The failure of our semiclassical "toy model" to fully account for atomic Lamb shift should come as absolutely no surprise. There are several layers of approximation between this model and a realistic hydrogen atom. A realistic hydrogen atom is described by Quantum Electrodynamics (QED). There is a great deal going on in QED that lies well beyond the scope of any model that approximates second quantization as the simple advection of space by vacuum fluctuations[dd]. Our simple model for second hydrogen atom in the absence of second quantization would be the Dirac equation, which describes a field with ½-integer spin. Rather than performing the FW transformation directly on the Dirac equation, we first replaced the Dirac equation with the Klein-Gordon equation describing a scalar (spinless) field[ee]. As described in Chapter 9 (pp. 202-203) of Ref. 57, such a field would describe a pionic atom. Replacing the hydrogen atom with a pionic atom therefore constitutes our second approximation. Now, it is important to note that Eq. (42) does not even provide a realistic model of a pionic atom. A realistic pionic atom would have a diagonal matrix potential imposed on the state space equation, while Eq. (42) involves a scalar potential directly in the original Klein-Gordon equation. Replacing the diagonal matrix potential with a bona fide scalar potential constitutes our third major approximation.

The problem loses some of its richness with each of the three approximations above. Quantum Electrodynamics is far beyond the scope of the discussion here, and we will not be able to go further into this fascinating topic. The Dirac equation is somewhat richer than the Klein-Gordon equation. In a realistic hydrogen atom, the effects of spin are fairly significant[ee], but also relevant to the discussion here is the fact that the Dirac equation contains first-order derivatives with respect to the spatial coordinates rather than second-order derivatives. This leads to a richer FW transformation with more terms, and so more physics. The significance of replacing the Dirac equation with the Klein-Gordon equation (what was called the second approximation in the paragraph above) is discussed a little further in Appendix F.1. The third major approximation mentioned in the paragraph above involves replacing the diagonal matrix potential of a pionic atom with a bona fide scalar potential that looks more like a sound speed function μ from the acoustic problem. As discussed in Appendix F.2, this leads to further loss in the rich structure of the problem. Since the so-called Darwin term associated with the atomic problem provides a window into

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[cc] In fact, this term corresponds to vacuum polarization, which should indeed be modest in size compared with the primary contribution to the Lamb shift, and it should also carry the opposite sign. See Section 4.4 for a little further discussion on this topic.

[dd] For example, quantum field theories such as QED address the symmetry properties of the particle field. Thus, electrons are fermions and their wave functions must be made antisymmetric, while solutions to the Klein-Gordon equation such as pions are bosons and their wave functions should be symmetrized. Such considerations are omitted from our semiclassical approach.

[ee] This is the most significant omission in our "toy model." A properly modified time-dependent Dirac equation would predict an anomalous magnetic moment, and this provides most of the missing shift. This will be discussed a little further in Section 4.4.

the diminishing richness of the problem, and it is in some contexts similar enough to the Lamb shift that it may cause some confusion, it is briefly examined in Appendix F.3.

3.2.5 The Key Insights to Emerge from these Examples

To conclude this section, note that there are two significant insights that we should take out of our examination of the classical Lamb shift. They both center on the discovery of the downrange Lamb shift (as noted in footnote cc, this is the classical equivalent of the "vacuum polarization" correction to the Lamb shift). This is a new physical effect that has not previously been included by classical field PEs, and in the future it may need to be incorporated to improve the accuracy of PE models. Perhaps even more significantly, we have discovered something profound about the PEs generated by the FW transformation. Let us take a moment to reflect on what we have just seen. The time (or downrange) fluctuations were introduced by hand. When the resultant [time/range]-dependent potential (or equivalently sound speed function μ) are [time/range]-averaged, these will induce a contact potential correction to the (now [time/range]-independent) average problem. This much constitutes Welton's model of the atomic Lamb shift. However, the externally imposed [time/range] dependence also induces secondary virtual fluctuations, and these automatically show up in the form of new terms in the FW transformation. This forms the new type of Lamb shift effect: the downrange Lamb shift. Very significantly, note that the FW transformation has automatically dressed the singularity, *even before there has been any explicit time averaging*. This will be very significant later, when we will count on the FW transformation to similarly dress the singularity associated with a density jump.

3.3 The Downrange Stepping Procedure Near an Interface

In quantum mechanics, the usual concern is determination of observables' expectation values. In a typical calculation, these are obtained using quantum mechanical perturbation theory. Needed in this case are a list of various (in some sense small) perturbing potentials to be added to the basic problem, and the eigenstates for the basic problem. In classical field theory, on the other hand, we are primarily interested in using the PE to simulate downrange propagation of the field, often for a specific deterministic problem. In problems involving propagation through large-scale features, this usually means propagating through an environment that has been mapped out by independent measurements. When the problem also involves a stochastic distribution of small (Bragg) scale features, the known large-scale deterministic environment may be augmented with a synthetic realization generated, for example, in the context of a Monte Carlo calculation. As discussed briefly in the introduction, it is possible to model a field propagating through such a complex environment by discretizing the problem onto a grid and using the PE to step downrange. When range-dependent interfaces (or a cusps) are present, this will entail stepping across tilted boundaries. This is a nontrivial operation, and we need to devise a robust procedure for doing so. Therefore, this section closely examines the mechanics of stepping across a tilted interface.

As noted in Section 2.1, the explicit formal development conducted in this report is restricted to a consideration of quasiplanar one-dimensional interfaces of the basic form $z = f(x)$ embedded in a two-dimensional space where x is the range and z is the depth (recall that the positive z-axis points upward by convention). In this case, the (now) scalar transverse gradient ∇_T will be used interchangeably with $\partial/\partial z$. The key ideas needed to generalize the procedure applicable to the restricted two-dimensional problem to the full three-dimensional problem are briefly outlined in Appendix G.

By our convention, in this report quantities above the interface (typically the water column) will be associated with a Roman numeral *I*, and those below the interface (typically the sub-bottom) will be associated with a Roman numeral *II*. Note that the positive z-axis then points from region *II* into region *I*.

3.3.1 Discretizing the PE

Consider some field χ that obeys a generic PE $-i\,\partial\chi/\partial x = H\chi$. The Hamiltonian H is a function of the transverse derivative ∇_T. The leading order term is proportional to $\nabla_T^m\chi$. The equation is discretized to first order in the step size Δx using the Mean Value Theorem. The basic stepping algorithm is[ff]:

$$\chi_{\text{new}} = \chi_{\text{old}} + i\left(H_{\text{old}}\chi_{\text{old}}\right)\cdot\Delta x + \mathrm{O}\left(\left(\Delta x\right)^2\right). \tag{55}$$

To implement this algorithm, set a certain default (maximum) downrange step size $\Delta x_{\max}$ and fix the vertical grid spacing Δz. Note that the slope is small and the transverse derivatives are of higher order than the downrange derivative. Both these observations independently suggest that the vertical grid spacing should be somewhat finer than the default step distance[gg] (i.e., $\Delta z < \Delta x_{\max}$). Next, adjust the downrange step size Δx so that the surface falls on a grid point at each and every step. (See Fig. 9; for the purposes of illustration, vertical distances have been exaggerated in the figure.) The default (downrange) step increment $\Delta x_{\max}$ only gets used when the surface is flat (i.e., range-independent). Since the slope of the interface is always small (we will see that it must be < 45°), the vertical grid spacing always remains finer than the horizontal step size, even when the adjusted downrange step size is smaller than the default step size (i.e., $\Delta z < \Delta x < \Delta x_{\max}$). If the surface does not reach the next higher vertical grid point during a maximum x-increment, the surface is effectively flat. The minimal resolvable slope is therefore determined by the size of the (fixed) vertical grid spacing Δz relative to the default (maximum) downrange step size $\Delta x_{\max}$.

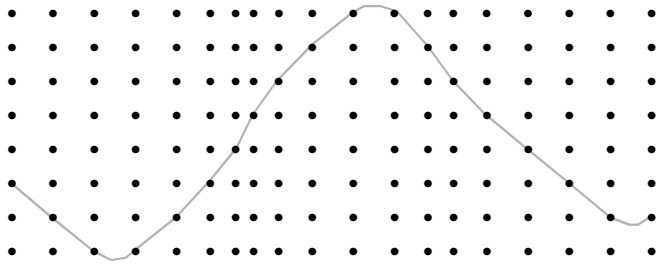


Fig. 9 — The grid to be used in the stepping algorithm is set up according to the following rules:

i. Choose a maximum downrange step size as the default step size.
ii. Choose vertical grid spacing (less than the default downrange step size).
iii. Adjust downrange stepping so the interface falls on a grid point.
iv. Minimal resolvable slope is determined by the size of the vertical grid spacing relative to the default downrange step size.

[ff] As discussed in Section 2.1, in practice this basic algorithm is modified using the Crank-Nicholson procedure, and sometimes also the Padé approximation. These modifications are not used in the formal development pursued here. It is straightforward to implement the Crank-Nicholson procedure on the results developed here, but the development of the appropriate Padé approximations necessitates future research.

[gg] Note that, in practice, one typically takes out an $\exp\left(ik_0 x\right)$ from the wave function, so away from the interface, the wave function's rate of change associated with x-dependence and that associated with z-dependence are comparable. Therefore, a higher-order derivative in the (vertical) z-direction indeed demands a finer step size in that direction.

Appendix Section G.1 discusses the major issues related to generalizing the stepping algorithm derived here (i.e., for a one-dimensional interface embedded in two-dimensional space) to the problem of a two-dimensional surface embedded in three-dimensional space. Assuming the third dimension is given by the unit vector $\hat{y}$, different $y = \text{constant}$ lines of grid points would have to be stepped separately so that they always hit the interface. Since, as discussed in Section 3.3.2.1, evaluation of $H\chi$ in a discretized space inherently involves a neighborhood of nearby points in the transverse grid, it is impossible to completely isolate $y = \text{constant}$ lines, and some fancy formal work must be used to address this issue. As we continue with the development of the basic problem begun here in Section 3.3.1, it is important to once again remind ourselves that along with the current report, virtually all other current implementations of the PE are also restricted to one-dimensional interfaces embedded in two-dimensional space (i.e., $z = f(x)$ and $\nabla_T = \partial/\partial z$).

The variable-step algorithm described here is useful for theoretical development. In a practical numerical implementation, it may prove useful to fix the step size. This simplifies the numerical procedure, particularly in the three-dimensional case or if there are multiple interfaces present. The alternative stepping algorithm with fixed step size is briefly examined at the end of Section 3.3.2.4.

3.3.2 Evaluating the Hamiltonian at a Penetrable Interface

3.3.2.1 Implementing the Stepping Procedure at a Boundary

As we begin our examination of the stepping procedure, assume that the wavefunction χ is continuous at the interface, but make no assumption about the continuity of the transverse derivative $\partial\chi/\partial z$ at the interface. The somewhat artificial, but nonetheless useful, case of χ discontinuous at the interface is considered separately in Section 3.3.4. On the other hand, there is little point in separately considering the case $\partial\chi/\partial z$ continuous. As is explained in Section 3.3.2.3 (just after Eq. (57)), very little simplification and no new insights emerge from the imposition of this condition.

The stepping procedure is iterative. Assume that the field χ is given at a certain value of the range, and that downrange stepping advances to the right. Along the old (i.e., already given) slice of grid points, specifically assume that where the interface crosses the grid, the field is known on the right side (i.e., the downrange side) of the interface. The stepping algorithm is now used to step infinitesimally close to, but just to the left of the next point where the grid intersects the interface. The field χ is continuous at the interface and so the value of the field χ is now known at all the new grid points to the right of the interface. The next step is to operate on χ with the discretized form of H in order to evaluate $H\chi$ (the generator of downrange stepping) just to the right of the interface. Once this quantity is obtained, a new downrange step follows immediately. The challenge lies in the mechanics of evaluating $H\chi$ in the vicinity of the interface. Specifically, recalling that the leading order term in $H\chi$ involves $\nabla_T^m\chi$, we need to take derivatives up to and including this order. It turns out that in order to do so, it is necessary to evaluate all the transverse derivatives ∇_T^l with l up to but not necessarily including this order *on both sides of the interface*. The m^{th} order derivative will then be obtained on one side of the interface and $H\chi$ is evaluated directly on that side. If that side happens to be to the right of the interface, then we are ready for the next step. If the side where $H\chi$ is known happens to be to the left of the interface, an implicit boundary condition will be used to obtain $H\chi$ on the right side.

3.3.2.2 Using Boundary Conditions to Evaluate Derivatives at an Interface

We now examine the procedure for using boundary conditions to take derivatives (up to the needed order) of the discretized field χ in the vicinity of the interface. The procedure is iterative. The lowest order is calculated first, and then this information is used to obtain the second derivative, and so forth[hh]. Thus, we begin by considering the first derivative. The discretized transverse derivative of χ is given by the difference between the values of χ evaluated at two adjacent vertical grid points divided by the separation distance Δz between them. Whether this discretized derivative is assigned to the top point or the bottom point is a matter of convention. For the first derivative, choose to identify it with the top point. Now there is an orphaned grid point: the point just above the interface. No finite difference can be assigned to it. This is where the boundary condition on the first derivative comes in. It is used to deduce the value of the grid point just above the interface from the value of the derivative just below the interface. All odd number derivatives will turn out to work the same way. (See Fig. 10a.) For the even derivative, things are just a little different.

The reason the second derivative and all even-order derivatives are different is that the derivatives should be kept roughly centered on the point to which they are assigned. For example, the second derivative of χ at the point labeled $j+1$ should be given by $\left[\partial^2\chi/\partial z^2\right]_{z=z_{j+1}} \approx \left(\chi^{j+2}-2\chi^{j+1}+\chi^{j}\right)\Big/\left(\Delta z\right)^2$. This is the value typically used in numerical implementations. To obtain this value, recall that the second derivative is the derivative of the first derivative, and postulate that the discretized *derivatives of the first derivative* must be assigned to grid points using the opposite convention from the one used to obtain the first derivative. Since the first derivative was assigned to the upper grid point, the derivative of the first derivative is assigned to the lower grid point. These conventions give us

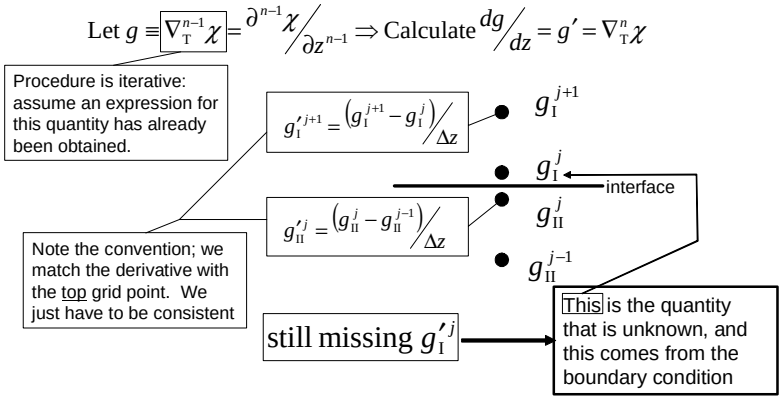
$$\frac{\partial}{\partial z}\left(\frac{\partial\chi}{\partial z}\right)\Bigg|_{z=z_{j+1}} = \left(\frac{\partial\chi}{\partial z}\Big|_{z_{j+2}} - \frac{\partial\chi}{\partial z}\Big|_{z_{j+1}}\right)\Big/\Delta z = \left(\frac{\chi\left(z_{j+2}\right)-\chi\left(z_{j+1}\right)}{\Delta z} - \frac{\chi\left(z_{j+1}\right)-\chi\left(z_{j}\right)}{\Delta z}\right)\Big/\Delta z\,,$$

and the desired result above follows immediately. Note that when we take the derivative of the derivative, the orphaned grid point lies below the interface, and now this value must be obtained from the result just above the interface using the boundary conditions. Since the procedure is iterative, it continues as described for the first and second derivatives, with the convention assigning derivatives to grid points alternating as described above[ii]. (See Fig. 10.)

[hh] In most cases, boundary conditions for derivatives of given order are independent of any higher-order derivatives, and the implementation is completely straightforward; if not, the iterative procedure outlined below at least produces the appropriate number of equations and unknowns, and the problem remains well-defined and soluble.

[ii] Note that as we continue to go up to higher orders *n*, the numerical evaluation of $\nabla_T^n\chi$ in the discrete problem will require the participation of an increasing number of vertical grid points.

a) For *n* odd:



b) For *n* even:

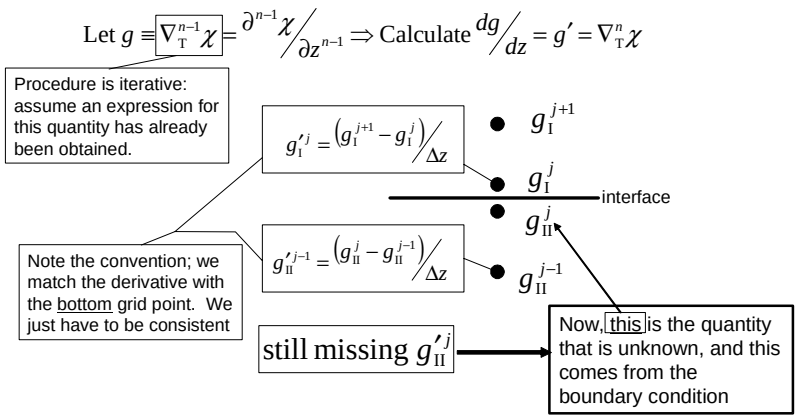


Fig. 10 — The conventions for discretizing the derivative $\nabla_{\mathrm{T}}^{n}\chi$ near an interface is shown for a) *n* odd and b) *n* even. When *n* is odd, the convention assigns finite difference approximations of the derivative to the top point. When *n* is even, the convention flips so that higher-order derivatives remain centered: for example for *n* = 2, the second derivative is assigned to the bottom point and we end up with

$$\left(\nabla_{\mathrm{T}}^{2}\chi\right)^{j+1} = \frac{\left(\nabla_{\mathrm{T}}\chi\right)^{j+2} - \left(\nabla_{\mathrm{T}}\chi\right)^{j+1}}{\Delta z} = \frac{\chi^{j+2} - 2\chi^{j+1} + \chi^{j}}{\left(\Delta z\right)^{2}}.$$

At the interface, there is always one orphaned value that must be evaluated using the boundary conditions**.**

3.3.2.3 The PE Spawns a New Family of Boundary Conditions

There is a subtle, but very important distinction between the PE and the Helmholtz equation. The latter is second order in the transverse derivative, so the solution is fully specified by two boundary conditions at a penetrable interface. However, a PE that is m^{th} order in the transverse derivative is well posed only once m boundary conditions have been specified on the penetrable interface [67, 68]. This formal issue

of well-posedness in the continuum limit is directly tied to the practical problem of how to calculate the higher-order derivative needed to numerically solve the discrete problem.

In practice, researchers have usually sidestepped this issue by truncating the entire PE (including the stepping algorithm) at the order $m = 2$ near the boundary (i.e., at first order in the PE expansion parameter λ), and in this way avoided the issue of determining the extra boundary conditions[jj]. In fact, as outlined in Ref. 69 (Appendix B), the technique developed above for evaluating derivatives near the interface has not been used in the standard implementation of the stair step PE[kk]. The alternate approach described in the reference does not lend itself to the use of the higher-order boundary conditions, and it is not appropriate for use with bona fide tilted surfaces (it only works for a step-like interface). In this report, however, a method for determining the higher-order boundary conditions is developed in Section 3.3.3. For the moment, we are exploiting the fact that these m boundary conditions must exist and must have been specified by the correct formulation of the problem.

The complete formulation of the problem involves m explicit boundary conditions, generally providing boundary conditions on χ to $\nabla_T^{m-1}\chi$. This allows our procedure for calculating the derivatives to work up to $\nabla_T^{m-1}\chi$. Although this formally specifies the problem, this all by itself is not yet enough to evaluate the quantity $H\chi$, which must be evaluated in order to proceed with our stepping algorithm. The reason is that this quantity contains a term proportional to $\nabla_T^m\chi$. Our technique for taking derivatives near the interface will allow us to determine $\nabla_T^m\chi$ on one side of the interface (for the conventions in Fig. 10, above the interface if m is even and below if m is odd), but we now do not have the value of $\nabla_T^m\chi$ on the other side. Recall that this quantity would be needed to directly evaluate $H\chi$ on that side of the interface. Since the Hamlitonians H for the PE problems that interest us always have leading order m that is even, we can evaluate $H\chi$ above the surface. If the slope is negative, we have all we need to proceed to the next step of the stepping procedure. On the other hand, if the slope is positive, we need to find an implicit boundary condition that allows us to deduce the value of $H\chi$ below the interface. (Note that we can circumvent the need to explicitly evaluate the missing partial derivative $\nabla_T^m\chi$ below the interface if we have some way to directly determine $H\chi$ on that side of the interface.)

The implicit boundary condition comes from the equation of motion tying $H\chi$ to the downrange derivative combined with the (a priori specified) boundary conditions on χ and $\partial\chi/\partial z$. The latter are used to deduce the boundary condition on $\partial\chi/\partial x$, which is then used in conjunction with the PE equation to deduce the boundary condition on $H\chi$. For most PE applications, it can be assumed that χ

[jj] This is a significant omission. Over the last 20 years, much of the research related to the PE has focused on obtaining ever-higher orders. For example, one of the key advantages of the Padé approximation is that it allows the efficient calculation of the high order PE. Progress in this direction has allowed the PE method to be applied to steep grazing angles, and to cases where the environmental parameters significantly vary as a function of the depth. The latter is of particular relevance to the issue of a density jump at the ocean bottom. Here, the density may jump by as much as a factor of two, usually the largest variation of the environmental parameters to be found in the entire problem. Furthermore, high grazing-angle results are suspect when such a crucial part of the problem is restricted to first order.

[kk] Instead, one places the interface in between two grid points. Then, one overlaps the upper and lower half-spaces by extending each out beyond the interface by one extra grid point. Lowest order theory (i.e., the one with a lead second order transverse derivative in the Hamiltonian) is used, so there are only two boundary conditions involved. The two boundary conditions are used to solve for the field at the extra (nonphysical) points. The extra points provide enough information to calculate the second transverse derivative in the first order Hamiltonian, which is the one used to generate downrange stepping right at the surface.

is continuous; however, density jumps will lead to discontinuities in $\partial\chi/\partial z$. The continuity of χ implies that the difference between the values of the field χ evaluated on the two sides of the interface is zero (i.e., $\chi_{\mathrm{II}} - \chi_{\mathrm{I}} \equiv \Delta\chi = 0$ on the surface), which implies the tangential derivative of the difference is also zero: $\hat{\mathrm{t}} \cdot \vec{\nabla}(\Delta\chi) = 0$. Writing out the tangential derivative in terms of $\partial\chi/\partial x$, $\partial\chi/\partial z$, and the local slope $\dot{f}$ leads to an equation for $\partial\chi/\partial x$:

$$\frac{\partial(\Delta\chi)}{\partial \mathrm{x}} + \dot{f}\frac{\partial(\Delta\chi)}{\partial \mathrm{z}} = 0 \Rightarrow \frac{\partial\chi_{\mathrm{II}}}{\partial \mathrm{x}} = \frac{\partial\chi_{\mathrm{I}}}{\partial \mathrm{x}} - \dot{f}\left[\frac{\partial\chi_{\mathrm{II}}}{\partial \mathrm{z}} - \frac{\partial\chi_{\mathrm{I}}}{\partial \mathrm{z}}\right] = 0, \tag{56}$$

and from the PE $\partial\chi/\partial \mathrm{x} = H\chi/-i$ we have for $H\chi$:

$$H_{\mathrm{II}}\chi_{\mathrm{II}} = H_{\mathrm{I}}\chi_{\mathrm{I}} + i\dot{f}\left[\frac{\partial\chi_{\mathrm{II}}}{\partial \mathrm{z}} - \frac{\partial\chi_{\mathrm{I}}}{\partial \mathrm{z}}\right]. \tag{57}$$

The slope $\dot{f}$ used is that of the upcoming step. The quantities on the right-hand side of Eq. (57) are known and used to calculate $H_{\mathrm{II}}\chi_{\mathrm{II}}$ (recalling that side II is below the interface, and so $H_{\mathrm{II}}\chi_{\mathrm{II}}$ cannot be determined directly under the conventions used in this report).

3.3.2.4 Some Final Thoughts Concerning the Hamiltonian at an Interface

Now we can see how little would have been gained had we separately considered the case $\partial\chi/\partial z$ continuous. Equation (57) would reduce to the simple condition that $H\chi$ be continuous at the interface, but this is the only gain and it represents a very minor simplification. The derivative $\nabla_T^m\chi$ can still jump dramatically at the boundary, since the continuity of $H\chi$ depends on delicate internal cancellations. For example, consider the very simple Hamiltonian $H = k_0 + \lambda$. Infinitesimal integration of the equation across the interface of the type discussed in Section 3.2.3 shows that χ and $\partial\chi/\partial z$ are both continuous. Then, from Eqs. (56) and (57), $\partial\chi/\partial x$ and $H\chi$, respectively, are continuous as well. Continuity of $H\chi$ implies that $H_I\chi_I - H_{II}\chi_{II} = 0$ and so we have shown that $\nabla_T^2\chi$ has a jump proportional to $k_0^2\mu\chi$. Note that just as for more complicated situations where we do not have continuity of $\partial\chi/\partial z$, we still will need to use our full set of boundary conditions to step across the interface.

Although the given set of boundary conditions that fully specifies our problem may or may not explicitly contain the slope, the algorithm nevertheless remains sensitive to the local slope. For instance, slope dependence is built into Eq. (57), the implicit boundary condition for $H\chi$. A very small slope that is below some minimum threshold will generate a flat surface where successive grid points on the interface remain at the same height. As illustrated in Fig. 11, such a flat interface may be punctuated by intermittent "boosts" where the slope takes on its minimum value for a single step. This minimum allowed value for the slope is fixed by the grid size: $\dot{f}_{\mathrm{fixed}} = \dot{f}_{\min} = \Delta x_{\max}/\Delta z$.

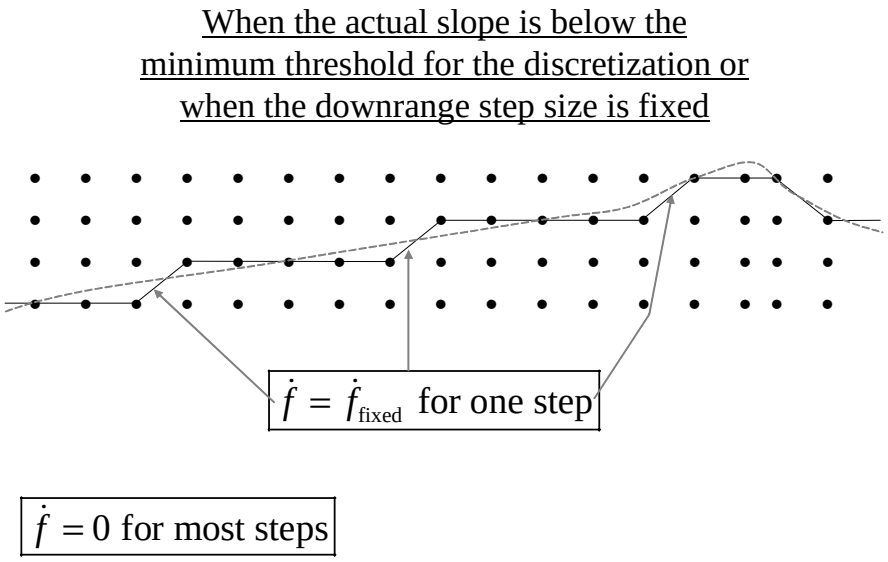


Fig. 11 — For a discretization to resolve smaller and smaller slopes, a vertical grid that is finer and finer relative to the default (downrange) step size is needed. If the vertical grid is too coarse relative to the step size, the interface remains at the same height during successive steps, and only jumps occasionally. Now, the discretization can no longer resolve the local slope. The presence of a small locally invisible slope can still cause a cumulative effect whereby after many downrange steps, a jump in the interface is eventually needed. At this jump, the slope is artificially high for one step. This is an artifact that can be made to disappear by using a finer vertical grid or a larger maximum step size, but this might not always be a viable option. At any rate, the occasional appearance of a "boost" that gives the slope a nonzero value for a single step is only a mild source of error since the slope here is just the minimum slope that our discretization would be capable of resolving. There are still no corners and steps on the surface, just mild steps in the slope associated with discretization. Note that since we always use the slope for the upcoming step, our procedure always gives $H\chi$ continuous along a horizontal portion of the interface. Also note that for the purposes of illustration, the slopes have once again been exaggerated. Finally, note that the figure also applies when the downrange step size is fixed. Now, the fixed slope is the maximum slope resolvable by the algorithm.

Fig. 11 also suggests an alternate to the variable-step-size algorithm presented in Section 3.3.1. Particularly in the three-dimensional case or if there are multiple interfaces present, it is useful to simplify the numerical implementation by dispensing with variable sizes Δx altogether, and fixing the downrange step: $\Delta x = \Delta x_{\text{fixed}}$. This would be similar to current implementations, but the (distorted) interface would lie right on top of the grid (rather than in the middle between grid points), and (more significantly) rather than having stair steps, the (distorted) interface would remain flat for a series steps before acquiring some fixed finite slope for a step (as in Fig. 11): $\dot{f}_{\text{fixed}} = \Delta x_{\text{fixed}} / \Delta z$. This fixed slope is now the maximum slope compatible with the given implementation (i.e., when the interface is at maximum slope, it would move vertically with every downrange step). In this case, the relative size of vertical and horizontal grid spacing would be determined by the desired *maximum* slope and not by the considerations mentioned in the second paragraph of Section 3.3.1 (i.e., now $\dot{f}_{\text{fixed}} = \dot{f}_{\max}$). In this case, note that the generalization of the stepping algorithm to three dimensions is now comparatively trivial (i.e., the need for interpolation described in Appendix G.1 has been eliminated). Also note that the presence of more than one surface poses no problems for this alternate stepping algorithm. Finally, in a practical implementation of the new

theory, one would expect streamlined efficient programs to work best. The stepping convention outlined in this paragraph avoids the complex code needed to vary the step size (along with its associated numerical overhead), and so it may well be the preferred choice for typical practical implementations. However, the variable-step-size algorithm described above provides a very nice context for the formal discussion that follows, and we implicitly assume that it is the one being used throughout the rest of this manuscript.

3.3.3 The Boundary Conditions

To facilitate our look at the manner in which boundary conditions arise from the formalism, let us begin by considering the standard two-dimensional problem with the range x and the transverse coordinate the depth z. The generalization to the three-dimensional problem with a two-dimensional transverse coordinate $\underline{R}_T = (y, z)$ will be briefly considered at the end of Section 3.3.3.2 and then further developed in Appendix G.2.

3.3.3.1 The Relationship Between Contact Potentials and Boundary Conditions

Boundary conditions such that $\nabla_{\mathrm{T}}^k \chi \quad (k \geq 1 \quad \text{for now})$ are discontinuous come from "distributions" in the Hamiltonian H. In this context, a distribution is a generalized function that constitutes a "spike" or a "contact" potential (such as the δ-function). For example, as we saw in Section 3.2.3, if H contains a δ-function at the interface, then as in the Kronig-Penny model in solid state physics (see Ref. 66) or equivalently as for the cusp in our discussion of the classical Lamb shift, we obtain a boundary condition by integrating the PE along the transverse dimension across an infinitesimal interval bracketing the interface ($\lim_{\varepsilon \to 0} \int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$ for the cusp in the two-dimensional problem; there is a very similar integral in the spatial dimension of the Kronig-Penny model for a one-dimensional lattice). With the leading derivative of second-order (i.e., a lead order term $\propto \nabla_T^2 \chi$), this procedure will generate a discontinuity in the first derivative of the wave function.

When higher-order derivatives of the δ-function are present, this example can be generalized by adapting a procedure originally derived by Heaviside [70, 71]. Before applying Heaviside's procedure, however, the rules for converting δ-functions times functions of the transverse coordinate variable z to δ-functions times something evaluated at the fixed point (on the surface) $z = f(x)$ need to be employed (specifically, use the equation taken from the classic text by Lighthill [72] and adapted in Eq. (59)). This leaves us with a sum of distributions times a "constant," where the "constant" is the field and its derivatives evaluated at the fixed height of the interface: $\chi(f)$ and $\nabla_T^k \chi\big|_{z=f}$. Now following Heaviside, the key step once again consists of an integration across the interface over an infinitesimal interval in the transverse direction (i.e., $\lim_{\varepsilon \to 0} \int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$ for the two-dimensional problem). This time, the definite integration over the infinitesimal interval *may* in general come after one or more indefinite integrations – or completely equivalently, integration over the interval from $-\infty$ to the new variable z_k, where it is understood that the field is "turned off" at $-\infty$.

To write all this symbolically, take the basic PE $H\chi + i\partial\chi/\partial x = 0$ and perform $n+1$ "indefinite" integrations followed by one definite integration. This gives us (for the two-dimensional problem):

$$\int_{f-\varepsilon}^{f+\varepsilon} dz \int_{-\infty}^{z} dz_1 \cdots \int_{-\infty}^{z_n} dz_{n+1} \left(H\chi \right)\Big|_{z_{n+1}} + \int_{f-\varepsilon}^{f+\varepsilon} dz \int_{-\infty}^{z} dz_1 \cdots \int_{-\infty}^{z_n} dz_{n+1} \left(i\frac{\partial \chi}{\partial x} \right)\Big|_{z_{n+1}} = 0, \tag{58}$$

where it is understood that we must always make the substitution[ll]:

$$\delta^{(k)}(z-f)\chi(z) \Rightarrow \sum_{p=0}^{k} \frac{(-1)^p (k)!}{p!(k-p)!} \delta^{(k-p)}(z-f) \frac{\partial^p \chi}{\partial z^p}\Big|_{z=f} = \delta^{(k)}(z-f)\chi(f) + \cdots. \tag{59}$$

The current assumption that the wave function χ is continuous implies that the first downrange derivative $\partial\chi/\partial x$ does not contain a distribution and so $\int_{f-\varepsilon}^{f+\varepsilon} dz \, \partial\chi/\partial x \to 0$ (or more generally $\int_{f-\varepsilon}^{f+\varepsilon} dz \int_{-\infty}^{z} dz_1 \cdots \int_{-\infty}^{z_n} dz_{n+1} \left(\partial\chi/\partial x \right) \to 0$), and only infinitesimal integration over $H\chi$ can give a nonzero contribution to Eq. (58). Thus, we can confine ourselves to integrating over $H\chi$ to obtain the boundary conditions:

$$\int_{f-\varepsilon}^{f+\varepsilon} dz \int_{-\infty}^{z} dz_1 \cdots \int_{-\infty}^{z_n} dz_{n+1} \left(H\chi \right)\Big|_{z_{n+1}} = 0. \tag{60}$$

Equation (60) is of course subject to the understanding given by Eq. (59). Note that when $n = 0$, we have

$$\int_{f-\varepsilon}^{f+\varepsilon} dz \int_{-\infty}^{z} dz_1 \left(H\chi \right)\Big|_{z_1} = 0,$$

and we additionally also have the equation

$$\int_{f-\varepsilon}^{f+\varepsilon} dz \left(H\chi \right)\Big|_{z} = 0. \tag{61}$$

The indefinite integrations pull off ∇_T's from the lead order derivative in H. After n indefinite integrations, the leading order term (in our notation, it is $\propto \nabla_T^m \chi$) is left with $m-n$ transverse derivatives operating on the wave function $\nabla_T^{m-n}\chi$. The infinitesimal *definite* integration peels off one more transverse derivative and then gives the difference between the value of this function evaluated on the two sides of the interface: $\nabla_T^{m-n-1}\chi_I - \nabla_T^{m-n-1}\chi_{II}$. Nonzero values for this difference come from the spike potentials. A δ-function provides a nonzero contribution after just one (infinitesimal) integration and in this way generates a jump in $\nabla_T^{m-1}\chi_I - \nabla_T^{m-1}\chi_{II}$. Since each indefinite integration also pulls off an order from the derivative in the spike potential, a δ'-function becomes a δ-function after one (indefinite) integration, and it therefore provides the jump after a total of two integrations. More generally, $\delta^{(n)}$-functions will generate jumps after a total of $n+1$ integrations[mm]. Note that if no distribution proportional to $\delta^{(n)}$ is present, then performing a total of $n+1$ integrations simply yields a continuity condition.

[ll] This equation can be derived using the following iterative argument: Take the derivative of the formula for $\delta^{(k-1)}(z-f)\chi(z)$, and expand using the product rule for differentiation. For example, treating *f* like a constant and taking $\chi(z)$ to be some general test function, take $\partial/\partial z$ of the equation $\delta(z-f)\chi(z) = \delta(z-f)\chi(f)$ and rearrange to get $\delta'(z-f)\chi(z) = \delta'(z-f)\chi(f) - \delta(z-f)\chi'(f)$. The procedure can then be repeated.

[mm] Note the integrals of these distributions are zero unless the number of integrations is just right: too few integrations, and the function integrates to zero under the definite (infinitesimal) intergration (i.e., the positive and negative areas under the curve cancel); too many, and the infinitesimal integration kills the term off (i.e., the δ-functions have all integrated out, leaving behind an integral of a bounded function over an infinitesimal interval).

3.3.3.2 Related Technical Issues that are Addressed Elsewhere in this Study

The needed distributions in $H\chi$ are generated both by higher-order cross-terms as we expand the standard square root operator ($\sqrt{1+2\lambda/k_0}$ when the density is the same everywhere) – e.g., see Appendix K.1.1 – as well as by the new FW correction terms – as we have seen in Section 3.2 and will again see in Section 4.1 and Appendix M. Note that by deriving the boundary conditions from distributions embedded within a *Hermitian* Hamiltonian, we guarantee energy conservation (and so stability as well).

If the needed "constant" coefficient of the distribution jumps (e.g., we have $\delta(z-f)\cdot\nabla_T^k\chi(f)$ where we have already determined that $\nabla_T^k\chi(f)$ is not continuous at the interface), use "δ-function bifurcation." This subtle issue is explored in Section 5.2 when an understanding of it becomes indispensable for considering an interface with a density jump at even the most rudimentary level. δ-function bifurcation will follow rules determined by examining a series of test cases for which the solution is known. For convenience, the rules are summarized in the footnote below[nn], but the topic is revisited in Section 5.2 and again in more detail in Appendix K.

Appendix G.2 presents a brief examination of the generalization to the full three-dimensional problem of the procedure developed here in Section 3.3.3. Again, the y-axis provides the extra dimension. The integrations used to determine the boundary conditions are now in the direction normal to the cut of interface in the $x=\text{constant}$ plane. Call this two-dimensional normal $\hat{n}_{2D}$. Call the two-dimensional tangent $\hat{t}_{2D}$. The boundary conditions are expressed in terms of $\hat{n}_{2D}$, $\hat{t}_{2D}$ and $\underline{\nabla}_T$, which in turn can be expressed in terms of $\partial f/\partial y$ and $\hat{y}\partial/\partial y+\hat{z}\partial/\partial z$. The downrange slope $\dot{f}$ is as before. (Keep in mind that the explicit boundary conditions obtained in Sections 4.1, 5.3.2, and 6.1 (specifically Eqs. (71), (99), and (120), respectively) will reflect only the basic formalism for the two-dimensional problem as developed here in Section 3.3.3.)

3.3.3.3 Relationship Between the Boundary Conditions in the PE Problem and those for the Full-wave Problem

As noted in Section 3.3.2 (and in Refs. 67 and 68), the boundary conditions that emerge from the procedure described here more or less substitute for a smaller set of boundary conditions associated with the full-wave problem. The manifest reason for the appearance of all these new boundary conditions is that as soon as powers of λ appear in the Hamiltonian, then the leading order derivative is some number $m>2$, and a full set of m boundary conditions must be *explicitly* specified in order that the PE problem be well posed. As the order of the PE approaches ∞, the number of required boundary conditions also goes to ∞, even though the full Helmholtz equation it approximates is only second order, and thus requires only two boundary conditions.

[nn] The basic rule is that the first δ-function obtained splits in half (i.e., bifurcates). The two halves are displaced in opposite directions away from the interface. Any other distributions in the product collapse since they are smooth functions in the half-spaces away from interface. The procedure is associative in the sense that it does not matter which δ-function is chosen to be the first one. On the way to generating that first δ-function, the chain rule for differentiation applies. The ∇_T operating on the δ-function will generate higher-order derivatives of the δ-function. It is permitted to multiply through by a density since it involves an undistorted step, but in general it is not permitted to multiply through by distorted steps produced by taking functions of steps. These rules, and the empirical evidence justifying them, are examined in Section 5.2 and in further detail in Appendix K.

There is a rather interesting complementary interpretation for these new boundary conditions. Along the tilted interface, these "new" boundary conditions also serve as replacements for the downrange derivative of the field in what would, in the full-wave problem, be the boundary condition on the normal derivative of the field. Specifically, when the normal has a downrange component, the normal derivative $\partial\chi/\partial\hat{n} = \hat{n}\cdot\vec{\nabla}\chi$ picks up a contribution from the downrange derivative, but in the PE, we now find that the *explicit* boundary conditions involve only transverse derivatives of the field. In other words, only the transverse portion of the normal derivative has survived to play a role in specifying the PE problem. This turns out to be a very desirable result, since the downrange derivative plays a special role in the PE: it is a downrange stepping operator, and as such it cannot appear in the Hamiltonian. Including the stepping operator $i\partial/\partial x$ into our boundary conditions would amount to inserting this operator into the Hamiltonian, in which case the equation would cease to be parabolic! (The implicit boundary condition (Eq. (56)) and its alternate form (Eq. (57)) are simply consequences of the continuity condition on χ. Note that they are *derived conditions on* the Hamiltonian, but they *do not add new information* to the Hamiltonian beyond that already contained within the continuity condition on χ, and so they play no role in the formal specification of the problem. Thus, they are fundamentally different from the explicit boundary conditions discussed here in Section 3.3.3. In particular, they do not contradict the assertions in this paragraph.)

Before taking a look at examples, which illustrate many of the ideas discussed here in Section 3.3.3, let us examine what happens if we relax the continuity condition on χ.

3.3.4 Relaxing the Continuity Condition on the Wave Function χ

We will shortly find it useful to consider a problem such that χ is discontinuous. This result is associated with the relatively artificial problem, where we consider "mixed orders." These are obtained by matching high order FW correction terms with low orders of the expansion of the $\sqrt{1+2\lambda/k_0}$ operator. For example, once again as in Section 3.2.2 include only λ's but not downrange derivatives in our power counting to get the quasi-first order Hamiltonian

$$H = k_0 + \lambda - \frac{\ddot{\lambda}}{8k_0^2}. \tag{62}$$

A χ-discontinuity boundary condition emerges from a Hermitian Hamiltonian (such as Eq. (62)) containing distributions as follows. Integrate down a vertical line as before. Given that the leading order of the PE is $\nabla_T^m\chi$, a $\delta^{(m-1)}$ in the "potential" will produce a jump in χ.

Now, given the needed boundary conditions, propagate to the interface as described above in Section 3.3.1, and use the boundary conditions on the field χ and its transverse derivatives to move to the far side and obtain the new value for $H\chi$ needed to perform the next step.

For our current purposes, we ignore the δ-function-like singularity generated by $\partial\chi/\partial x$ when the interface of χ-discontinuity is range-dependent (i.e., tilted). There are two justifications for this. In the examples that will interest us, the missing term is of higher order than the Hamiltonian (for constant density theory, the missing terms are $\mathrm{O}\left(\dot{f}^3\right)$ or $\mathrm{O}\left(\dot{f}\cdot\ddot{f}\cdot\nabla_T\right)$) and it vanishes completely in the purely coherent part of the stochastic case. More significantly, χ will jump at an interface in only a handful of

relatively artificial cases. Using a full higher-order theory, where for example $-\ddot{\lambda}/8k_0^2$ is considered third order and matched with the $\mathrm{O}(\lambda^3)$ leading term, then the δ'-function in $-\ddot{\lambda}/8k_0^2$ will not lead to a discontinuity in χ (much more is given in Section 4.2 about changes in the meaning of a given contact potential as the lead order of the PE changes). The continuity of χ is also used extensively in Appendix G.2 to extend the procedure for extracting boundary conditions to the full three-dimensional problem. Thus, it will ultimately prove fortuitous that all consistent and fully realistic problems will have χ continuous. Nevertheless, the Hamiltonian (Eq. (62)) will prove useful in isolating the new physics associated with the downrange Lamb shift generated by an interface such as the ocean bottom, and assessing its possible significance in underwater acoustics, so we will press on with the analysis.

Finally, let us generalize the implicit boundary condition. Assume $\chi_{\mathrm{I}} = a\chi_{\mathrm{II}}$ at the surface. Now, we have

$$
\begin{aligned}
& a\chi_{\mathrm{II}} - \chi_{\mathrm{I}} = 0 \text{ on the surface} \\
& \Rightarrow \text{ tangential derivative of } a\chi_{\mathrm{II}} - \chi_{\mathrm{I}} \text{ is zero} \\
& \Rightarrow \text{ i.e., } \hat{\mathrm{t}} \cdot \vec{\nabla}\left(a\chi_{\mathrm{II}} - \chi_{\mathrm{I}}\right) = 0 \\
& \Rightarrow \partial\left(a\chi_{\mathrm{II}} - \chi_{\mathrm{I}}\right)/\partial \mathrm{x} + \dot{f}\,\partial\left(a\chi_{\mathrm{II}} - \chi_{\mathrm{I}}\right)/\partial \mathrm{z} = 0 \\
& \Rightarrow a\left(\partial\chi_{\mathrm{II}}/\partial \mathrm{x}\right) = \partial\chi_{\mathrm{I}}/\partial \mathrm{x} - \dot{f}\left[a\left(\partial\chi_{\mathrm{II}}/\partial \mathrm{z}\right) - \partial\chi_{\mathrm{I}}/\partial \mathrm{z}\right] = 0 \\
& \Rightarrow \text{use } \partial\chi/\partial \mathrm{x} = H\chi/-i \\
& \Rightarrow H_{\mathrm{II}}\chi_{\mathrm{II}} = \frac{H_{\mathrm{I}}\chi_{\mathrm{I}}}{a} + i\dot{f}\left[\partial\chi_{\mathrm{II}}/\partial \mathrm{z} - \frac{1}{a}\left(\partial\chi_{\mathrm{I}}/\partial \mathrm{z}\right)\right].
\end{aligned}
\tag{63}
$$

Thus, we have all we need to apply the technique outlined in Sections 3.3.1 to 3.3.3 for the instance where χ is discontinuous. This will prove useful in Section 4, as we move first to an interface where the sound speed jumps and then also consider the case where the density is allowed to jump as well.

4. THE SOUND SPEED JUMP—TILT-INDUCED SMEARING AND THE CLASSICAL LAMB SHIFT

In this section we consider a sound speed to jump and closely examine two examples where the surface roughness buffers the singularity (i.e., smears it out):

- uprange/downrange smearing induced by a deterministic tilt and associated with the new term introduced by the FW transformation
- the classical Lamb shift induced by a stochastic rough interface, and associated primarily with smearing in the transverse direction.

In Sections 5.3.2. and 5.3.4, the study here in Section 4 is extended to the case where the density jumps as well. We study these phenomena both to assess the effects' potential importance in underwater acoustics, and also as a vehicle for the further development of our formal structure in anticipation of the development of a PE suitable for modeling Bragg scattering from a rough interface where the density jumps. We begin here in Section 4 with the case of a sound speed jump alone in order to fully develop our understanding of the problem in this relatively simple context. In Section 4.1, we once again consider a quasi-first-order theory that combines first PE theory with the new nominally third-order term introduced by the FW transformation. This term is the one associated with new tilt and curvature-induced

effects. Next, in Section 4.2 we set the curvature of the interface to zero, leaving us with an effect associated with tilt-induced smearing. The resultant boundary conditions along a deterministic interface are examined in detail. We find that the relationships between some of the boundary conditions for the PE and their corresponding manifestations in the full-wave problem are often quite apparent at a specific order, only to become surprisingly obscure at other orders. In Section 4.3, we examine the stochastic problem and obtain the classical Lamb shift associated with a sound speed jump. Unlike for the cusp, the tilt/curvature-induced correction (essentially smearing in the uprange/downrange direction) associated with the new FW term disappears from this stochastic problem, leaving us only with smearing in the transverse direction. In Section 4.4, the new physics associated with the tilt/curvature-induced correction and with the classical Lamb shift is placed into the context of other physical phenomena. In particular, we see at the end of Section 4.4.3 that tilt-induced smearing is related to vacuum polarization in the quantum problem.

This prepares us for Sections 5 and 6, where the density jump is introduced into our study. The possible relevance in underwater acoustics of the classical Lamb shift is considered in Section 5.4, and the crucial tools needed to consider Bragg scattering from a rough interface where the density jumps are considered in Section 6.1. As discussed in Section 6.1.3, our study of tilt-induced smearing will be valuable primarily for the insights it gives us in the way that the PE buffers singularities.

4.1 A Simple Model for a Sound Speed Discontinuity at the Interface

Here, we consider an interface where the sound speed jumps and pursue a calculation much like that for the cusp (where the sound speed gradient jumps) in Section 3.2.3.

We consider the standard two-dimensional ($x-z$) space, where (for now) the sound speed is constant in the half-spaces I and II, and the reference sound speed is the sound speed in Region I. The two regions are separated by the rough surface $z=f(x)$. The conventions for this problem are summarized in Fig. 12.

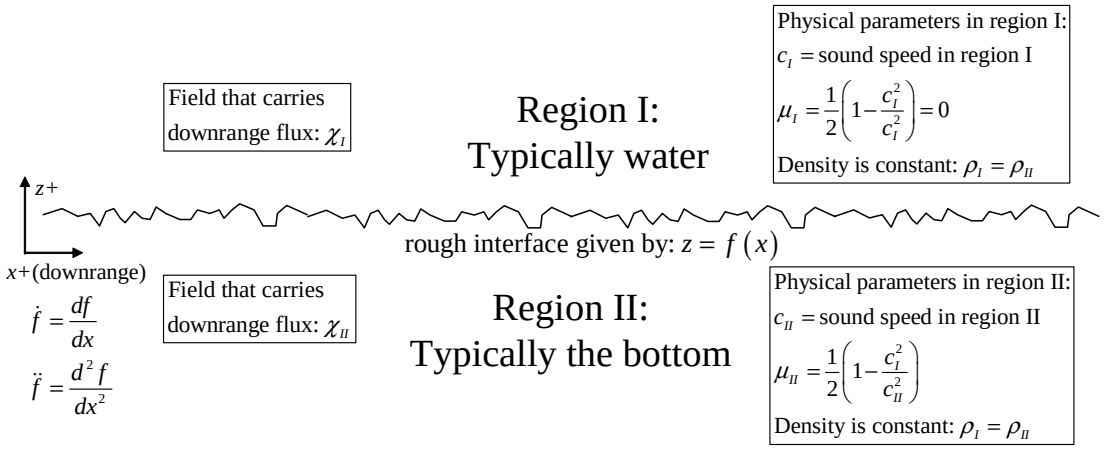


Fig. 12 — The conventions for a rough interface where the sound speed jumps. Regions I and II are separated by a rough surface $z=f(x)$ along which the sound speed jumps. As before, $\mu \equiv \left(1-n^2\right)/2$ (this will be generalized later), where $n=c_0/c$ such that $k=nk_0$. Here, $c_0=c_I$. For the moment, both regions are still assumed to have the same density.

4.1.1 The Boundary Conditions for Quasi-first Order Theory

Let us also use the quasi-first order Hamiltonian

$$H = k_0 + \lambda - \ddot{\lambda}/8k_0^2 = k_0 + \lambda + \ddot{\mu}/8k_0 \,, \tag{64}$$

where

$$\mu \equiv \left(1-\left({}^{c_I}\!/_{c}\right)^2\right)\Big/2 = \left[\left(1-\left({}^{c_I}\!/_{c_{II}}\right)^2\right)\Big/2\right]\Theta\left(-z+f(x)\right) = \mu_{II}\Theta\left(-z+f(x)\right). \tag{65}$$

Note that Eq. (65) simply restates the fact that $\mu = 0$ in Region I and $\mu = \mu_{II}$ in Region II. Now, we have

$$\begin{aligned} \dot{\mu} &= \dot{f}\mu_{II}\delta(-z+f) = \dot{f}\mu_{II}\delta(z-f) \\ \ddot{\mu} &= \ddot{f}\mu_{II}\delta(z-f) - \dot{f}^2\mu_{II}\delta'(z-f). \end{aligned} \tag{66}$$

So now we have

$$\frac{\ddot{\mu}}{8k_0} = -\frac{\dot{f}^{\,2}}{8k_0}\mu_{II}\delta'(z-f) + \frac{\ddot{f}}{8k_0}\mu_{II}\delta(z-f). \tag{67}$$

These δ- and δ'-functions generate perfectly good Hermitian contact potentials. Now use Eq. (59) with $k = 1$ to get

$$\delta'(z-f)\chi(z) = \delta'(z-f)\chi(f) - \delta(z-f)\left.\frac{\partial\chi}{\partial z}\right|_{z=f}. \tag{68}$$

The equation of motion $-i\,\partial\chi/\partial x = H\chi$ with the Hamiltonian (Eq. (64)) becomes

$$\frac{\nabla_T^2\chi}{2k_0} - \frac{\mu_{II}}{8k_0}\dot{f}^2\delta'(z-f)\chi(f) + \frac{\mu_{II}}{8k_0}\delta(z-f)\left(\ddot{f}\chi(f) + \dot{f}^2\left.\frac{\partial\chi}{\partial z}\right|_{z=f}\right) + \cdots = 0 \tag{69}$$

where the ellipsis "$\cdots$" stands for terms that are at worst steps and are delta functions or their derivatives. As discussed in Section 3.3.4, we are throwing out the step in $\partial\chi/\partial x$ because it is higher order in the variables $\ddot{f}, \dot{f}$ and because it is an artifact of the unusual power counting convention implicit in the quasi-first order Hamiltonian (Eq. (64). We can use the transverse integrations given in Eq. (60) with $n = 0$ and in Eq. (61) to get

$$\begin{aligned} \chi_I - \chi_{II} &= \frac{\mu_{II}}{4}\dot{f}^2\chi(f) \\ \left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} &= -\frac{\mu_{II}}{4}\left(\ddot{f}\chi(f) + \dot{f}^2\left.\frac{\partial\chi}{\partial z}\right|_{z=f}\right), \end{aligned} \tag{70}$$

respectively. Note that there is an ambiguity concerning the proper way to evaluate $\chi(f)$ and $\left[\partial\chi/\partial z\right]_{z=f}$, since these quantities jump at the interface. The discontinuity is generated by δ- and δ'-

functions that are multiplied by $\dot{f}^2$ and $\ddot{f}$, and so the discontinuities themselves are $O\left(\ddot{f}, \dot{f}^2\right)$. When such discontinuities are inserted back into the δ- and δ'-terms, the overall order of the ambiguity becomes $\mathrm{O}\left(\dot{f}^4, \dot{f}^2\ddot{f}, \ddot{f}^2\right)$. This is a higher order than concerns us in the present context. Thus to $O\left(\ddot{f}, \dot{f}^2\right)$, on the right-hand sides of Eqs. (70) we can choose to evaluate χ anywhere in the interval $\chi \in \left[\chi_I, \chi_{II}\right]$, and $\partial\chi/\partial z$ anywhere in the interval $\partial\chi/\partial z \in \left[\partial\chi_I/\partial z, \partial\chi_{II}/\partial z\right]$. Anticipating the intuitively appealing δ-function bifurcation result (see footnote nn, as well as Section 5.2 and Appendix K), we can choose to evaluate $\chi(f)$ and $\left[\partial\chi/\partial z\right]_{z=f}$ at the midpoint of the intervals (i.e., at the averages denoted by a bar "$\overline{\chi}, \overline{\partial\chi/\partial z}$"). This would leave us with

$$\begin{aligned} \chi_{II} &= \chi_I - \frac{\dot{f}^2}{4}\mu_{II}\overline{\chi} \\ \frac{\partial\chi_{II}}{\partial z} &= \frac{\partial\chi_I}{\partial z} + \frac{\mu_{II}}{4}\left(\ddot{f}\,\overline{\chi} + \dot{f}^2\overline{\frac{\partial\chi}{\partial z}}\right). \end{aligned} \tag{71}$$

Recall that other conventions implicit in Eq. (71) were summarized in Fig. 12. (In the analyses in Section 4.2, and then again beginning with Eq. (83) in Section 4.3), we choose to simplify our work a little bit by selecting $\chi_I(f)$ and $\left[\partial\chi_I/\partial z\right]_{z=f}$ rather than the average values. To the order that concerns us here, this is a perfectly valid thing to do.

4.1.2 The Boundary Conditions Only Conserve Energy When Taken Together as a Pair

Our "toy model" provides us with interesting subtleties concerning energy conservation. For example, since δ and δ' act just like bona fide functions, the Hamiltonian (Eq. (64)) is Hermitian, and so energy must be conserved by the resultant boundary conditions (Eq. (71)). However, recall that in deriving Eq. (71), we made the substitution Eq. (68):

$$\delta'(z-f)\chi(z) = \delta'(z-f)\chi(f) - \delta(z-f)\left.\frac{\partial\chi}{\partial z}\right|_{z=f}.$$

These two terms only correspond to a Hermitian operator times the field χ when taken together. Since the δ'-term gives the χ discontinuity, and the δ-term contributes to the $\partial\chi/\partial z$ discontinuity, we can conclude that these contributions to the boundary conditions only conserve energy when taken together as a pair. Similarly, a close examination of the boundary conditions (Eq. (71)) reveals that the horizontal and vertical interfaces in a discretization conserve energy in concert, but not individually. To see this, note that a boundary condition of the general form $\chi \to a\chi$ cannot conserve energy along a vertical interface, since χ is basically a carrier of the downrange flux. The missing energy must be made up along the horizontal interface. This is acceptable, since the vertical and horizontal interfaces are artifacts of discretization, and our formalism actually applies to a sloping interface.

4.2 The Deterministic Interface and a Look at How Boundary Conditions "Migrate" with Increasing Order

4.2.1 A Deterministic Interface with Tilt, but No Curvature

To explore the meaning of the contribution of the new term $\ddot{\mu}/8k_0^2$ to the behavior of the PE near an interface, where the sound speed (but not yet the density) jumps, let us consider an interface with tilt ($\dot{f} \neq 0$), but no curvature ($\ddot{f} = 0$). As mentioned in Section 2.3, here there is no backscatter, and so the PE should model the full-wave result to arbitrary precision. Thus, we should be able to find a fairly straightforward explanation for all aspects of the PE result.

4.2.1.1 Tilt-induced Boundary Conditions are Difficult to Interpret in Quasi-First-Order Theory

We begin with the simple model as in Eq. (6)

$$H = k_0 + \lambda - \ddot{\lambda}/8k_0^2 = k_0 + \lambda + \ddot{\mu}/8k_0^2$$

and note that for a tilted interface without curvature, the resultant boundary conditions (Eq. (13)) now lead to the boundary following conditions

$$\begin{aligned} \chi_{II} &= \left(1 - \frac{\dot{f}^2}{4}\mu_{II}\right)\chi_I \\ \frac{\partial \chi_{II}}{\partial z} &= \left(1 + \frac{\dot{f}^2}{4}\mu_{II}\right)\frac{\partial \chi_I}{\partial z} \end{aligned} . \tag{72}$$

(Here we are exploiting the fact that χ and $\partial\chi/\partial z$ are continuous at 0th order in *f*.)

At first glance, the $\mathrm{O}\left(\dot{f}^2\right)$ terms contributed by the new term $\ddot{\mu}/8k_0^2$ do not seem to make any sense. To be specific, these boundary conditions (Eq. (72)) are a step in the wrong direction compared with the boundary conditions that emerge from the simplest possible Hamiltonian $H = k_0 + \lambda$. For this Hamiltonian, we can use infinitesimal integrations to show that χ and $\partial\chi/\partial z$ are continuous. Thus, $\partial\chi/\partial x$ and so $H\chi$ are continuous, and so to $\mathrm{O}(\lambda)$, so is λ, and consequently so is the $\mathrm{O}(\lambda)$ expansion of $H^{-1/2}\chi$. This gives us continuity of A and $\partial A/\partial z$, where A solves the Helmholtz equation. So far, this is exactly what we would expect.

Now, note that continuity of $H\chi$ also gives a boundary condition on $\nabla_T^2\chi$ and so also on $\nabla_T^2 A$. Note that the boundary condition on $\nabla_T^2\chi$ does not involve $\dot{f}^2$, and the transformation connecting χ to A only involves $\lambda\chi$ and χ, so it cannot introduce a dependence on $\dot{f}^2$, nor can a further operation by the ∇_T^2 operator to take us from an equation connecting $\chi \leftrightarrow A$ to one connecting $\nabla_T^2\chi \leftrightarrow \nabla_T^2 A$. Thus, the boundary conditions on $\nabla_T^2\chi$ and $\nabla_T^2 A$ are the same as for a flat $z = 0$ interface, noting in particular that there is no $\mathrm{O}\left(\dot{f}^2\right)$ connection. In Appendix H, it is shown that the boundary condition on

$\nabla_T^2 A$ should in fact contain a term that goes as $\dot{f}^2$. This is an indication that the $\mathrm{O}\left(\dot{f}^2\right)$ term that leads to boundary conditions (Eq. (72)) is ultimately somehow related to the boundary condition on $\nabla_T^2 A$ rather than to those on A and $\partial A/\partial z$.

Before exploring this further, let us note a very interesting aspect to the result in Appendix H. The term proportional to $\mathrm{O}\left(\ddot{f}\right)$ back in Eq. (71) (which is set to zero in Eq. (72)) is apparently associated with the implicit boundary condition on $\partial^3 A/\partial z^3$. This $\mathrm{O}\left(\ddot{f}\right)$ term induces physical effects that are implicit in full-wave theory, but have to be made explicit in the context of the PE[oo]. The new physical effect introduced by the $\mathrm{O}\left(\ddot{f}\right)$ term appears to involve coupling to interface waves. These interface waves are briefly discussed in Appendix H, and the effect is be examined again in Section 5 and in Appendices N.2 and O. For the moment, it is valuable to develop a better understanding of the comparatively straightforward $\mathrm{O}\left(\dot{f}^2\right)$ terms without having to become enmeshed in these issues. That is the reason we concentrate on a surface without curvature here.

Before seeking the needed $\mathrm{O}\left(\dot{f}^2\right)$ contribution to the boundary conditions in the exotic new terms generated by the FW transformation, let us first eliminate the conventional higher-order terms in the PE (i.e., those that come from expanding the square root operator $\sqrt{1+2\lambda/k_0}$) as possible sources for the missing contribution to the boundary conditions. Considering the $\mathrm{O}\left(\lambda^2\right)$ Hamiltonian $H = k_0 + \lambda - \lambda^2/2k_0$, we can use the standard infinitesimal integrations to find that χ and $\partial\chi/\partial z$ are constant, and that the boundary conditions on $\nabla_{\mathrm{T}}^2\chi$ and $\nabla_{\mathrm{T}}^3\chi$ come from δ- and δ'-functions generated by cross-terms in λ^2. These are exactly the same boundary conditions as those for a flat horizontal surface ($f = 0$), and there is no source for $\mathrm{O}\left(\dot{f}^2\right)$ terms in the boundary condition for $\nabla_T^2\chi$. The transformation from the auxiliary field χ back to the actual pressure field A involves powers of λ (the transformation is performed an infinitesimal distance on either side of the interface), and again there is no source for terms explicitly proportional to $\dot{f}^2$.

4.2.1.2 Using $\mathrm{O}\left(\lambda^2, \ddot{\lambda}\right)$ Theory to Understand the Tilt-induced Boundary Conditions

Now, let us add the new FW $-\ddot{\lambda}/8k_0^2 = \ddot{\mu}/8k_0$ term to the second order Hamiltonian to get

$$H = k_0 + \lambda - \frac{\lambda^2}{2k_0} - \frac{\ddot{\lambda}}{8k_0^2}.$$

[oo] This is somewhat similar to backscatter as discussed in Appendix B. Note that $\ddot{f}$ is the curvature of the surface, and in a sense (for the shallow grazing angles that we are implicitly restricting ourselves to here, and operating within the PE picture based on small perturbations from range independence) backscatter is basically induced by the curvature of the surface, and not the tilt. (Recall that with shallow tilt and grazing angles, an interface with tilt, but no curvature, will not backscatter.)

This qualitatively recovers the expected behavior. The term proportional to $\dot{f}^2\delta'(z-f)$ generates a jump in $\nabla_T^2\chi$, but infinitesimal integration reveals that there is no jump in χ and $\partial\chi/\partial z$ (we would need terms proportional to a δ''' and δ'', respectively, to generate jumps in these quantities). Expanding the so-called WKB operator $H^{-1/2}=(1+2\lambda/k_0)^{-1/4}$ to $O(\lambda^2)$, and using it to convert from χ back to A on either side of the interface, there are cancellations between the implicit jump in $\nabla_T^4\chi$ and the explicit one in $\nabla_T^2\chi$ so that A and $\partial A/\partial z$ remain continuous[pp]. Using the usual infinitesimal integration, it is easy to show that to within a factor of 2, the boundary condition on $\nabla_T^2\chi$ that is proportional to $\dot{f}^2$ is indeed like that expected for $\nabla_T^2 A$ (and given in Eq. (H.9)) $\nabla_T^2 A$ depends not only on $\nabla_T^2\chi$ but also on $\nabla_T^4\chi$ and $\nabla_T^6\chi$, and so the precise relationship between $\nabla_T^2 A$ and $\nabla_T^2\chi$ is quite complicated. A rigorous as opposed to qualitative rederivation of Eq. (H.9) would involve much more effort than is warranted here. For our current purposes, it is enough that we have been able to demonstrate qualitatively that the new FW terms are indeed needed to reproduce the boundary conditions for $\nabla_T^2 A$ that properly include a component that is proportional $\dot{f}^2$ (as in Eq. (H.9)).

4.2.1.3 A More Informed Second Look at Quasi-First-Order Theory

Now, if we drop the "$\lambda^2/2k_0$" term, and just use the quasi-first-order Hamiltonian

$$H = k_0 + \lambda - \frac{\ddot{\lambda}}{8k_0^2},$$

then the formalism retains a memory of the jump in $\nabla_T^2\chi$, albeit in modified form. Recall that the quasi-first order Hamiltonian generates jumps in χ and $\partial\chi/\partial z$ (Eq. (70))

$$\begin{aligned} \chi_I - \chi_{II} - \frac{\dot{f}^2}{4}\mu_{II}\chi_I &= 0 \\ \frac{\partial\chi_I}{\partial z} - \frac{\partial\chi_{II}}{\partial z} + \frac{\dot{f}^2}{4}\mu_{II}\chi_I &= 0 \end{aligned}. \tag{73}$$

[pp] Here we demonstrate that the cancellations needed so that A and $\partial A/\partial z$ like χ and $\partial\chi/\partial z$ are continuous in $O(\lambda^2,\ddot{\lambda})$ theory. First consider the artificial problem where the interface is flat, but we insert by hand the $O(\dot{f}^2)$ boundary condition for the fixed value of $\dot{f}^2$ (recall we are here considering the tilted interface with a constant slope). This range-independent problem is now an eigenvalue problem. Decompose χ into eigenvectors χ_m, and use χ_m continuity to show that $H^{-1/2}\chi = A$ is continuous. Thus, for this case, the boundary conditions on in $\nabla_T^4\chi, \nabla_T^2\chi$, and χ must lead to algebraic identities that conspire to produce cancellations such that A (and similarly $\partial A/\partial z$) are continuous. Now, restore a true tilt and show the same algebraic identities still apply. The boundary conditions on $\nabla_T^3\chi, \nabla_T^2\chi$, $\partial\chi/\partial z$, and χ must all remain the same, since these all come from δ-functions in the Hamiltonian (or in the case of continuity conditions, the lack thereof). As always, we can use tangential differentiation to show that continuity of χ and $\partial\chi/\partial z$ imply continuity of $\partial\chi/\partial x$, which via the PE implies continuity of $H\chi$, and this also fixes the boundary condition on $\nabla_T^4\chi$. These fix the algebraic relations between $\nabla_T^4\chi, \nabla_T^2\chi$, and χ, and we already know that these lead to cancellations in the $O(\lambda^2)$ transformation from χ to A that produce the continuity of A.

If we take the tangential derivative ($\propto \partial/\partial x + \dot{f}\,\partial/\partial z$) of the first equation in Eq. (73), we have (recalling $\ddot{f} = 0$)

$$\frac{\partial \chi_I}{\partial x} - \frac{\partial \chi_{II}}{\partial x} - \frac{\dot{f}^2}{4}\mu_{II}\frac{\partial \chi_I}{\partial x} + \dot{f}\left(\frac{\partial \chi_I}{\partial z} - \frac{\partial \chi_{II}}{\partial z}\right) + \frac{\dot{f}^3}{4}\mu_{II}\frac{\partial \chi_I}{\partial z} = 0\,.$$

Using the second boundary condition and as always retaining only terms to $\mathrm{O}\left(\dot{f}^2\right)$[qq], we have the rescaling

$$\left(1 - \frac{\dot{f}^2}{4}\mu_{II}\right)\frac{\partial \chi_I}{\partial x} = \frac{\partial \chi_{II}}{\partial x}\,.$$

Substituting back into the PE, it follows that $H\chi$ obeys the same rescaling and we now have

$$\left(1 - \frac{\dot{f}^2}{4}\mu_{II}\right)\nabla_T^2 \chi_I = \nabla_T^2 \chi_{II} - 2k_0^2 \mu_{II}\chi_{II}$$

or

$$\nabla_T^2 \chi_I - \nabla_T^2 \chi_{II} = \frac{\dot{f}^2}{4}\mu_{II}\nabla_T^2 \chi_I - 2k_0^2 \mu_{II}\chi_{II}\,.$$

Again noting that $H^{-1/2}\chi = A$, and more specifically that in quasi-first-order theory this gives us in the half-spaces $A = H^{-1/2}\chi = \left(k_0 - \lambda/2\right)\chi$, we can see that A (and its transverse derivative) picks up similar behavior. We no longer have a boundary condition similar in form to Eq. (H.9). We have discovered that quasi-first-order theory picks up jumps in χ and A to compensate for modifications to the jumps in $\nabla_T^2\chi$ and $\nabla_T^2 A$.

In other words, quasi-first-order theory is characterized by jumps in χ and A that do not appear in the full-wave theory – these jumps are, however, placeholders for a bona fide physical effect that is present in full-wave theory. In that sense, the effect is real and must be taken seriously. The same is true for the cusp, and the atomic Lamb shift. For example, for the cusp, the tilt-generated (i.e., $\propto \dot{f}^2$) contact potential is really related to a jump in $\nabla_T^3 A$, and so the boundary condition on $\nabla_T A$ that was obtained earlier is a residual of this effect. A close look at the derivation of the traditional (transverse) Lamb shift (i.e., the one proportional to $k_0^2\left\langle f^2\right\rangle$) also reveals that it is related to a discontinuity in the third derivative $\nabla_T^3\chi$. Nevertheless, we know from quantum mechanics that the predicted contact potential indeed leads to an observable physical effect, even when inserted into the standard (nonrelativistic) Schrödinger equation. This teaches us that the artificial boundary conditions of quasi-first-order theory can be productively used to model the legitimate physical result.

[qq] Recall that at $\mathrm{O}\left(\dot{f}^3\right)$, the quasi-first-order model would begin to pick up very problematic δ-functions in $\partial\chi/\partial x$.

4.2.2 Migrating Boundary Conditions

4.2.2.1 Changing Boundary Conditions as the Lead Order of the PE Changes

The interpretation of a contact potential in terms of induced boundary conditions depends on its context. For example, consider what happens as we modify the order p ($p = m/2$ following the notation of Section 3.3.2) of the expansion of the square root operator $\sqrt{1+2\lambda/k_0}$. Then, rather obviously, the leading-order term λ^p in the Hamiltonian H changes, and with it the leading order derivative of the field $\nabla_T^{2p}\chi/(2k_0)^p$. We have just seen in Section 4.2.1 that as this happens, a given fixed contact potential will induce different boundary conditions. In particular, we saw how the boundary conditions induced by a δ'-function potential morphed from discontinuities in $\nabla_T^2\chi$ and $\nabla_T^3\chi$ only into a different and somewhat larger set of discontinuities that now also includes the discontinuity of the wave function χ itself and its first derivative. The implications of this statement are illustrated in Fig. 13.

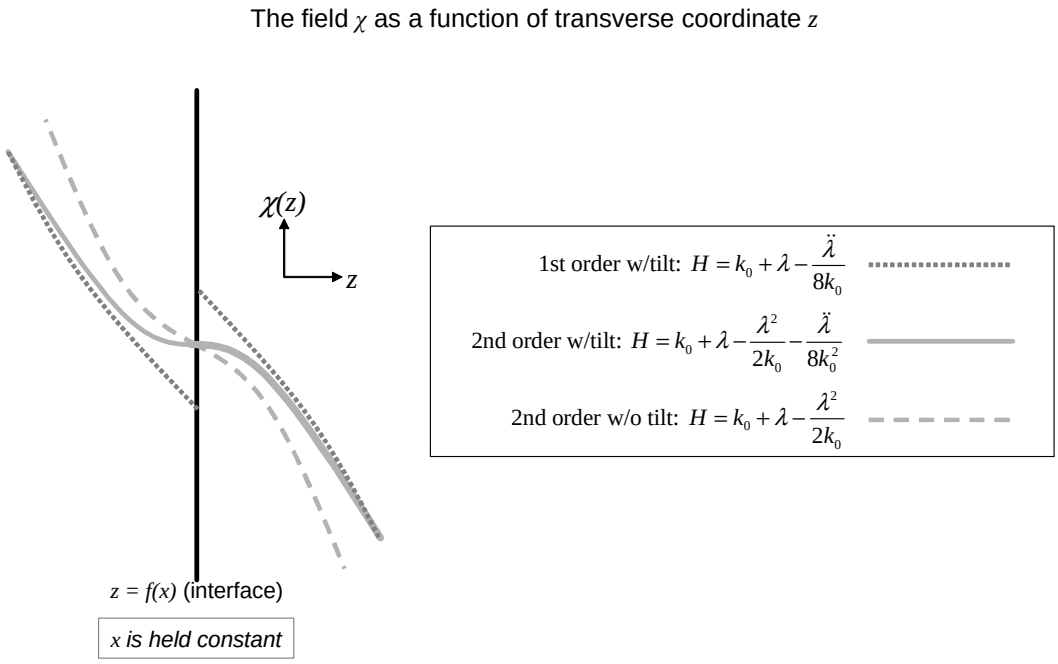


Fig. 13 — The FW transformation introduces a term proportional to $\ddot{\lambda}$ into the Hamiltonian *H*. This term becomes a δ'-function along a tilted interface where the sound speed jumps. In the context of second order (i.e., $O(\lambda^2)$) theory, this tilt-induced contact potential introduces an expected jump in boundary conditions for the second derivative of the auxiliary field χ: $\partial^2\chi/\partial z^2$. In the context of first order (i.e., $O(\lambda)$) theory, this tilt-induced effect changes, and partly becomes a jump in the auxiliary field χ. The behavior of the corresponding full acoustic field *A* would be similar. Note that the sketch is an illustration of the concepts involved, and not an actual numerical calculation. (The numerical calculation of these concepts will be a topic for follow-on research.) For the purposes of comparison, the field behavior with the $\ddot{\lambda}$ term entirely removed is sketched as well.

The δ'-function potential discussed in Section 4.2.1 and in Fig. 13 results when the new FW term was evaluated at an interface where the sound speed jumps. For the case of the cusp (i.e., a jump in the gradient of the sound speed; see Section 3.2.3), replace the field in Fig. 13 with its transverse derivative $\chi(z) \to \partial\chi/\partial z$. Recall that a similar contact potential occurs in the stochastic problem, where it is

called a "Lamb shift." For the classical Lamb shift associated with a sound speed cusp (see Section 3.2.3), replace the average field with its derivative $\langle\chi\rangle(z) \to \partial\langle\chi\rangle/\partial z$, and for the "toy model" of the atomic Lamb shift (see Section 3.2.4), replace the stochastic field in Fig. 13 with its gradient $\langle\varphi\rangle \to \vec{\nabla}\langle\varphi\rangle$.

Note that in higher-order theory, a contact potential acting at a point leads to a nonlocal change in the field that can be interpreted as a diffuse cloud. Specifically, the higher-order boundary conditions are changed in a way such that the wave function is "launched" differently. This modifies the behavior of the field not just at the one point where the contact potential is located, but also in the vicinity of the point. The difference between the field with and without the contact potential present can be interpreted as a cloud in the vicinity of the contact potential. Thus, we see that this physically real cloud is ultimately touched off by boundary conditions on higher-order derivatives, which are implicit in full wave theory, and explicit in higher-order PEs. At lower order theory (say in the world of the nonrelativistic Schrödinger equation), the contact potential induces a local field discontinuity in lieu of the effect of the diffuse cloud. This does not look much like a cloud, but it provides a model of sorts for the effects related to the physically real cloud.

4.2.2.2 General Principles Regarding the Migration of Boundary Conditions

Let us now draw a general conclusion based on the set of examples we have just considered. We stipulate that boundary conditions are in reality contact potentials, and then we take the consequences of that statement seriously. These assertions mean that as we:

- convert the boundary conditions into contact potentials,
- add terms that increase the order of the lead derivative in the differential equation,
- translate the contact potentials (e.g., δ-functions) back into explicit boundary conditions on the wave-function and its derivatives,
- ➢ then we find that the given phenomenon at the interface now influences the solution via the boundary conditions on higher-order derivatives than was previously the case. In other words, it migrates up to higher-order transverse derivatives of the wave function.

The converse happens if we remove the leading order derivative in a differential equation:

- ➢ a given effect will now induce explicit boundary conditions on *lower-order derivatives* of the solution to the wave equation. In other words, it migrates down to lower-order transverse derivatives of the wave function.

Thus, *boundary conditions migrate as leading order derivatives are added or subtracted.*

In the discussion just concluded here and in the previous subsection, we considered an effect that occurs naturally in $O(\lambda^2)$ theory, and migrated down to the $O(\lambda)$ theory. Specifically, when the $O(\lambda^2)$ PE is used, the effect spawns associated boundary conditions that are obviously related to the corresponding boundary condition for the solution of the Helmholtz equation: there is a discontinuity in the second derivative of the wave function: $\nabla_T^2\chi$. However, the effect migrates down to the $O(\lambda)$ theory in a very nonintuitive way: for example, there is now also a discontinuity in the wave function χ itself. However, we saw that the $O(\lambda)$ theory retains physical significance.

Later in Section 6.1 as we examine density jumps, we come across an effect that naturally migrates *up from* $O(\lambda)$ theory *to* the $O(\lambda^2)$ (and higher) PE. This turns out to be the most important application of the concept of migrating boundary conditions, so it is worthwhile to take a moment to foreshadow the following result: The known attributes of the solution to the (full-wave) Helmholtz equation suggest that the wave function χ, which is a carrier of downrange flux, should be discontinuous along a tilted interface where the density jumps. This discontinuity should already be apparent in $O(\lambda)$ theory. Nevertheless, the discontinuity in χ is automatically forced upward into the $O(\lambda^2)$ theory (and higher orders) by the structure that the FW procedure imposes on the PE. In this context, the discontinuity in χ automatically migrates up to become a discontinuity in its second derivative: $\nabla_T^2\chi$. The needed discontinuity in χ can only be placed into $O(\lambda)$ theory by hand, and then only in an incomplete form that is not entirely consistent with the other physical demands on the theory.

4.3 Sound Speed Discontinuity Along a Stochastic Interface: The Lamb Shift for a Sound Speed Jump

Here the calculation for a sound speed cusp given in Section 3.2.3 is adapted to calculate the effective boundary conditions induced by a sound speed discontinuity along a stochastic rough interface. Since it both reinforces many of the basic insights obtained in Section 3.2.3 and additionally provides insights into the core issue of our study – incorporating discontinuities of the environmental parameters into the PE – the calculation is once again explicitly considered here rather than being relegated to an appendix as are some comparable calculations later in this study.

4.3.1 The Effective Boundary Conditions for the Sound Speed Jump

Begin with the boundary conditions (Eq. (71)). Now follow the stochastic procedure outlined in Section 3.2.3. Once again, convert the boundary conditions at $z = f$ to effective boundary conditions down at $z = 0$ by performing, independently on each of the two sides of the interface, Taylor series expansions of the function χ and its derivative. Incorporating boundary conditions (Eq. (71)), we have an updated version of Eq. (32):

$$\begin{aligned}
&\chi_I(0) - \chi_{II}(0) \\
&= \chi_I(f) - \chi_{II}(f) - f\left(\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f}\right) + \frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right) \\
&= \frac{\dot f^2}{4}\mu_{II}\overline{\chi}(0) - f\left(-\frac{\mu_{II}}{4}\ddot f\,\overline{\chi}\right) + \frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right) \\
&= \frac{\dot f^2 + f\cdot\ddot f}{4}\mu_{II}\overline{\chi}(0) + \frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right)
\end{aligned} \quad . \tag{74}$$

whereas for the cusp, we used the boundary condition (Eq. (71)) on $\partial\chi/\partial z$, but now it is nonzero at first-order in $\ddot f$. Similarly, we see that χ is continuous at the surface $z = f$ to $\mathrm{O}\left(\dot f^2\right)$, so the tangential derivative

$$\hat t\cdot\vec\nabla\chi \propto \frac{\partial\chi}{\partial x} + \dot f\frac{\partial\chi}{\partial z}$$

is continuous to $\mathrm{O}\left(\dot{f}^2\right)$. Since $\partial\chi/\partial z$ is continuous to $\mathrm{O}\left(\ddot{f}\right)$, $\partial\chi/\partial x$ at the surface is continuous to $\mathrm{O}\left(\dot{f}^2, \dot{f}\cdot\ddot{f}\right)$, and from the PE, so must $H\chi$. Evaluating $H_I\chi_I - H_{II}\chi_{II} = 0$, we have to $\mathrm{O}\left(\dot{f}^2, \dot{f}\cdot\ddot{f}\right)$

$$\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f} = -2k_0^2\mu_{II}\chi + O\left(\dot{f}^2, \dot{f}\cdot\ddot{f}\right) \tag{75}$$

and

$$\chi_I(0) - \chi_{II}(0) = \frac{\dot{f}^2 + f\cdot\ddot{f}}{4}\mu_{II}\overline{\chi}(0) - k_0^2 f^2\mu_{II}\overline{\chi}(0) + \mathrm{O}\left(f^3\right). \tag{76}$$

Similarly, modifying Eq. (35) we find:

$$\begin{aligned}
\left.\frac{\partial\chi_I}{\partial z}\right|_{z=0} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=0} &= \left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} - f\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right) \\
&\quad + \frac{f^2}{2}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right) \\
&= -\frac{\mu_{II}}{4}\left(\ddot{f}\overline{\chi}(f) + \dot{f}^2\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}\right) + 2k_0^2 f\mu_{II}\overline{\chi}(f) \\
&\quad + \frac{f^2}{2}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=0} - \left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=0}\right) + \mathrm{O}\left(f^3\right) \\
&= -\frac{\mu_{II}}{4}\left(\ddot{f}\overline{\chi}(0) + \ddot{f}f\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0} + \dot{f}^2\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}\right) + 2k_0^2 f\mu_{II}\overline{\chi}(0) \\
&\quad + 2k_0^2 f^2\mu_{II}\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0} + \frac{f^2}{2}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=0} - \left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=0}\right) + \mathrm{O}\left(f^3\right).
\end{aligned} \tag{77}$$

Again adapting the technique originally developed by Kuperman for a slightly different context [65], break the wave function into coherent and incoherent parts: $\chi|_{z=0} = \langle\chi\rangle(0) + \delta\chi$, and average these boundary conditions. This gives us

$$\begin{aligned}
\langle\chi_I\rangle(0) - \langle\chi_{II}\rangle(0) &= \frac{\langle\dot{f}^2\rangle + \langle f\cdot\ddot{f}\rangle}{4}\mu_{II}\langle\overline{\chi}\rangle(0) - k_0^2\langle f^2\rangle\mu_{II}\langle\overline{\chi}\rangle(0) + \mathrm{O}\left(f^3\right) \\
&= -k_0^2\langle f^2\rangle\mu_{II}\langle\overline{\chi}\rangle(0) + \mathrm{O}\left(f^3\right) \\
\left.\frac{\partial\langle\chi_I\rangle}{\partial z}\right|_{z=0} - \left.\frac{\partial\langle\chi_{II}\rangle}{\partial z}\right|_{z=0} &= -\frac{\mu_{II}}{4}\left(\langle\ddot{f}\overline{\delta\chi}\rangle + \left[\langle\ddot{f}\cdot f\rangle + \langle\dot{f}^2\rangle\right]\left.\overline{\frac{\partial\langle\chi\rangle}{\partial z}}\right|_{z=0}\right) + 2\mu_{II}k_0^2\langle f\overline{\delta\chi}\rangle \\
&\quad + 2k_0^2\langle f^2\rangle\mu_{II}\left.\overline{\frac{\partial\langle\chi\rangle}{\partial z}}\right|_{z=0} + \frac{\langle f^2\rangle}{2}\left(\left.\frac{\partial^3\langle\chi_I\rangle}{\partial z^3}\right|_{z=0} - \left.\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right|_{z=0}\right) + \mathrm{O}\left(f^3\right).
\end{aligned} \tag{78}$$

Note that quite generally, $\left\langle \ddot{f} \cdot f \right\rangle + \left\langle \dot{f}^2 \right\rangle = 0$, so the downrange Lamb shift for a sound speed jump disappears immediately from Eq. (78).

4.3.2 Converting the Smearing Term to Familiar Form

Now, let us look at the smearing term in the boundary condition for $\partial \langle \chi \rangle / \partial x$ given by the last part of Eq. (78). This term involves the boundary condition for the third derivative $\partial^3 \langle \chi \rangle / \partial x^3$. To obtain this, flatten the interface so that $f = 0$, and take the transverse derivative $\nabla_T = \partial / \partial z$ of the stochastic Helmholtz equation on either side of the interface:

$$\begin{aligned} &\nabla_T \cdot \left[-i \frac{\partial \langle \chi \rangle}{\partial x} = [H](z) \langle \chi \rangle = \frac{\nabla_T^2 \langle \chi \rangle}{2k_0} - k_0 [\mu](z) \langle \chi \rangle \right] \Rightarrow \\ &-i \frac{\partial \nabla_T \langle \chi \rangle}{\partial x} = \frac{\nabla_T^3 \langle \chi \rangle}{2k_0} - k_0 \left(\nabla_T [\mu](z) \right) \langle \chi \rangle - k_0 \left([\mu](z) \right) \nabla_T \langle \chi \rangle + \mathrm{O}\left(\langle f \delta\chi \rangle, \langle f^2 \rangle \right), \end{aligned} \tag{79}$$

and evaluate the second equation an infinitesimal distance on both sides of the interface and subtract. So far, Eq. (79) is the same as Eq. (38). However, here we are assuming that the sound speed is constant in the half spaces, so $\nabla_T [\mu](z) = 0$ away from the interface. On the other hand, $[\mu]$ now jumps at the interface. Also, to $\mathrm{O}(f^0)$, $\nabla_T \chi$ is still continuous, so subtracting Eq. (79) evaluated just inside the two regions gives us

$$\begin{aligned} 0 &= \frac{\nabla_T^3 \langle \chi_I \rangle \big|_{z=0} - \nabla_T^3 \langle \chi_{II} \rangle \big|_{z=0}}{2k_0} - k_0 \left([\mu_I] \big|_{z=0} - [\mu_{II}] \big|_{z=0} \right) \nabla_T \langle \chi_{II} \rangle + \mathrm{O}(f) \\ \nabla_T^3 \langle \chi_I \rangle \big|_{z=0} - \nabla_T^3 \langle \chi_{II} \rangle \big|_{z=0} &= -2k_0^2 \mu_{II} \nabla_T \langle \chi_{II} \rangle + \mathrm{O}(f), \end{aligned} \tag{80}$$

and Eq. (78) becomes

$$\begin{aligned} \langle \chi_I \rangle(0) - \langle \chi_{II} \rangle(0) &= -k_0^2 \left\langle f^2 \right\rangle \mu_{II} \langle \bar{\chi} \rangle(0) + \mathrm{O}\left(f^3 \right) \\ \left. \frac{\partial \langle \chi_I \rangle}{\partial z} \right|_{z=0} - \left. \frac{\partial \langle \chi_{II} \rangle}{\partial z} \right|_{z=0} &= -\frac{\mu_{II}}{4} \left\langle \ddot{f} \overline{\delta\chi} \right\rangle_{z=0} + 2\mu_{II} k_0^2 \left\langle f \overline{\delta\chi} \right\rangle \\ &\quad + 2k_0^2 \left\langle f^2 \right\rangle \mu_{II} \left. \overline{\frac{\partial \langle \chi \rangle}{\partial z}} \right|_{z=0} - k_0^2 \left\langle f^2 \right\rangle \mu_{II} \nabla_T \langle \chi_{II} \rangle + \mathrm{O}\left(f^3 \right) \\ &= -\frac{\mu_{II}}{4} \left\langle \ddot{f} \overline{\delta\chi} \right\rangle + 2\mu_{II} k_0^2 \left\langle f \overline{\delta\chi} \right\rangle \\ &\quad + k_0^2 \left\langle f^2 \right\rangle \mu_{II} \left. \overline{\frac{\partial \langle \chi \rangle}{\partial z}} \right|_{z=0} + \mathrm{O}\left(f^3 \right). \end{aligned} \tag{81}$$

4.3.3 Terms Associated with Diffuse Scattering

Note that unlike for the cusp (e.g., Eq. (40)), there are now lossy diffuse (Bragg) scattering terms (proportional to $\left\langle \ddot{f}\overline{\delta\chi}\right\rangle$ and $\left\langle f\overline{\delta\chi}\right\rangle$) in the boundary conditions for the coherent field. Although they will be ignored for the moment so that we may concentrate on the purely coherent effects, these terms provide a window into a very interesting set of physical processes. They both contribute an overall energy sink.

$\overline{\delta\chi}$ is typically proportional to f, and it follows that the term proportional to $\left\langle f\overline{\delta\chi}\right\rangle$ is proportional to $\left\langle f^2\right\rangle$. This term corresponds to the well-known Bragg scattering phenomenon associated with the first-order perturbation result of rough surface scattering theory (for an general overview of first-order perturbation theory and Bragg scattering, see, for example, Ref. 73). S. McDaniel presents a nice discussion bringing the Bragg scattering term $\left\langle f\overline{\delta\chi}\right\rangle$ (for a rough surface where the sound speed jumps) into the context of the PE (Ref. 74, Section II.A). As in the discussion here, she bases her discussion on the normal-mode work of Kuperman [65].

The term proportional to $\left\langle \ddot{f}\overline{\delta\chi}\right\rangle$ is particularly interesting. It describes curvature-induced diffuse Bragg scattering, and again noting that $\overline{\delta\chi}$ is typically proportional to f, this type of incoherent scattering phenomenon is proportional to $\left\langle f\cdot\ddot{f}\right\rangle = -\left\langle \dot{f}^2\right\rangle$. This quantity, the mean square of the slope, is related to the need for renormalization in scattering theory. This very interesting topic is explored a little further in Section 4.4.

4.3.4 Pure Coherent Field Effects

4.3.4.1 The Effective Boundary Conditions on the Coherent Field

Until then, however, we will drop the diffuse scattering terms and concentrate on the propagation of pure coherent field effects. This is not unlike dropping the diffuse scattering contribution from *volume* scattering surrounding (but not right on top of) the sound speed cusp of Section 3.2.3 or the $1/r$ potential in the atomic problem of Section 3.2.4, and calculating only the coherent radiation. We also need to keep in mind that the coupling between coherent and incoherent radiation should be relatively modest, even if previous incoherent scattering has produced a great deal of incoherent radiation. To see why this is true, note that in $\left\langle \ddot{f}\overline{\delta\chi}\right\rangle$ and $\left\langle f\overline{\delta\chi}\right\rangle$, f and $\ddot{f}$ are only correlated to the *locally* generated part of the incoherent field $\overline{\delta\chi}$ (i.e., that having been generated within a distance of the correlation length of the interface), and not that generated by the entire surface. The local part of the incoherent field $\overline{\delta\chi}$ should thus remain relatively modest, and the Bragg terms should never overwhelm the rest of Eq. (81). Keeping all this in mind, we eliminate the diffuse scattering terms from Eq. (81), and are left with

$$\begin{aligned}\left\langle \chi_I\right\rangle(0) - \left\langle \chi_{II}\right\rangle(0) &= -k_0^2\left\langle f^2\right\rangle \mu_{II}\left\langle \bar{\chi}\right\rangle(0) + \mathrm{O}\left(f^3\right)\\ \left.\frac{\partial\left\langle \chi_I\right\rangle}{\partial z}\right|_{z=0} - \left.\frac{\partial\left\langle \chi_{II}\right\rangle}{\partial z}\right|_{z=0} &= k_0^2\left\langle f^2\right\rangle \mu_{II}\left.\overline{\frac{\partial\left\langle \chi\right\rangle}{\partial z}}\right|_{z=0} + \mathrm{O}\left(f^3\right).\end{aligned} \tag{82}$$

Once again, note that the downrange Lamb shift for an interface has disappeared for an interface with a sound speed jump, and we are only left with the traditional (transverse) Lamb shift phenomenon.

For our subsequent analysis, it will be useful to take advantage of the fact that

$$\langle \bar{\chi} \rangle = \langle \chi_I \rangle = \langle \chi_{II} \rangle + \mathrm{O}\left(\langle f^2 \rangle \right)$$

to rewrite Eq. (82) as

$$\begin{aligned} \langle \chi_{II} \rangle(0) &= \left(1 + k_0^2 \langle f^2 \rangle \mu_{II}\right) \langle \chi_I \rangle(0) \\ \left. \frac{\partial \langle \chi_{II} \rangle}{\partial z} \right|_{z=0} &= \left(1 - k_0^2 \langle f^2 \rangle \mu_{II}\right) \left. \frac{\partial \langle \chi_I \rangle}{\partial z} \right|_{z=0} \end{aligned} \quad . \tag{83}$$

(Note that the conventions implicit in Eq. (83) are illustrated in Fig 12. Most relevantly, recall that the curve $z = f(x)$ separates region *I* from region *II*, that the reference sound speed is the one in region *I*, and $\mu \equiv \left(1 - c_I^2 / c^2\right)/2$. This implies that $\mu_I = 0$ and $\mu_{II} = \left(1 - c_I^2 / c_{II}^2\right)/2$. The positive *z* axis points from region *II* into region *I*.)

4.3.4.2 Understanding the Coherent Field Boundary Conditions

An interesting interpretation for both Eq. (83) and the earlier result (Eq. (40)) is illustrated in Fig. 14. A sound speed jump along a stochastic rough interface looks like a dipole sheet, while a jump in the sound speed gradient along the same surface looks like a monopole (charge sheet).

Fig. 14 — In the stochastic problem, a rough interface decomposes into contributions that look like a monopole sheet, a dipole sheet, etc. A jump in the sound speed gradient generates the former, while the dipole is generated by a jump in the sound speed itself.

Finally, note that Eq. (83) indicates that the stochastic wave function $\langle \chi \rangle$ is discontinuous at the horizontal interface separating the two regions. This boundary condition is perfectly compatible with the straightforward eigenvalue problem. To justify this general assertion, use the generic field χ rather than the stochastic field $\langle \chi \rangle$, and assume that $-i \partial \chi / \partial x = H \chi$ for range-independent H and that $\chi_I = a \chi_{II}$ along a horizontal line (say $z = 0$). Now $\chi_I - a \chi_{II} = 0$ along the line, and the same is true for the tangential derivative

$$0 = \partial(\chi_I - a \chi_{II}) / \partial x = \partial \chi_I / \partial x - a \, \partial \chi_{II} / \partial x \, .$$

In other words, χ and $\partial \chi / \partial x$ jump in tandem. Recalling that a given eigenfunction χ_n obeys the eigenvalue equation $\chi_n = k_n \left(\partial \chi_n / \partial x \right)$, note the tandem jumps in χ_n and $\partial \chi_n / \partial x$ are crucial if this

equality is to hold at the interface. While this may seem obvious in hindsight, a failure to recognize this result can lead to considerable confusion as we pursue our analysis.

4.4 The "New Physics" in Context

The new physics discovered so far is placed into a broader physical context in Fig. 15. In this section, we explore some of the implications of the figure.

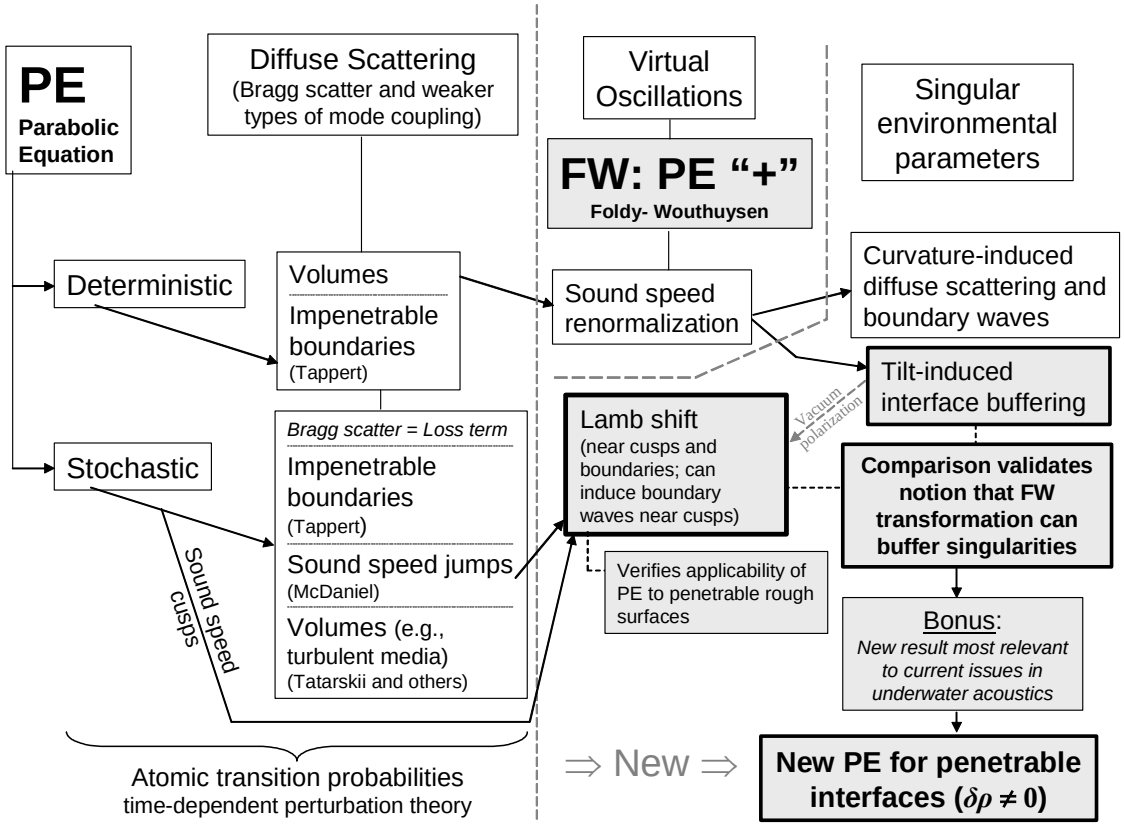


Fig. 15 — The classical Lamb shift in context. The PE (cf. the Schrödinger equation in atomic physics) is used to propagate the field (cf. the electron wave function), often in the vicinity of a rough interface (cf. the world line of the nucleus advected by vacuum fluctuations). Along the interface, the sound speed (or more generally any environmental parameter) or its transverse derivative (in atomic physics, the gradient of the potential) is discontinuous. It is well known that the rough interface couples eigenstates (or modes to use the terminology of a classical wave guide). The most pronounced manifestation of this is Bragg scattering. The stochastic problem also generates a shift of the eigenstates (and associated eigenvalues) in addition to the mixing of eigenstates. This is the Lamb shift. More obscure is the fact that the slope and curvature of such interfaces spawn a new class of effects (for the atomic problem, the slope of the world line corresponds to the velocity of the nucleus as it is advected by vacuum fluctuations, and the curvature is the acceleration). For instance, tilt buffers the interface in a way that is very reminiscent of the Lamb shift, but it is automatically generated by the deterministic formalism without the need for stochastic averaging. The formalism built up also suggests a method for modeling an interface characterized by a density jump. Since the Lamb shift is a true rough surface effect, the proven success of the method in modeling this class of effects validates its use in modeling a rough interface where the density jumps. As discussed in Section 6.1, the formalism buffers a density jump much like it buffers a tilted interface. The aspects of the problem most closely examined in the current paper are shaded.

4.4.1 The Classical Lamb Shift in Context

Note that the Lamb shift emerges from the stochastic problem. The transverse (or traditional) Lamb shift is proportional to the mean square surface height $\left\langle f^2 \right\rangle$, and it is a result of smearing of the interface in the transverse direction. This is a purely coherent field effect, and as such it involves mode shifts rather than mode mixing. The corresponding eigenvalues for the modes (the modes are eigenfunctions) shift as well. This is noted in the classic quantum mechanics textbook by Cohn-Tanoudji et al. [75], where it is pointed out that there are in fact two types of effects associated with the time-dependence introduced by vacuum fluctuations (or similarly range-dependent roughness in the acoustic waveguide problem):

- The mixing of eigenstates producing transition probabilities and characterized by time-dependent perturbation theory. (This corresponds to Bragg scattering described by the Born series in the acoustic scattering problem.)
- The Lamb shift modifying eigenstates — i.e., time-averaging creates a new stochastic problem that is effectively static (time-independent). (For the acoustic problem, replace "time" with "range" in this statement.)

In the deterministic problem, a similar effect is introduced by surface tilt. Once again the interface is smeared, this time by the shielding (or buffering) by a cloud of virtual particle pairs (i.e., bound uprange-downrange oscillations). The FW transformation automatically generates this without the need for explicit stochastic averaging. This forms an important precedent, which will help us understand how the PE deals with Bragg-scale vorticity, an effect that occurs along an interface where the density jumps (see Section 6.1). Sometimes, tilt-induced buffering survives into the stochastic problem. This is called the "downrange Lamb shift," because it is caused by smearing in the downrange direction rather than in the transverse direction (as is the traditional Lamb shift). The downrange Lamb shift occurs when there is a sound speed cusp along a stochastic rough surface and, as we will soon see, apparently a weak form of this effect also occurs when there is a density jump along such an interface.

4.4.2 Terms Proportional to Surface Curvature and Tilt

Figure 15 also takes note of the fact that in Eq. (81), there is an exotic new curvature-induced diffuse scattering term: $-(\mu_{II}/4)\left\langle \ddot{f}\delta\chi \right\rangle_{z=0}$. This interesting scattering effect couples modes, but it will not be considered very deeply in the present context. However, assuming the incoherent field is proportional to the surface height (i.e., $\delta\chi \propto f$), the term involves the important expansion parameter $\left\langle \ddot{f} \cdot f \right\rangle = -\left\langle \dot{f}^2 \right\rangle$, which is worth a closer look.

Recall that tilt-induced buffering associated with a sound speed jump is proportional to $\dot{f}^2$ (e.g., see Eq. (72)), and similarly, if the surface corresponds to a jump in the first derivative of the sound speed, there is also a virtual cloud that generates a term proportional to $\dot{f}^2$ (see Eq. (31)). The Foldy-Wouthuysen procedure will eventually add higher-order downrange derivatives that create terms proportional to higher powers of $\dot{f}$. This makes $\dot{f}$ a true expansion parameter, limiting the slope $\dot{f} < 1$ and so the interface grade to under 45 deg. This a trait shared with rough surface scattering theories based on the Kirchhoff approximation or perturbation theory. For the sound speed cusp and apparently also for a density jump, there is a "downrange Lamb shift" effect that is proportional to the mean square slope $\left\langle \dot{f}^2 \right\rangle$. As we have just seen, this quantity also shows up in the stochastic diffuse scattering problem,

where we would obtain a term proportional to $\left\langle \ddot{f} \cdot [\text{incoherent field}] \right\rangle \propto \left\langle \ddot{f} \cdot f \right\rangle = -\left\langle \dot{f}^2 \right\rangle$. The expansion parameter $\left\langle \dot{f}^2 \right\rangle$ is a broad-spectrum parameter in the sense that it is sensitive to all scales. For the typical scenario where surface roughness is characterized by a power-law tail such that the quantity $\left\langle \dot{f}^2 \right\rangle$ blows up (e.g., the spectrum $S(\underline{k}) \sim 1/k^p$; $p \leq 4$ for a two-dimensional rough surface), we have to impose a cutoff. For the PE, we follow the convention from quantum mechanics (e.g., Ref. 57, p. 60) and cut off the wave number at the reference wave number k_0. This cutoff is associated with a limit of spatial resolution. From the uncertainty principle, an allowed wave number range of 0 to k_0 corresponds to a maximum spatial resolution of $1/2k_0 = \lambda_0/4\pi$, where λ_0 is the reference wavelength. The sensitivity to an upper cutoff of the downrange Lamb shift and the curvature-induced diffuse scattering is associated with a sensitivity of the underlying physical effect to all scales down to this length scale.

Several more remarks are appropriate concerning the need to provide a cutoff beyond which the field cannot resolve features of the surface. There are two related, but distinct scenarios at issue here:

1. The first is when $\left\langle \dot{f}^2 \right\rangle$ and perhaps also $\left\langle f^2 \right\rangle$ blow up. Specifically for a two-dimensional surface, if the tail of the spectrum goes as a power $p \leq 2$, $\left\langle f^2 \right\rangle$ blows up and the cumulative effect of small-scale features causes the surface height to be unbounded, and if the tail of the spectrum goes as a power $p \leq 4$, the mean square slope $\left\langle \dot{f}^2 \right\rangle$ does not exist and the surface is a fractal. Clearly, some cutoff is necessary if our theory is to avoid unphysical infinities[rr].
2. The second is when $\left\langle f^2 \right\rangle$ and $\left\langle \dot{f}^2 \right\rangle$ are both finite, but scales very much smaller than the wavelength nevertheless make a major contribution to these values. This can occur if the power law is integrable for $k \to \infty$, or if some external physical constraint forces the spectrum to cutoff at some large value of k. For example, when $p > 2$, $\left\langle f^2 \right\rangle$ is finite and when $p > 4$, then $\left\langle \dot{f}^2 \right\rangle$ is finite, but there may still be a significant contribution from scales that are very small compared to the wavelength of the field. Alternately, note that for all naturally occurring classical phenomena, the spectrum must cut off at some scale (at latest at the atomic scale). Even if that occurs at far below the Bragg scale, $\left\langle f^2 \right\rangle$ and $\left\langle \dot{f}^2 \right\rangle$ must still exist even if $p \leq 4$ and/or $p \leq 2$, and so the surface is never really of infinite height, nor does it continue to behave like a fractal all the way down to the smallest scales. When $\left\langle f^2 \right\rangle$ and $\left\langle \dot{f}^2 \right\rangle$ exist, but depend on the characteristics of the surface at very small scales, then the question becomes: do the scales well below a wavelength really matter as far as the field is concerned? The answer is no. Since the field cannot possibly react to what happens at scales far below that allowed by the uncertainty principle, it cannot, for example, directly depend on the nature of some physical cutoff in the far UV (i.e., large k). (It can indirectly depend on these scales via the values of the environmental parameters, but that is another issue.) The theory as currently constituted is thus overly sensitive to small scales.

[rr] On a semantic note, once we introduce the cutoff on the fractal surface, it is no longer, strictly speaking, a true fractal. It is now known as a self-affine surface. By this we mean that the surface behaves like a fractal within the length scales that matter to the physical process that concerns us. Any naturally occurring "fractal" is really a self-affine surface.

Both of these scenarios imply that some *imposed* cutoff at the limits set by the uncertainty principle is absolutely necessary. In the first case, that fact is impossible to ignore. This happens, say, in unrenormalized Quantum Electrodynamics (QED). In the second case, the issue is really the same (an imposed cutoff is necessary because small scales are oversampled), but now it is easier to ignore, and in fact it is often overlooked. This is an illustration of an important issue Weinberg addresses in his field theory text [76, p. 441] "… the renormalization of masses and fields has nothing directly to do with the presence of infinities, and would be necessary even in a theory in which all momentum space integrals were convergent." In other words, tractable approximations to field theory tend to be overly sensitive to small scales, and they need to be cured of it.

4.4.3 Understanding the Cutoff as a Crude Form of Renormalization

Our artificially imposed cutoff is a crude form of renormalization (valid in the PE /Schrödinger equation (PE/SE) limit). The Lamb shift was historically the phenomenon that first raised the issue of renormalization [76, pp. 31-38]. Interestingly, as noted by Weinberg (p. 38), "A fully relativistic calculation of the Lamb shift including positrons in intermediate states could have been attempted in the 1930's, using the old non-relativistic perturbation theory" [76]. In this report, we present a variant on the idea that classical PE/SE theory can be used to obtain Lamb shift phenomena. It is based on Welton's approach as described in Refs. 57 and 62, but additional information is also extracted from the new terms introduced by the FW transformation.

Note that in the "toy model" of the atomic Lamb shift, it is already $\left\langle \delta r^2 \right\rangle$ that diverges, and not only $\left\langle \delta \dot{r}^2 \right\rangle = \left\langle \mathrm{v}^2 \right\rangle$. This is analogous to the case where both $\left\langle f^2 \right\rangle$ and $\left\langle \dot{f}^2 \right\rangle$ diverge for a rough one- or two-dimensional surface. In other words, the roughness of the vacuum fluctuations[ss] corresponds, for example, to the $p = 2$ case for a rough two-dimensional surface. Renormalization is thus necessary to handle divergences in both components of the Lamb shift that appear in our "toy model."

It is also instructive to approach the issue of renormalization from another point of view. In the "toy model" of the atomic Lamb shift, the new term imposed by the FW transformation is associated with a virtual electron-positron pair (note the quote in the paragraph above). This becomes a loop diagram in the language of Feynman diagrams, and it is loop diagrams that force the issue of renormalization. The electron-positron loop is associated with a phenomenon known as vacuum polarization[tt], and it is the root cause behind the divergence of $\left\langle \delta \dot{r}^2 \right\rangle = \left\langle \mathrm{v}^2 \right\rangle$. (The loop diagram associated with vacuum polarization is shown, for example, in Fig. 8-4, p. 152 of Ref. 57.) Similarly, the fluctuations introduced into the Schrödinger equation by hand correspond to virtual photon-electron loops. These virtual photon-electron loop diagrams also diverge unless some kind of renormalization procedure is invoked, but more slowly than do the loops generated by electron-positron pairs. The photon-electron loops are connected to the vertex correction term and to some extent also to the electron self-energy, and these loop diagrams (also shown in Fig. 8-4, p. 152 of Ref. 57) are the root cause behind the divergence of $\left\langle \delta r^2 \right\rangle$. The photon-electron loops[uu] (connected to the transverse Lamb shift) form the bulk of the atomic Lamb shift effect.

[ss] Recall that in this context, the fluctuations are imposed artificially by hand since our model imposes second quantization as an ad hoc modification to first quantization.

[tt] Vacuum polarization also involves a virtual photon, since it is a consequence of the interaction of the electron with vacuum fluctuations, which in turn involve virtual photons.

[uu] Recall that these are associated with the transverse Lamb shift.

The vacuum polarization[vv] is much smaller, and it has the opposite sign. This leaves a small shortfall in the effect, which is mostly made up by the contribution from an anomalous magnetic moment [77]. There are also small higher-order corrections.

4.4.4 Towards Incorporating the New Physics into Underwater Propagation

Having developed a general understanding of the context of the classical Lamb shift relative to other field effects, the next step in examining this effect is to explore the significance of the classical Lamb shift in the context of underwater propagation. The rough sound speed cusp Lamb shift may appear when the acoustic field is confined in a duct, and propagates for long ranges (see Fig. 16). The ducting occurs because the sound speed profile is downward refracting on the top portion of a layer (or alternately the air-sea interface bounds the field from above), and upward refracting below, and thus it is not directly caused by the cusp. However, this ducting causes a significant amount of acoustic energy to be concentrated in the vicinity of the cusp, and this provides the cusp with an opportunity to influence its behavior. This may cause a significant phase shift of the acoustic wave. Futhermore, the rich impedance boundary conditions induced by the classical Lamb shift for a cusp permit the existence of interface waves trapped near the stochastic rough interface. These boundary waves form a part of the coherent field that decays exponentially away from the interface. In other words, some fraction of the acoustic energy is confined to the immediate vicinity of the interface. This is a kind of localization. For a one-dimensional interface embedded in two-dimensional $x-z$ space, this is a one-dimensional localization effect, while for the atomic Lamb shift, we would have localization in three-dimensional space. This explains why the Lamb shift is sometimes tied to Anderson localization (for example, see Ref. 78, especially the top of column ii, p. 39).

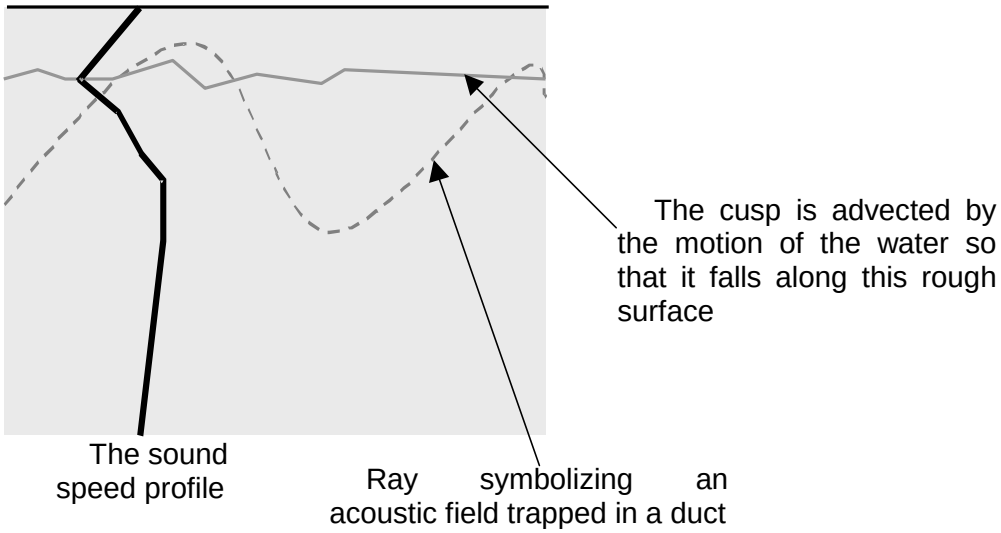


Fig. 16 — The acoustic Lamb shift associated with a rough cusp may appear in long-range propagation associated with a duct formed by pronounced near-surface layering.

[vv] Recall that this is associated with the downrange Lamb shift, and so with the new terms introduced by the FW transformation. Note that this implies that structure of the field equations automatically forces vacuum polarization once photon loops such as the vertex term are introduced.

The acoustic Lamb shift associated with a sound speed jump may affect shallow water propagation via the interaction of the field with a rough ocean bottom. Here the effect shifts the downrange wave number of the coherent field in a way that may accumulate within the phase. However, the sound speed jump is typically quite modest for ocean bottoms that acoustically behave like a fluid such as mud, sand, and relatively unconsolidated rock (as opposed to elastic solids such as limestone and basalt), while the density jump can approach a factor of two. Thus, to properly model a rough ocean bottom, it will be necessary to consider a density jump as well as a sound speed jump. In the next section, we will see that a straightforward generalization of the FW ansatz permits us to include a density jump.

5. INTRODUCING A DENSITY JUMP

The density jump as found, for example, at the ocean bottom, is introduced here in Section 5. In Section 5.1, the basic components of the FW procedure are adapted to the case where the density jumps, and then Section 5.2 discusses δ-function bifurcation, an important new tool needed for adapting the results to *interfaces* where the density *jumps*. In Section 5.3, the interface where the density jumps is examined for the first time. Tilt-induced smearing is examined in the context of the deterministic problem, and then the resultant insights are used to obtain the classical Lamb shift associated with a density and sound speed jump. Here, as with the sound speed cusp but unlike the sound speed jump, we obtain a small tilt/curvature-induced "vacuum polarization" correction to the classical Lamb shift. The examination of the classical Lamb shift concludes with a discussion of its possible relevance to underwater acoustics.

In addition to their direct effect on the scattering problem, the phenomena examined in Sections 4 and 5 also teach us something very important about the PE. They use the dominant component of the Lamb shift, transverse smearing induced by stochastic averaging, to develop a solid understanding of stochastic smearing (i.e., buffering) of a singularity associated with the environmental parameters. Juxtaposing this phenomenon with tilt-induced smearing in the deterministic problem, we discover that the PE buffers (i.e., smears out) singularities in the deterministic problem in a way that closely mimics the buffering imposed by the stochastic problem.

Section 5 also serves to build our understanding of some of the issues associated with the density jump. In Section 6, the knowledge acquired in Sections 4 and 5 will be used to examine a very important, but also very subtle issue that must be addressed if density jumps are to be properly incorporated into the PE.

5.1 The Basic Formalism

When the density varies, the problem generalizes in a rather straightforward manner. In the formulas below, the changes associated with density variation are enclosed in boxes.

The formal development in this section applies equally to two-dimensional and three-dimensional spaces. Interfaces are explicitly introduced in Section 5.2. Once interfaces are considered, consideration will once again be restricted by convention to two-dimensional spaces.

5.1.1 The Ansatz

Recalling Eq. (1), the Helmholtz equation generalizes to

$$\vec{\nabla}\cdot\left(\boxed{\frac{1}{\rho}}\vec{\nabla}A\right)+\frac{k_0^2n^2}{\boxed{\rho}}A=0\,, \tag{84}$$

where ρ is the density. Now, the Foldy-Wouthuysen ansatz becomes

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix} = \frac{1}{2}\left(A \pm \frac{i}{k_0}\boxed{\frac{\rho_0}{\rho}}\frac{\partial A}{\partial x} \right), \tag{85}$$

where ρ_0 is some reference density. The time-averaged downrange energy flux

$$S_x = \frac{1}{2\rho\omega}\mathrm{Im}\left(A^* \frac{\partial A}{\partial x} \right)$$

is proportional to a factor of $1/\rho$ and this is built into θ and χ, so that

$$|\theta|^2 - |\chi|^2 = -2\rho_0 c_0 S_x ,$$

and so θ and χ are indeed carriers of flux as before (the reference density ρ_0 and the reference sound speed $c_0 = \omega/k_0$ are just constants). In Appendix I, it is shown that the state space equation is once again

$$i\frac{\partial \Phi}{\partial x} = \mathcal{H}\Phi \quad \text{with} \quad \mathcal{H} \equiv \mathcal{O} + \mathcal{E} + k_0\eta ,$$

where now

$$\begin{aligned} \mathcal{O} &= \lambda\xi \\ \mathcal{E} &= \left(\lambda - \boxed{2k_0\gamma} \right)\eta \end{aligned}, \tag{86}$$

with the matrices η and ξ as before, and

$$\begin{aligned} \lambda &= \frac{\underline{\nabla}_T \cdot \left(\boxed{\frac{\rho_0}{\rho}} \right)\underline{\nabla}_T}{2k_0} - k_0\mu + \boxed{k_0\gamma} \\ \mu &\equiv \frac{1}{2}\left(1 - \frac{\mathrm{K}}{\mathrm{K}_0} \right) = -\frac{\Delta \mathrm{K}}{2\mathrm{K}_0} = \frac{1}{2}\left(1 - \frac{\rho_0}{\rho}n^2 \right). \\ \gamma &\equiv \frac{1}{2}\left(1 - \frac{\rho}{\rho_0} \right) = -\frac{\Delta\rho}{2\rho_0} \end{aligned} \tag{87}$$

Note that now μ is defined in terms of the compressibility $K = 1/\left(c^2\rho\right)$ rather than the sound speed squared, but the definition for μ reduces to the previous expression if the density is everywhere the same. K_0 is some reference compressibility. Note also that λ (the coefficient of the odd matrix ξ) is still Hermitian, but it acquires an extra term related to the departure of the local density ρ from its reference value ρ_0. The state space equation is very similar to what it was when the density was everywhere the same, but now the even operator $\mathcal{E}$ has also acquired an extra factor proportional to γ that measures how much the local density differs from its reference value.

5.1.2 The Diagonalized Hamiltonian

To obtain the diagonalized matrix Hamiltonian $\mathcal{H}$ to fourth order, consider the general results shown in Eqs. (14) and (15), which are reproduced here for convenience:

$$\tilde{\mathcal{H}}^{IV} = k_0\eta + \mathcal{E}^{II} \tag{88}$$

where

$$\mathcal{E}^{II} = \begin{array}{l} \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\left[\mathcal{O},[\mathcal{O},\mathcal{E}]\right] - \frac{i}{8k_0^2}\left[\mathcal{O},\dot{\mathcal{O}}\right] \\ + \frac{\eta}{8k_0^3}\left(-[\mathcal{O},\mathcal{E}]^2 - i\left\{\dot{\mathcal{O}},[\mathcal{O},\mathcal{E}]\right\} + \dot{\mathcal{O}}^2\right) + \text{ 5}^{\text{th}}\text{ order} \end{array}, \tag{89}$$

and insert the definitions for $\mathcal{E}$ and $\mathcal{O}$ from Eq. (86). This gives us $\mathcal{H}$ to fourth order (counting powers of λ, γ and $\partial/\partial x$ (acting on λ, γ) as orders):

$$\begin{array}{l} \mathcal{H} = \\ \eta k_0 \left(\begin{array}{l} 1 - 2\gamma + \frac{\lambda}{k_0} - \frac{\lambda^2}{2k_0^2} + \frac{\lambda^3}{2k_0^3} - \frac{5\lambda^4}{8k_0^4} - \frac{\dot{\lambda}^2}{8k_0^2} \\ - \frac{1}{4k_0^2}\left\{\lambda,\{\lambda,\gamma\}\right\} + \frac{1}{2k_0^3}\left\{\lambda^2,\{\lambda,\gamma\}\right\} - \frac{1}{2k_0^3}\{\lambda,\gamma\}^2 \end{array} \right) \\ + \frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right] - \frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right] + \frac{i}{4k_0^2}\left[\{\lambda,\gamma\},\dot{\lambda}\right] + 5\text{th order} \end{array}. \tag{90}$$

The details of the derivation of Eq. (90) are given in Appendix J.1 on the CD. Note that we wave-dropped the tilde and the superscript IV. (Recall that the commutator $[,]$ and anti-commutator $\{,\}$ are defined in footnote f.)

The next step is to modify Eq. (90) for the special case where the density variation is a jump. This is particularly useful, since the density is often fairly constant within a given material, but jumps as one passes from one material to another. As long as the transition region from material to material is very small on the order of a wavelength (and it often is, particularly in the context of low frequency acoustic scattering from the ocean bottom), it is a good approximation to model the jump in the density function by a step function along a precisely defined interface dividing the two materials. However, before proceeding to develop a form of the Hamiltonian $\mathcal{H}$ given by Eq. (90) fine-tuned for such density jumps, we have to explore a very important formal result: δ-function bifurcation.

5.2 δ-function Bifurcation

Once steps are introduced into the environmental parameters, the field theory will invariably generate scenarios where distributions are multiplied. From a mathematical standpoint, there is no completely general way to define such quantities. However, it is possible to develop empirical rules for interpreting these quantities in the context of field theory. This reflects the fact that the mathematics in this context describes underlying physical effects that are well behaved.

5.2.1 The Bifurcation Rules

To deduce the rules for the multiplication of distributions, consider two prototypical problems, which cover the key physical circumstances of interest in the current discussion, and where we know an acceptable interpretation for a product of derivatives must exist. Specifically demand that:

- It must be possible to use the chain rule in the full wave equation to recover the boundary conditions for an interface where the density jumps:

$$\vec{\nabla}\cdot\left(\rho^{-1}\vec{\nabla}A\right)+\frac{k_0^2n^2}{\rho}A=0\Rightarrow\text{continuity of } A,\frac{1}{\rho}\frac{\partial A}{\partial n}$$

- In the constant density PE ($\delta\rho=0$), where the sound speed jumps along a flat (range-independent) surface, adding orders to the PE recovers the explicit boundary conditions for the higher-order derivatives of the field (i.e., the boundary conditions on $\nabla_T^n\chi$, $n>2$)[ww].

These conditions force δ-function bifurcation. This means that the first time a step function is differentiated to form a δ-function, that δ-function bifurcates into two half-δ-functions an infinitesimal distance on either side of the interface:

$$\frac{\partial\Theta(z-f)}{\partial z}=\delta(z-f)\Rightarrow\frac{\delta^+(z-f)}{2}+\frac{\delta^-(z-f)}{2}.$$

Now, other factors in the product are no longer distributions, since all are evaluated just inside the half-space on either side of the interface.

5.2.2 δ-function Bifurcation in Other Contexts

This result has in the past appeared in another context. Green's function integral formulas for the solution to the Helmholtz equation in a bounded region pick up factors of ½, and this ultimately comes from a similar δ-function bifurcation at the normal derivative of the Green's function on the boundary [79-81]. (The first two references do not *explicitly* use the terminology of distribution theory, but the result is the same.)

The issues related to the multiplication of distributions are relatively hidden in quantum mechanics, and to some extent also for the sound speed cusp. Since the wavefunction itself is continuous, the products that involve distributions occur in third and higher-order terms in the Hamiltonian H – examples include the terms proportional to

$$\left(\nabla^2V\right)\nabla^2,\nabla V\left(\nabla^2V\right)\nabla,V\left(\nabla^2V\right)\nabla^2,\left(\nabla^2V\right)^2. \tag{91}$$

(On the other hand, products of distributions are already in Section 4.1, where we consider quasi-first order theory for an interface where the sound speed jumps.) Obscuring the whole issue even further is the

[ww] In considering this range-independent problem, we will exploit the fact that the eigenvector structure of the solution will force the orders in the operator λ to decouple. Basically, this means that any distribution generated in $\lambda^n\chi$ must cancel internally, and so adding a higher order to the PE will add new boundary conditions, but not change preexisting boundary conditions extracted from lower order theory. The details of this assertion are discussed at the beginning of Appendix K.2.1.2.

fact that in quantum mechanics, one typically calculates expectation values, often using decompositions of unity to simplify the evaluation of these expressions. Specifically, physical quantities are characterized by expectation values of (Hermitian) operators, and products within these expectation values can be broken apart by interjecting decompositions of unity of the form $\sum_n |\varphi_n\rangle\langle\varphi_n|$ (where the set of eigenvectors $\{\varphi_n\}$ (for the time-independent problem) form a basis for the solution set). Then, products of distributions such as in Eq. (91) seem to go away. Decompositions of unity are also useful because they reduce the number of distinct expectation values that need to be calculated, and the technique is particularly appealing when used in the context of the atomic problem, because it helps to skirt the issue that V itself is already infinite at the origin[xx].

5.2.3 Caveats

It is important to keep in mind that the multiplication of distributions is not defined in general. Thus, the δ-function bifurcation prescription only applies in certain specified contexts, and it must be applied with care. The prescription works well when the associated step functions are raised to simple powers (e.g., a term proportional to $\Theta^n\left(z-f\left(x\right)\right)\delta\left(z-f\left(x\right)\right)$), and when it is used in conjunction with the ordinary rules of differentiation such as the chain rule and the product rule. An example of the proper use of the δ-function bifurcation prescription in conjunction with the chain rule would be if we are given some function of the step function $g\left(\Theta\left(z-f\left(x\right)\right)\right)$, and then define its derivative

$$\partial g\left(\Theta\left(z-f\right)\right)/\partial z = g'\left(\Theta\left(z-f\right)\right)\cdot\partial\Theta\left(z-f\right)/\partial z = \left[dg/dy\right]_{y=\Theta(z-f)}\delta\left(z-f\left(x\right)\right)$$

(and similarly for $\partial g/\partial x$). Similarly, the product rule would imply that

$$\frac{\partial}{\partial z}\left[g\left(\Theta\left(z-f\left(x\right)\right)\right)\cdot h\left(\Theta\left(z-f\left(x\right)\right)\right)\right] =$$
$$\frac{\partial g\left(\Theta\left(z-f\left(x\right)\right)\right)}{\partial z}\cdot h\left(\Theta\left(z-f\left(x\right)\right)\right) + g\left(\Theta\left(z-f\left(x\right)\right)\right)\cdot\frac{\partial h\left(\Theta\left(z-f\left(x\right)\right)\right)}{\partial z}.$$

However, naively multiplying through by functions of the step function will cause problems. For example, multiplications such as $\left[\sqrt{1+\text{constant}\cdot\Theta}\right]\cdot\delta$ or $\left[1/\left(1+\text{constant}\cdot\Theta\right)\right]\cdot\delta$ will produce incorrect results when combined with the bifurcation prescription (at least if both sides are weighted equally). These functions apparently distort the step and change the weighting factor. On the other hand, we can expand these functions in a Taylor series expansion, which consists of a sum of terms that are products of the form $\Theta^n\cdot\delta$. Now, for these clean undistorted steps we can use the δ-function bifurcation prescription.

[xx] However, keep in mind that for the time-*in*dependent case, the higher-order Hamiltonian *H* is strictly made up of powers of $\lambda = -\hbar^2\nabla^2/2m_0 + V$, and as noted in the previous footnote, λ is, crudely speaking, interchangeable with an eigenvalue. Thus, $\lambda^n\varphi \propto \varphi$ and so the infinities associated with powers of *V*, with the distributions of the type shown in Eq. (91), and with derivatives of the wavefunction φ, must cancel when all are taken together. (Also note that there must be internal cancellations between infinities generated by the operators ∇^2 and *V* associated with *each specific application* of the operator λ.)

The observation that δ-function bifurcation works for undistorted steps is an intuitively sensible result. On the other hand, it is not a priori clear that there would not be a problem with distorted steps generated *internal* to the chain rule. In other words it is somewhat surprising that in this context the step in $g'(\Theta)$ is apparently undistorted with respect to the step Θ. For present purposes, it is sufficient to note that the result seems to hold in the two rather different examples we consider in the Appendix K[yy] as well as in the Green's function integral formula in scattering theory, and that these examples are typical of scenarios that arise in the context of the PE. Development of a full mathematical theory of the general result (including possible restrictions on its validity) will be deferred to future research[zz]. Similar issues apply to the product rule. For our purposes, we note that the product rule is used in one form or another in all four examples discussed in the Appendix K as well as in the Green's function integral formulas from scattering theory, and that it consistently produces correct results. Thus, in this context the steps in $g(\Theta)$ and $h(\Theta)$ are apparently undistorted and the product rule can be used in conjunction with δ-function bifurcation. (There is some further discussion concerning the need for undistorted steps in Appendix K.2.2.)

5.2.4 Plausibility Arguments

Appendix K provides a plausibility argument for the δ-function bifurcation rules given above. Section K.1 considers two cases where the rules apply:

- Subsection K.1.1 examines a flat interface where the sound speed jumps, but not the density,
- Subsection K.1.2 considers the full two-fluid interface in the full wave (Helmholtz equation) problem.

Then, Section K.2 examines two cases where the prescription only seems to work to first order:

- The substitution $\alpha = 1/\rho$ is analyzed in Subsection K.2.1.1 and
- Tappert's change of variable substitution $u = A/\sqrt{\rho}$ is evaluated in Subsection K.2.1.2.

In Section K.2.2, we examine why some cases only seem to work to first order. In particular, the need for undistorted steps is discussed in this section, and then our observations are verified in Subsection K.2.3, when the $\alpha = 1/\rho$ case is extended to second order using a Taylor series expansion. Finally, the associative property for our prescription is briefly examined in Section K.3.

Before closing this subject, it should be emphasized that it is implicitly assumed in the δ-function-bifurcation rules that the parameters jump at an interface, but do not otherwise vary in the vicinity of the interface. As we see in Appendix J.2 (the argument leading to Eq. (J.19)), extra care must be exercised if we apply δ-function bifurcation in situations where this condition is violated. In particular, the associative property (see Appendix K.3) in choosing which distributions to bifurcate may not hold, and explicit symmetrization may be necessary.

[yy] The chain rule for differentiation and the product rule for differentiation are both used in the full wave two-fluid problem considered in Appendix K.1.2, and following a more complicated scenario, they are also ultimately needed for the successful implementation of the change of variable (COV) substitution discussed in Appendix K.2.1.2.

[zz] The result appears to be related to the fact that in $g'(\Theta(z)) = [dg/dy]_{y=\Theta(z)}$, the discontinuous function $\Theta(z)$ is not really embedded inside the function dg/dy. Instead, it is applied after the fact to produce a "clean" (i.e., undistorted) step. In fact, given the discontinuities in both g and Θ, there does not appear to be any way to make sense of $g'(\Theta)$ other than the interpretation $g'(y)$ with y first treated as a general, continuous function, and only subsequently set equal to a discontinuous function.

5.3 The Interface Where the Density Jumps

In Section 5.3.1, the Hamiltonian (Eq. (90)) is converted to a form that is useful for the special case where the density jumps along an interface, but is otherwise constant in the half-spaces. This section also examines the transformation between the pressure field A and the auxiliary field χ associated with the PE. Section 5.3.2 generalizes to the density jump the discussion of Section 4.1 by examining the boundary conditions in quasi-first-order theory. The previous discussion is extended as the new FW terms are examined closely in Section 5.3.3. Section 5.3.4 examines the classical Lamb shift for a rough interface where the density and compressibility jump and so it is a generalization of Section 4.3. Finally, Section 5.4 examines the significance of the classical Lamb shift in a typical scenario for acoustic propagation in a shallow water (coastal) environment.

5.3.1 The Basic Formal Structure

5.3.1.1 The Form of the Hamiltonian Useful When the Density Jumps

We are now in a position to use the δ-function-bifurcation prescription established in Section 5.2 to tailor the general fourth-order Hamiltonian for an acoustic field in an environment where the density varies (Eq. (90) of Section 5.1) to the special case where the density jumps at interfaces, but is otherwise constant:

$$\mathcal{H} = \eta k_0 \left(\begin{array}{l} 1 - 2\gamma + \dfrac{\lambda}{k_0} - \dfrac{\lambda^2}{2k_0^2} + \dfrac{\lambda^3}{2k_0^3} - \dfrac{5\lambda^4}{8k_0^4} - (1+4\gamma)\dfrac{\ddot{\lambda}}{8k_0^3} + \dfrac{3\{\lambda,\ddot{\lambda}\}}{16k_0^4} \\ -\dfrac{1}{4k_0^2}\{\lambda,\{\lambda,\gamma\}\} + \dfrac{1}{2k_0^3}\{\lambda^2,\{\lambda,\gamma\}\} - \dfrac{1}{2k_0^3}\{\lambda,\gamma\}^2 \end{array} \right) + 5^{\text{th}} \text{ order.} \tag{92}$$

This result is derived in Appendix J.2. In the derivation, it is assumed that a quasi-planar interface separates two half-spaces, where the compressibility K (or equivalently $\mu = \tfrac{1}{2}(1 - K/K_0)$) is assumed to be range-independent in the half-spaces and the density ρ (or equivalently $\gamma = \tfrac{1}{2}(1 - \rho/\rho_0)$) is assumed to be constant in the half-spaces. Both quantities may jump along the range-dependent interface. The assumption that there are only two half-spaces is made to keep the discussion straightforward, but there is nothing in the derivation itself that disallows a scenario where several interfaces are present.

As discussed in Appendix J.2 (and to a lesser extent later here in Section 5.3.1), in the half-spaces where the density is constant, the terms involving the anticommutator $\{\lambda,\gamma\}$ simplify dramatically. Equation (92) maintains the more complicated form because these terms will generate δ-functions at the interface, and only the full form involving these anticommutators will produce the correct distributions along the interface.

During the derivation in Appendix J.2, we also monitor the possibility that the compressibility K (or equivalently μ) may be range-dependent in the half spaces. At the end of the derivation, we will find that if μ is range-dependent in the half-spaces, we pick up an extra (nominally fourth-order) term in $\mathcal{H}$:

$$\eta k_0 \left[\frac{1}{4k_0^4} \cdot \frac{1}{2} \left\{ \left(\frac{\partial \lambda}{\partial x} \right)^{\pm}, \dot{\lambda}_S \right\} + \text{PV}\left(\frac{\dot{\lambda}^2}{4k_0^4} \right) \right] = \eta k_0 \left(-\frac{1}{4k_0^3} \cdot \frac{1}{2} \left\{ \frac{\partial \mu^{\pm}}{\partial x}, \dot{\lambda}_S \right\} + \text{PV}\left(\frac{\dot{\mu}^2}{4k_0^2} \right) \right). \tag{93}$$

The subscript S indicates that $\dot{\lambda}_S$ is to be evaluated precisely on the interface S. The superscript $\pm$ serves to remind us that as $\dot{\lambda}_S$ bifurcates, $\partial\mu/\partial x$ is evaluated just inside the half-spaces. Furthermore, since we are now allowing μ and, consequently, λ to depend on the range away from the interface, the usual term proportional to $\dot{\lambda}^2$ must also be added to the Hamiltonian $\mathcal{H}$ in the half-spaces away from the interface. Indicating that this quantity is evaluated in its standard form everywhere except right on top of the interface, we identify the standard $\dot{\lambda}^2$-term as a principal value (PV). Note that if μ is range-*in*dependent in the half-spaces, then both sides of Eq. (93) indeed reduce to zero.

Equations (92) and (93) define a diagonal matrix Hamiltonian $\mathcal{H}$ to be used in a wave equation of the form

$$i\frac{\partial}{\partial x}\begin{pmatrix}\theta\\ \chi\end{pmatrix} = \mathcal{H}\begin{pmatrix}\theta\\ \chi\end{pmatrix}, \tag{94}$$

where θ and χ are decoupled scalar fields that propagate in the uprange and downrange direction, respectively (as always, we will study the behavior of χ). (The fields θ and χ differ from the fields of the same name defined in Eq. (85) by a sequence of FW transformations. As with the Hamiltonian $\mathcal{H}$, we have dropped the tildes that we sometimes associate with quantities that come out of the FW procedure. Once the diagonalization procedure has been completed, these tildes have outlived their usefulness.)

Note that the assumption that the density is constant within a given medium, and only changes when one passes from one medium to another, is very reasonable. The compressibility is much more likely to vary significantly within a medium. Indeed, sound speed fluctuations within a given medium are typically generated by fluctuations of the compressibility rather than of the density.

5.3.1.2 The Hamiltonian in the Half-spaces

The PE formalism not only picks out a specific downrange direction, but also reference values for the density and compressibility. These are typically chosen to be the maximum values of these quantities. For the basic interface problem, there are two values of the density in play, and γ will be nonzero on the side where the density is smaller (i.e., different from the reference value $\rho_0 = \rho_{\text{maximum}}$). On that side of the interface, the Hamiltonian will involve an expansion not only in λ as before, but also in γ, the measure of the departure of the local value of the density from its reference value. (In power counting, both λ and γ contribute equally.) As before, the expansion must eventually converge to the "exact" square root operator (neglecting any local range dependence in the half-spaces). There are several ways to combine terms to verify that this is indeed the case. In the Appendix L.1, one of these is derived:

$$H = \frac{k_0}{\boxed{\alpha}}\sqrt{1+\frac{2\boxed{\alpha}\lambda}{k_0}} = \sqrt{\bar{\nabla}_T^2 + k^2}\,, \tag{95}$$

where $\alpha \equiv \rho_o/\rho$. (Note that this result is only valid in half-spaces where ρ is locally constant and the range dependence in K is locally weak.) The second instance of α in Eq. (95) (i.e., the one in the product $2\boxed{\alpha}\lambda$) comes from the series

$$1+(2\gamma)+(2\gamma)^2+(2\gamma)^3+(2\gamma)^4\cdots=\frac{1}{1-2\gamma}=\frac{\rho_0}{\rho}=\alpha, \tag{96}$$

and the factor of $1/\alpha$ in front simply comes from $1/\alpha=1-2\gamma$. Note that this expansion indeed recovers the correct result $H=\sqrt{\tilde{\nabla}_T^2+k^2}$. The result (Eq. (95)) emerges from a resummation of terms that misses out on some cancellations, and therefore implies a more stringent convergence condition than is really the case. It is, however, a particularly compact form of the full expansion, and therefore useful as a mnemonic for reproducing the new PE expansion in the half-spaces. α should always be written in terms of γ, and the result for H should be expanded in λ and γ to the desired order (with λ and γ counting equally in determining the order).

An alternate closed form for ∞-order H that is based on a different grouping of the terms in the λ-γ expansion is derived in Appendix Subsection L.2. This form more accurately reflects the convergence properties of the expansion – in fact, the infinite-order result looks just like the traditional form of the Hamiltonian in the water column (i.e., the form that leads to an expansion in the sound speed deviation only, Eq. (4)). This result suggests that we will be able to proceed as before and use traditional PE codes in the water column, even though formally the Hamiltonian in the water column now contains an expansion in the parameter measuring the density jump: γ. However, note that to determine the *actual order* of such a result, we will still have to formally expand in λ and γ the Hamiltonian we actually use.

5.3.1.3 The Transformation Between the Pressure Field and the Auxiliary Field Associated with the PE

As briefly discussed near the beginning of Appendix C.2.1, the fact that the FW transformation is by construction pseudo-unitary guarantees that the integral over transverse space of the quantity $|\theta|^2-|\chi|^2$ always remains proportional to the total energy flux in the uprange/downrange direction. This is true even if θ and χ are the decoupled fields that have emerged after repeated applications of the FW transformation (e.g., as in Eq. (94)). This implies that χ will always be some kind of carrier of downrange flux. Specifically, $|\chi|^2$ should differ from the downrange energy flux by no more than an integration by parts. This leads us to surmise that the carrier of flux χ must have a relationship vis-à-vis the pressure field A that is similar to the one it had when the density was constant; however, now an extra factor of $1/\sqrt{\rho}$ must be thrown in because the square of this quantity is in the energy flux, but it is no longer globally constant. The result (again valid in half-spaces where the density is locally constant and the range dependence of the compressibility is locally weak) is

$$\frac{1}{\sqrt{\rho}}\sqrt{-i\frac{\partial}{\partial x}}\cdot A\propto\sqrt{\frac{\alpha}{k_0}}\sqrt{H}\cdot A=\left(1+\frac{2\alpha\lambda}{k_0}\right)^{1/4}A=\chi. \tag{97}$$

Examining the first and second orders explicitly verifies that our conjecture is correct (see Appendix D.2). Again note that Eq. (97) is essentially a mnemonic for the corresponding finite order expansion in λ and γ. Also note that $\sqrt{H}$ is still a near-eigenoperator and so nearly cancels in weakly range-dependent environments, but now there is also a factor $\sqrt{\alpha}$ that cannot be dropped even if there is no range dependence at all. (For this argument to work, we also need to recall that the commutator of $\sqrt{\alpha}$ and

$\sqrt{H}$ is nonzero only right on top of the interface, where Eq. (97) is not valid anyway, and where we do not need to transform from the auxiliary field χ back to the pressure field A.) Note that, strictly speaking, the result for the endpoint calculation is only as accurate up the same order in λ and γ as the Hamiltonian used.

5.3.2 Deterministic Quasi-First-Order Theory

We now have everything we need to examine quasi-first-order deterministic theory for the case where the density jumps along an interface. This study extends the calculation in Section 4.1 (which is itself an extension to a sound speed jump of the discussion in Section 3.2.3 for the sound speed cusp).

The current situation is similar to that described toward the end of Section 5.3.1, but here we specifically restrict ourselves to the standard two-dimensional $x-z$ space. Regions I and II are separated by a rough surface $z=f(x)$ along which the density ρ and the compressibility K jump. These parameters are now *both* assumed to be constant in Regions I and II (but this will again be relaxed for K in Section 5.4). The reference values for these parameters are in general ρ_0 and K_0. Since the density is no longer globally constant, μ generalizes to $\mu \equiv \left(1-{}^{K}\!/_{K_0}\right)\!/2 = \left(1-n^2\cdot{}^{\rho_0}\!/_{\rho}\right)\!/2$, where as before $n=c_0/c=\sqrt{[\rho K]/[\rho_0 K_0]}$. Similarly, $\gamma \equiv \left(1-{}^{\rho}\!/_{\rho_0}\right)\!/2$. As just noted in Section 5.3.1, the reference parameters ρ_0 and K_0 are typically chosen to be their maximal values. In the conventions used here, ρ_{II} and K_I are the maximal quantities, and so $K_0=K_I$ and $\rho_0=\rho_{II}$. This corresponds to the prototypical case where Region I is the water column and Region II is sediment in the sub-bottom (generally of the ocean). These conventions are summarized in Fig. 17.

As in Section 3.1, express the diagonalized matrix Hamiltonian in terms of a scalar Hamiltonian: $\mathcal{H}=\eta H$. The quasi-first order scalar Hamiltonian H based on Eq. (92) is then

$$H = k_0 + \lambda - 2k_0\gamma - {}^{\ddot{\lambda}}\!/_{8k_0^2}\,. \tag{98}$$

From Eq. (94), we see that this Hamiltonian is associated with the usual scalar PE (Eq. (18)) for downrange propagation:

$$-i\frac{\partial \chi}{\partial x} = H\chi\,.$$

The δ-function-bifurcation rules outlined in Section 5.2 are used as needed to evaluate H. The infinitesimal transverse integrations described in Section 3.3.3 (and already used in the simpler version of this problem described in Section 4.1) are applied to the PE. The boundary conditions that emerge are

$$\begin{aligned}
\chi_{II} &= \chi_I + \frac{\dot{f}^2}{8\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I}-\frac{\delta\rho}{\rho_{II}}\right)\overline{\rho\chi} + \frac{\delta\rho}{8k_0^2}\left(\ddot{f}\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]} + \dot{f}^2\overline{\left[\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}\right]}\right) \\
\frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z} &= \frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z} - \frac{1}{8\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I}-\frac{\delta\rho}{\rho_{II}}\right)\left(\ddot{f}\,\overline{\chi} + \dot{f}^2\overline{\frac{\partial\chi}{\partial z}}\right)
\end{aligned}\,. \tag{99}$$

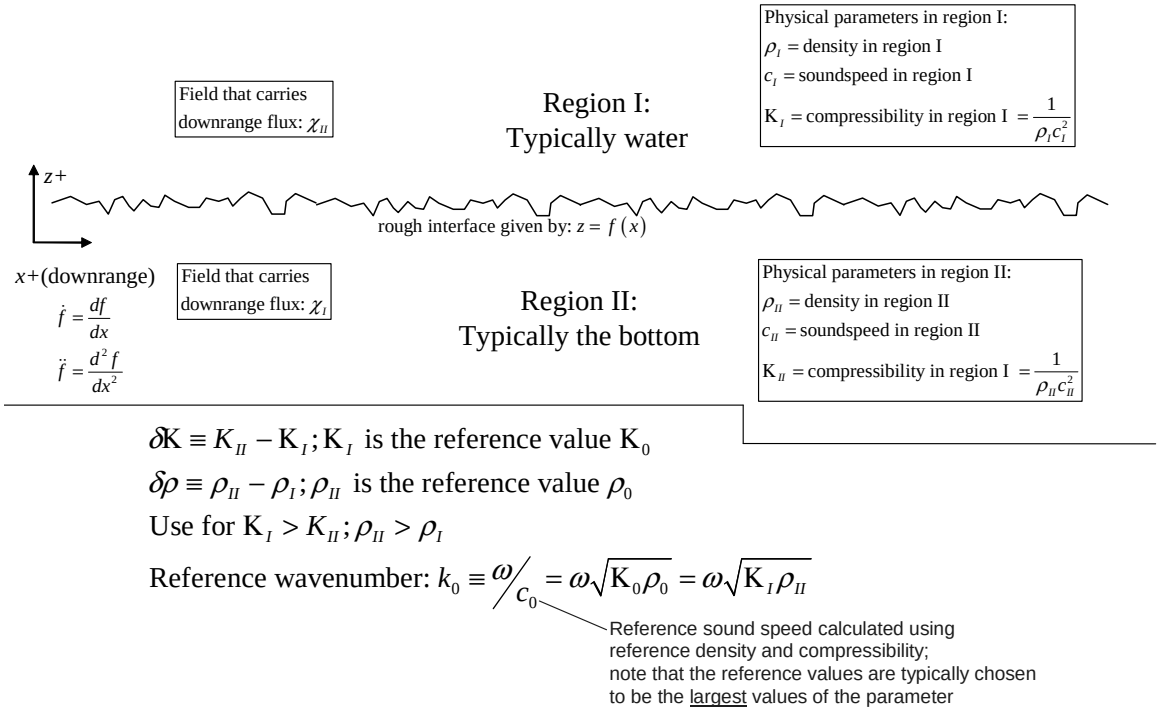


Fig. 17 — We consider the standard two-dimensional $x-z$ space. Regions I and II are separated by the rough surface $z = f(x)$. The positive *z*-axis points from Region II into Region I. The density ρ and (for the moment) also the compressibility *K* are constant in the half-spaces. Region I is typically the water column, and Region II is typically sediment in the sub-bottom. In order to minimize the related PE expansion parameters γ and μ, the reference values should be chosen to be the maximum values of the parameters. In this case, this means that the reference density is chosen to be that in Region II (the bottom) and the reference compressibility is chosen to be that in Region I (the water column).

A $\overline{\text{bar}}$ denotes an average between the respective quantities evaluated on the two sides of the interface. Details of the derivation of boundary conditions (Eq. (99)) are given in Appendix M. Setting $\delta K / K_I = -2\mu_{II}$ and $\delta\rho = 0$, we verify that Eq. (99) is indeed a straightforward generalization of Eq. (71).

We defer the extension of the discussion in Section 4.2.1 to Section 6.1.5. In that section, we again use the full-wave boundary conditions to gain an understanding of the deterministic boundary conditions generated by distributions in $\ddot{\lambda}$ — this time, the more general $\ddot{\lambda}$ responsible for the boundary conditions given by Eq. (99).

Having derived the boundary conditions for quasi-first-order theory, let us gain further insight into the new terms uniquely generated by the FW transformation (i.e., those with an explicit range derivative; as we have already argued, such terms are loosely associated with “vacuum polarization”). This is done in the next section. There, Section 5.3.4 examines the stochastic problem.

5.3.3 A Close Look at the New Foldy-Wouthuysen Terms

5.3.3.1 Higher-order FW Terms

As frequently discussed above, the FW procedure generates a Hamiltonian that uniquely includes a series of terms explicitly associated with the range dependence. It was noted in Section 4.4 that the terms of this series that are proportional to $\ddot{\lambda}$ correspond to the phenomenon of "vacuum polarization" known from quantum mechanics (because this type of term involves virtual particle pairs)[aaa]. The lowest-order member of this class of terms is the third-order term $-\ddot{\lambda}/\left(8k_0^2\right)$, that was just evaluated in Section 5.3.2. Examining Eq. (92), we see that there are also two nominally fourth-order terms in this class:

$$\frac{3\left\{\lambda,\ddot{\lambda}\right\}}{16k_0^4} \quad \text{and} \quad -4\gamma\frac{\ddot{\lambda}}{8k_0^3}.$$

Below, we present an estimate for the magnitude of these terms for typical values of the environmental parameters, and verify that they are indeed getting smaller. Furthermore, δ-function bifurcation can be used to convert the $-(4\gamma)\ddot{\lambda}/\left(8k_0^3\right)$ term into a form that suggests an infinite series encountered previously. The infinite series can be evaluated in closed form. This allows us to examine the boundary conditions for Dirichlet ($\chi = 0$) and Neumann ($\partial\chi/\partial n = 0$ for the full wave problem, but this changes a little bit for the PE) boundary conditions. The Neumann boundary condition for the PE implies the existence of curvature-induced boundary waves. Curvature-induced boundary waves have not yet been fully incorporated into modern scattering theory, and the PE based on the FW transformation presents a promising new technique for doing so. Curvature-induced boundary waves were studied by Biot and Tolstoy in a line of development that has until now run parallel to mainstream rough-surface scattering theory. The relationship between the Biot-Tolstoy scattering theory and the curvature-induced boundary waves predicted by the parabolic equation based on the FW transformation is discussed at the end of this subsection.

5.3.3.2 Specific Examples

As in Section 5.3.2, we consider two-dimensional $x-z$ space, and Regions I and II separated by the rough surface $z = f(x)$. Values ρ and K are constants in the half-spaces, but jump at the interface. The reference compressibility is K_I, and the reference density is ρ_{II}. This implies that $\mu_I = \gamma_{II} = 0$. In this section, we choose the values

$$\begin{aligned} &K_{\text{water}} = K_I = K_0 = 3K_{II} = 3K_{\text{sand}} \\ &2\rho_{\text{water}} = 2\rho_I = \rho_0 = \rho_{II} = \rho_{\text{sand}} \\ &c_{\text{water}} = 1500\,\text{m/s} \quad \Rightarrow \quad c_{\text{sand}} \approx 1840\,\text{m/s} \end{aligned} \qquad . \tag{100}$$

These parameter values are representative of underwater acoustics scenarios.

Comparing the fourth-order term $\frac{3}{16k_0^4}\left\{\lambda,\ddot{\lambda}\right\}$ with the third-order term $-\ddot{\lambda}/\left(8k_0^3\right)$, we find terms that differ from the corresponding (bifurcated) third-order contributions in one of two basic ways:

[aaa] An example of a new term introduced by the FW that is not of the "vacuum polarization" class of terms would be the term given by Eq. (93).

- Terms that differ from the corresponding third-order term by a factor $\left([-3K_{\pm}]/[4K_0]\right)\left(\nabla_T^2/k_{\pm}^2\right)$ (operating on the wave function $\chi_{\pm}$).
- Terms that differ from the corresponding third-order term by a factor $3\left(\mu_{\pm}-\gamma_{\pm}\right)$.

(Recall that the subscript $\pm$ indicates that the parameters are to be evaluated just inside Region I (+) or Region II (-).)

In Appendix N.1.1, it is argued that for the parameters given in Eq. (100), terms of the first sort will typically provide a negligible correction on the order of 1% to 2% while terms of the second sort introduce a still-modest 12.5% correction.

In Appendix N.1.2, it is established that for the usual scenario, where $\gamma_{II}=0$ (i.e., the reference density is in Region II), δ-function bifurcation reduces the term $-4\gamma\left(\ddot{\lambda}/8k_0^3\right)$ to

$$-4\gamma\frac{\ddot{\lambda}}{8k_0^3}=-2\gamma_I\frac{\ddot{\lambda}}{8k_0^3}. \tag{101}$$

Given the parameters listed in Eq. (100), this represents a 50% correction to the third-order term $-\ddot{\lambda}/8k_0^3$. This error is significant enough to cause concern that in many practical instances, it may prove necessary to use higher-order theory to correctly evaluate this term. Therefore, in Appendix N.2, the result is extrapolated to infinite orders.

5.3.3.3 Infinite-order Theory

The extrapolation is obtained as follows. The term given in Eq. (101) hints at the sequence of terms

$$\left(1+2\gamma_+\right)\frac{-\ddot{\lambda}}{8k_0^3},$$

which contains the familiar factor $\left(1+2\gamma_+\right)$. This hints at the beginning of a series that plays a prominent role in our expansion of the PE, namely the series given in Eq. (96): $1+(2\gamma)+(2\gamma)^2+(2\gamma)^3=\rho_0/\rho$. This suggests that at infinite order, we have $-\left(\ddot{\lambda}/8k_0^3\right)\cdot\left(\rho_{II}/\rho_I\right)$.

Modifying the boundary conditions accordingly, and then taking the limits $\rho_{II}\gg\rho_I$ and $K_{II}\ll K_I$, we get the Dirichlet boundary conditions for the field in Region II and the Neumann boundary conditions for the field in Region I[bbb]. The details are in Appendix N.2. The Dirichlet boundary condition is unchanged, but note what happens to the Neumann boundary condition. It becomes

$$\nabla_T\chi_I=-\frac{\ddot{f}}{4}\chi_I. \tag{102}$$

[bbb] Note that these boundary conditions would apply, for example, if Region II represents the water column under an air-sea interface or Region I represents the water column above a very hard bottom. Note, this implies that the Dirichlet boundary condition would apply for an acoustic field incident from a hard bottom onto the water column and the Neumann boundary conditions would apply on a sound field incident from the air onto the ocean surface.

This is significant because such boundary conditions allow solutions containing transverse dependence of the form $\exp\left(-\ddot{f}\cdot z/4\right)$ — i.e., boundary waves. As noted above, these curvature-induced boundary waves have not yet been fully incorporated into modern scattering theory, and the PE based on the FW transformation presents a promising new technique for doing so.

5.3.3.4 Boundary Waves

Boundary waves have proven to be quite problematic in scattering theories based on the full-wave acoustic equation. For example, they do not show up at low orders of perturbative, small-slope or Kirchhoff scattering theory. If they show up at all, boundary wave phenomena creep in as multiple scattering effects at high orders of these approximations. As Thorsos and others have pointed out [82-85], the fact that a given order can ignore boundary waves is intimately connected to the fact that the above rough surface scattering theories do not conserve energy at each order. A prominent example is lowest order perturbation theory for the Neumann boundary condition, which predicts a scattered field even at glancing incidence, when the energy flux incident on the surface goes to zero. The perturbation, small-slope, and Kirchhoff approximation (and others less well known) are all part of a closely related family of approximations, and therefore they share many advantages and deficiencies, including their problems associated with boundary wave phenomena such as the lack of order-by-order energy conservation. Note that the PE has energy conservation built in, so a rough surface scattering theory directly based on it should include the phenomenon of roughness-induced boundary waves. This is a key distinction between traditional theories of rough surface scattering and the energy-conserving PE, and it is potentially a fruitful topic for future research.

Appendix O presents a closer look at curvature-induced boundary waves in the context of modern acoustic scattering theory and points to ways in which the PE based on the FW transformation may contribute to our understanding of this issue. This appendix also notes that effects that explicitly depend on the square of the local slope[ccc] raise issues that are similar to the ones posed by curvature-induced boundary waves. Both effects are artificially pushed to high orders by the various perturbative approximations in widespread use, and both involve physics that is new to the theoretical framework and is uniquely sensitive to the size scale between the Bragg (wavelength) scale and $\left[\text{wavelength}\right]/2\pi$ (this is a third scale in addition to the large (> wavelength) scale and the Bragg scale). The new physics is a consequence of the fact that the curvature $\ddot{f}$ and the square of the slope $\dot{f}^2$ typically remain sensitive to subwavelength scales, while the surface displacement f does not[ddd]. However, this sensitivity to small scales also causes trouble. Such terms fail to properly cut themselves off at very small scales, and, therefore, they raise the issue of renormalization. The PE provides a serviceable solution to the renormalization problem: the issue of renormalization can be sidestepped with the use of a single upper cutoff. The advantages of the PE are, then, that it brings curvature and tilt-induced effects to their natural place at low order, and that it presents a serviceable solution to the renormalization problem.

[ccc] This refers to effects explicitly proportional to $\dot{f}^2$ such as those discussed in Section 4.2.1, and not to effects that implicitly depend on the slope, such as tilting of the diffraction grating introduced by the small slope approximation (see Appendix O).

[ddd] This statement applies to the rough surfaces typically encountered by classical fields. As noted in Section 4.4, this does *not* hold in the analogous problem from atomic physics, where even the equivalent of *f* becomes sensitive to small scales.

5.3.3.5 Relationship to Other Approaches Such as Biot-Tolstoy Theory

There is an independent line of research that shares many of these advantages. However, it has remained outside the mainstream of scattering theory. M. A. Biot and I. Tolstoy have developed a theory for scattering from bossed surfaces that predicts curvature-induced boundary conditions that are very similar to those generated by the "vacuum polarization" term. This work was outlined in a series of articles beginning in the late 1950s. A flavor of the effort is provided by Refs. 86 through 88, and a more complete reference list is available in the annotated bibliography at the end of Ref. 8. Their boundary conditions contain terms that are proportional to the curvature $\ddot{f}$, and resemble the $\mathrm{O}\left(\ddot{f}\right)$ contribution to boundary conditions on $\partial\chi/\partial z$ given Eq. (71) for a sound speed jump, Eq. (99) for a density and compressibility jump, and Eq. (102) for the Neumann boundary condition. (For that matter, the $\mathrm{O}\left(\dot{f}^2\right)$ term in the $\partial\chi/\partial z$ boundary term associated with the sound speed cusp and given in Eq. (31) is similar as well.)

The similarities reflect profound links between the results obtained using the two very different approaches. The physics of Biot-Tolstoy theory is basically the same as that associated with the curvature-generated component of the "vacuum polarization" term. The dependence on the curvature ensures that the associated physical effects are sensitive to a broad spectrum of wave numbers in the rough surface spectrum. Therefore, via the uncertainty principle, we know that they are also sensitive to scales smaller than a wavelength. The associated physical effects include curvature-induced boundary waves and other emergent multiple scattering phenomena. Although these effects are obscured by perturbation theory, they are not vanishingly small. Biot-Tolstoy boundary waves have been observed in the laboratory [89-90].

There are also several differences between the "vacuum polarization" contribution to the PE and Biot-Tolstoy scattering. The PE deals with both cusps and jumps in the environmental parameters, while Biot-Tolstoy theory only handles jumps. The remaining differences between the two approaches reflect the different ways that the rough surface is constructed. Biot-Tolstoy theory constructs the surface using bosses (hemispheres, sections of hemispheres, and indentations of the same shape). Generally speaking, Biot-Tolstoy theory allows for surfaces that are rougher than those allowed by the PE, which only allows surfaces that are smooth displacements from the range-independent problem and have modest slope and curvature. The PE thus operates towards the smooth-surface end of Biot-Tolstoy theory. To use Biot and Tolstoy's terminology, the parabolic equation is restricted to surfaces with small form factors. Thus, it can only generate boundary waves along concave deterministic surfaces (associated with parameter jumps) or along cusps. Bossed surfaces of the type addressed by Biot-Tolstoy theory can have non-zero *average* curvature, and so boundary waves are possible even in the stochastic problem. On the other hand, the parabolic equation deals directly with the surface relief function f, and so it can easily handle relatively smooth deterministic surfaces. More generally, there are a number of complications associated with decomposing surfaces into bosses, and these are avoided by the PE.

Finally, we should also note that Barbone and Spivak have also combined effective impedance boundary conditions (vaguely like Eq. (102) above) with the PE to model scattering from the ocean bottom [91]. Here acoustic scattering from the bottom is modeled using an apparent impedance that is treated as a perturbation from the boundary conditions for a rough pressure-release (i.e., Dirichlet boundary condition) surface. The physics here is not the same as the phenomena described by the "vacuum polarization" term in the PE.

Next, let us consider the stochastic problem for the PE where the density and compressibility both jump.

5.3.4 The Classical Lamb Shift for $\delta\rho \neq 0$

This section examines the stochastic boundary conditions corresponding to a field that obeys the boundary conditions shown in Eq. (99) in the deterministic case. All the assumptions described by Fig. 17 must, of course, continue to hold here. Specifically, assume that $K_I > K_{II}$ and $\rho_I < \rho_{II}$, and that the reference values are chosen to be the larger value. As in Sections 3.2.3 and 4.3, adapt the technique originally developed by Kuperman [65]. Project the boundary conditions at $z = f$ down to the line $z = 0$. Then break the wave function evaluated at $z = 0$ into coherent and incoherent parts: $\chi|_{z=0} = \langle\chi\rangle(0) + \delta\chi$, and average these boundary conditions.

The stochastic version of the boundary conditions shown in Eq. (99) turns out to be:

$$\begin{aligned}
\langle\chi_I\rangle\big|_{z=0} &= \langle\chi_{II}\rangle\big|_{z=0} + \langle f^2\rangle\frac{\delta\rho}{2}\left[\overline{\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}}\right]_{z=0}\left[\overline{\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}}\right]_{z=0} + \frac{k_0^2\langle f^2\rangle}{2\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I} - \frac{\delta\rho}{\rho_{II}}\right)\overline{\left[\rho\langle\chi\rangle\right]}_{z=0} \\
&\quad - \frac{\delta\rho}{8k_0^2}\left[\overline{\frac{1}{\rho}\left\langle \ddot{f}\frac{\partial(\delta\chi)}{\partial z}\right\rangle}\right]_{z=0} + \delta\rho\left[\overline{\frac{1}{\rho}\left\langle f\frac{\partial(\delta\chi)}{\partial z}\right\rangle}\right]_{z=0} + \mathrm{O}\left(f^4\right) \\
\frac{1}{\rho_I}\frac{\partial\langle\chi_I\rangle}{\partial z}\bigg|_{z=0} &= \frac{1}{\rho_{II}}\frac{\partial\langle\chi_{II}\rangle}{\partial z}\bigg|_{z=0} + \frac{\langle\ddot{f}\overline{\delta\chi}\rangle}{8\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I} - \frac{\delta\rho}{\rho_{II}}\right) - \frac{k_0^2\langle f\overline{\delta\chi}\rangle}{\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I} - \frac{\delta\rho}{\rho_{II}}\right) \\
&\quad - \frac{k_0^2\langle f^2\rangle}{2\rho_{II}}\left(\frac{\delta \mathrm{K}}{\mathrm{K}_I} - \frac{\delta\rho}{\rho_{II}}\right)\overline{\frac{\partial\langle\chi\rangle}{\partial z}}\bigg|_{z=0} - \langle f^2\rangle\frac{\delta\rho}{2}\left[\overline{\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}}\right]_{z=0} \\
&\quad - \langle\dot{f}^2\rangle\frac{\delta\rho}{8k_0^2}\left[\overline{\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}}\right]_{z=0} + \mathrm{O}\left(f^4\right).
\end{aligned} \tag{103}$$

As always, an overbar $\bar{\ }$ indicates an averaging between the values from Regions I and II. Note that if we set $\rho_I = \rho_{II}$, $\delta\rho = 0$ and $\delta K/K_I = -2\mu_{II}$, we recover Eq. (81). Recall that as always, the surface spectrum used to calculated $\langle\dot{f}^2\rangle$ and $\langle\ddot{f}\,\delta\chi\rangle$ cuts off at $k_0 = \sqrt{K_I\rho_{II}}$. The details of the derivation of Eq. (103) are presented in Appendix P.

In the $\partial\chi/\partial z$ boundary condition of Eq. (103), there is an apparent "vacuum polarization" term (i.e., downrange Lamb shift):

$$-\langle\dot{f}^2\rangle\frac{\delta\rho}{8k_0^2}\left[\overline{\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}}\right]_{z=0}.$$

This time, unlike for the sound speed cusp and our "toy model" for the hydrogen atom (Eqs. (40) and (51), respectively), this "vacuum polarization" contribution has the same sign as has the "traditional" (or transverse) Lamb shift (caused by smearing). That is because this term is generated by a "hole." In other words, it results from the absence of a term rather than from the active presence of a term. The term that is "missing" from the deterministic boundary conditions (Eq. (99)) is

$$\dot{f}^2 \frac{\delta\rho}{8k_0^2}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}.$$

This is the first time that we have encountered a "hole" like this, and for the time being, the result will be treated as tentative. These issues are discussed further in Section P.2.

Appendix P.3 discusses the stepping algorithm for the discretization of the stochastic problem characterized by the stochastic boundary conditions shown in Eq. (103). The complications discussed there are all related to the boundary conditions involving the second and third derivatives of the stochastic field $\langle\chi\rangle$. To get a quick and dirty idea of the magnitude of the classical (acoustic) Lamb shift in the context of shallow water acoustics, these problematic terms are dropped in the calculation in Section 5.4. For shallow grazing angles, these higher-order transverse derivatives of the field are small and this approximation is perfectly legitimate. The remaining boundary conditions still conserve energy.

5.4 The Significance of the Classical Lamb Shift in Underwater Acoustics

5.4.1 The Basic Formalism

In this section, we consider long-range ducted propagation in a realistic shallow-water environment. The depth of the water column is on the order of 100 m and the penetrable bottom is composed of rough sand, mud, or soft fluid-like rock.

In many such shallow-water scenarios there are also sound speed gradients in the water column and in the bottom, and these gradients are not the same in magnitude. This generates a sound speed cusp along the seafloor. Furthermore, the gradients in the sound speed may even experience discontinuities within the media, and these too may occur along rough interfaces. Thus, both the surface and cusp Lamb shifts are present. To describe downrange propagation under such a scenario, we employ the quasi-first order stochastic variable density result with the sound speed cusp included. Note that Eq. (93), which adds a term associated with a variable sound speed in the half-spaces, is nominally fourth order, while the term proportional to $\ddot{\lambda}$ that is present in quasi-first order theory is nominally third order. Thus, to obtain quasi-first order theory where there are parameter jumps and sound speed cusps, we should simply combine the boundary conditions shown in Eqs. (40) and (103). In order to put the results into a form suited for numerical studies, we use boundary conditions Eqs. ((P.14) and (P.20)) in lieu of those in Eq. (103). These alternate boundary conditions introduce the variables A and B:

$$\begin{aligned}
&\langle\chi_I\rangle\big|_{z=0} - \langle\chi_{II}\rangle\big|_{z=0} = 4k_0^2\langle f^2\rangle B\overline{\left[\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}\right]}_{z=0} + 4k_0^2\langle f^2\rangle A\overline{\rho\langle\chi\rangle}\Big|_{z=0} \\
&\underbrace{-B\overline{\left[\frac{1}{\rho}\left\langle \ddot{f}\frac{\partial(\delta\chi)}{\partial z}\right\rangle\right]}_{z=0} + 8k_0^2\cdot B\overline{\left[\frac{1}{\rho}\left\langle f\frac{\partial(\delta\chi)}{\partial z}\right\rangle\right]}_{z=0}}_{\text{Diffuse (Bragg) scatter terms}} + 4^{\text{th}}\text{ order.} \\
&\frac{1}{\rho_I}\frac{\partial\langle\chi_I\rangle}{\partial z}\bigg|_{z=0} - \frac{1}{\rho_{II}}\frac{\partial\langle\chi_{II}\rangle}{\partial z}\bigg|_{z=0} = \underbrace{A\langle\ddot{f}\overline{\delta\chi}\rangle_{z=0} - 8k_0^2A\langle f\overline{\delta\chi}\rangle_{z=0}}_{\text{Diffuse (Bragg) scatter terms}} \\
&-4k_0^2\langle f^2\rangle A\overline{\frac{\partial\langle\chi\rangle}{\partial z}\bigg|_{z=0}} - 4k_0^2\langle f^2\rangle B\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}_{z=0} + B\langle f\cdot\ddot{f}\rangle\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}_{z=0} \\
&+k_0^2\langle f^2\rangle\left[\frac{\partial[\mu_I]}{\partial z}\bigg|_{z=0} - \frac{\partial[\mu_{II}]}{\partial z}\bigg|_{z=0}\right]\langle\chi\rangle\big|_{z=0} - \frac{\langle\dot{f}^2\rangle}{4}\left[\frac{\partial[\mu_I]}{\partial z}\bigg|_{z=0} - \frac{\partial[\mu_{II}]}{\partial z}\bigg|_{z=0}\right]\langle\chi\rangle\big|_{z=0} \\
&+4^{\text{th}}\text{ order},
\end{aligned} \tag{104}$$

where

$$A = \frac{1}{8\rho_{II}}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right) \quad ; \quad B = \frac{\delta\rho}{8k_0^2}.$$

As in Section 4.3 (specifically, the discussion leading to Eq. (82)), we now drop the terms associated with diffuse (Bragg) scattering. Furthermore, as discussed at the end of Section 5.3.4, we also drop the terms proportional to the second and third derivatives of the stochastic field $\langle\chi\rangle$.The latter is a good approximation for shallow grazing angles. Here in Section 5.4, as we are considering long-range ducted propagation in a shallow-water environment, mode-stripping rapidly eliminates any high-grazing angle modes, leaving us only with shallow-grazing angle modes. Thus, in the present context it is perfectly legitimate to eliminate the wide-angle terms proportional to second and third derivatives of the stochastic field $\langle\chi\rangle$. The result of these approximations is

$$\begin{aligned}
&\langle\chi_I\rangle\big|_{z=0} - \langle\chi_{II}\rangle\big|_{z=0} = 4k_0^2\langle f^2\rangle A\overline{\rho\langle\chi\rangle}\Big|_{z=0} + 4^{\text{th}}\text{ order.} \\
&\frac{1}{\rho_I}\frac{\partial\langle\chi_I\rangle}{\partial z}\bigg|_{z=0} - \frac{1}{\rho_{II}}\frac{\partial\langle\chi_{II}\rangle}{\partial z}\bigg|_{z=0} = \\
&-4k_0^2\langle f^2\rangle A\overline{\frac{\partial\langle\chi\rangle}{\partial z}}\bigg|_{z=0} + k_0^2\langle f^2\rangle\left[\frac{\partial[\mu_I]}{\partial z}\bigg|_{z=0} - \frac{\partial[\mu_{II}]}{\partial z}\bigg|_{z=0}\right]\langle\chi\rangle\big|_{z=0} \\
&-\frac{\langle\dot{f}^2\rangle}{4}\left[\frac{\partial[\mu_I]}{\partial z}\bigg|_{z=0} - \frac{\partial[\mu_{II}]}{\partial z}\bigg|_{z=0}\right]\langle\chi\rangle\big|_{z=0} + 4^{\text{th}}\text{ order.} \\
&A = \frac{1}{8\rho_{II}}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right) \quad ; \quad B = \frac{\delta\rho}{8k_0^2}.
\end{aligned} \tag{105}$$

Next, let us relate this result to the acoustic pressure field. Let us define a new field $w \equiv \left(\sqrt{H}\right)^{-1}\chi$. Now

$$\left[\left(\sqrt{H}\right)^{-1}, H\right] = \left[\left(\sqrt{H}\right)^{-1}, \sqrt{H}\sqrt{H}\right] = \sqrt{H} - \sqrt{H} = 0,$$

and so w obeys the same wave equation and consequently the same boundary conditions as does χ. Also note that in the half-spaces, we have

$$\sqrt{\frac{\rho}{\rho_0}}\left(\sqrt{H}\right)^{-1}\chi = A = \sqrt{\frac{\rho}{\rho_0}}\cdot w.$$

Thus, with the usual choice $\rho_0 = \rho_{II}$, in Region I we have

$$\sqrt{\frac{\rho_I}{\rho_{II}}}\cdot w_I = A_I,$$

and in Region II, $w_{II} = A_{II}$. Now, let us define a new field by multiplying w by the constant $\sqrt{\rho_{II}/\rho_I}$:

$$\tilde{w} = \sqrt{\frac{\rho_{II}}{\rho_I}} \cdot w \,.$$

The field $\tilde{w}$ obeys the same PE and the same boundary conditions as w and χ, and in Region I it is equal to the pressure field: $\tilde{w}_I = A_I$. Taking stochastic averages, we now have $\langle \tilde{w}_I \rangle = \langle A_I \rangle$, where $\langle \tilde{w}_I \rangle$ obeys boundary conditions (Eq. (105)). This effectively means that we are free to apply boundary conditions (Eq. (105)) directly to the stochastic acoustic field $\langle A \rangle$ in Region I (the water column). In other words, given the initial acoustic field in Region I, we *implicitly* convert to $\langle \tilde{w}_I \rangle$, propagate and then perform the (trivial) conversion back to the acoustic field $\langle A_I \rangle$. To perform the conversion from $\langle \tilde{w}_{II} \rangle$ to $\langle A_{II} \rangle$, we would have to multiply by $\sqrt{\rho_{II}/\rho_I}$, but we will not need this at present.

Boundary conditions (Eq. (105)) apply to a stochastic quasi-planar rough surface. It is important to appreciate that there is a fundamental difference between scattering from this kind of rough interface and a simpler problem such as, for example, propagation through a simple penetrable wedge. A theory describing the wedge problem can be checked against an analytical solution. On the other hand, recalling the discussion in Section 2.3, we know that theories describing rough surface scattering phenomena, such as diffuse (Bragg) scattering and the Lamb shift, cannot be similarly benchmarked against closed-form solutions. Like chaos, these phenomena appear when analytical solutions are not available. The validity of the theories and numerical implementations related to such phenomena must somehow be evaluated by comparing existing stochastic data sets (taken either in the field or in the laboratory) to ensemble averages of deterministic calculations, or (a little more easily) to stochastic theories. The classical Lamb shift given by boundary conditions (Eq. (105)) is a stochastic result that can be used in this manner. Thus, it is useful to employ boundary conditions (Eq. (105)) to simulate this phenomenon for typical values of the relevant environmental parameters, and then examine the feasibility of using experimental results to validate the theory.

5.4.2 A Numerical Study

Ralph Baer of NRL has conducted such a study. His calculations are based on the NRL Range-dependent Acoustic Model (RAM) PE code [92], a standard PE code in widespread use today. Baer incorporated boundary conditions (Eq. (105)) into this code, and used the result to simulate the classical Lamb shift for a realistic shallow water environment. The results are presented in Fig. 18. In Fig. 18(a), we show a typical shallow water sound speed profile, where a cusp (i.e., a knee in the sound speed profile) is advected by internal waves, and the interface between the water (light gray area) and the bottom (dark grey area) is stochastically rough. A typical water-column depth is 100 m. The internal waves are given stochastically by the Garret-Munk spectrum, and the bottom roughness by a spectrum typically taken from the work of Darrell Jackson [93-96] or Essen [97]. In Fig. 18(b), the transmission loss (TL) as a function of range is graphed for a simple example. The solid line corresponds to the traditional theory, while the dashed line is the result when the classical Lamb shift is included. The range shown varies from 24 to 25 km. The source and receiver depths are both 50 m — i.e., midway in the water column. In this particular example, the sound speed varies linearly from 1500 m/s at the flat air-sea boundary to 1530 m/s at the rough bottom. The bottom roughness is characterized by the two-dimensional spectrum $S(k) = \left(0.002 \text{ m}^4\right) \cdot \left(h_0 k\right)^{-3.5}$ (with $h_0 = 1$), which is then used to calculate $\langle f^2 \rangle$ and $\langle \dot{f}^2 \rangle$. These values are then brought over to the one-dimensional problem. The peak of the bottom spectrum k_p is assumed to be $k_p = 0.1 \text{ m}^{-1}$ (corresponding to a period in the undulations along

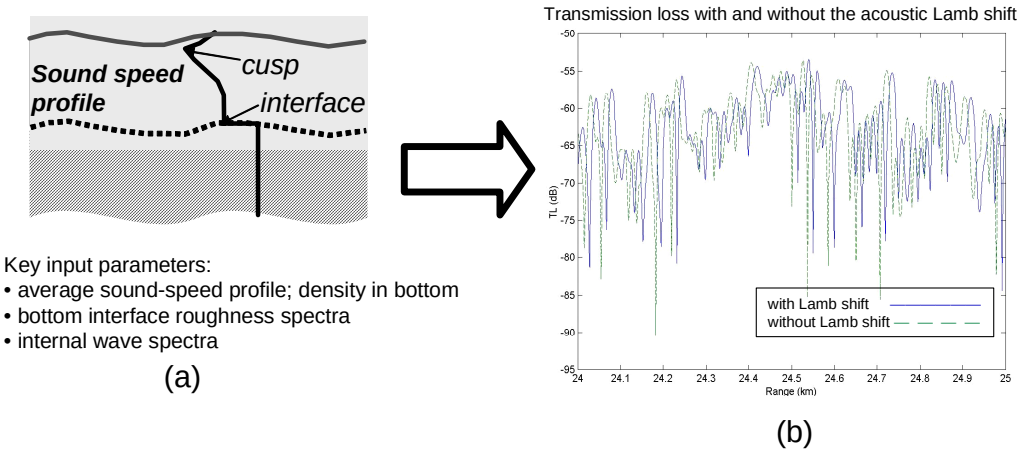


Fig. 18 — (a) A typical shallow water sound speed profile, where a cusp (i.e., a knee in the sound speed profile) is advected by internal waves, and the interface between the water (light gray area) and the bottom (dark gray area) is stochastically rough. (b) The transmission loss as a function of the range is graphed for a simple example in a realistic shallow water environment: a 100 m-deep water column over a rough sandy, muddy, or fluid-like rock bottom. Typical values are used for the various environmental parameters involved. (The precise values are laid out in the text.) The solid line corresponds to the traditional theory, while the dashed line is the result when the classical Lamb shift is included. For this example, note that there is no cusp advected by internal waves; but there is a cusp at the rough bottom. Note that the classical Lamb shift illustrated above resembles a spatial shift. The actual Lamb shift is in the downrange wave number, and after downrange propagation, this translates approximately into a spatial shift (the different modes are shifted by different distances, and so overall there is a little more going on than a simple spatial shift). When mode stripping eliminates all but a very small number of modes, this spatial shift becomes clearly defined as seen above. Ralph Baer performed this calculation.

the bottom on the order of 60 m). The sound speed in the bottom is a constant 2000 m/s, and the density in the bottom is 1.5 times the density of water. For this particular example, note that there is no cusp advected by internal waves; but there is a cusp at the rough bottom.

5.4.3 The Significance of the Results

The Lamb shift appears for all types of rough interfaces, and in principle its effect can be quite large. Examining Fig. 18(b) it is immediately apparent that the classical Lamb shift, at least in this typical case, represents a spatial shift. As discussed in the figure caption, this is no surprise since the actual shift is in the downrange wave numbers, and after propagation this translates into a shift in the pattern of the transmission loss as a function of the range. Unfortunately, in underwater acoustics, such a shift may be relatively difficult to measure since both the field and the environment are usually sampled only intermittently. The best way to measure the acoustic Lamb shift would be to isolate modes and look for roughness-induced changes to the beat frequency between pairs of low modes. This effect could be most easily measured in the laboratory. Such an experiment would certainly be instructive and have scientific value, but from the point of view of systems development, it may not be of crucial importance, since the directly analogous phenomenon has been measured in the quantum problem. On the other hand, interface waves (i.e., localization) associated with the Lamb-shift effect near (stochastically advected) cusps could have significant practical applications, and the full development of our understanding of such phenomena will require further study.

Furthermore, as noted at the end of Section 5.3.3, the curvature-induced (for a parameter jump) and tilt-induced (for a cusp) boundary waves that we have found in the *deterministic* problem are related to acoustic Biot-Tolstoy boundary waves and these have also been observed in the laboratory [86-90]. This effect is probably quite small, but this assertion also requires further study.

In the context of underwater acoustics, an additional value of considering the acoustic Lamb shift lies in the role it plays as a thought experiment that establishes the validity of the techniques being employed. Detailed experiments on the hydrogen atom have established the atomic Lamb shift as a bona fide physical effect. This experience teaches us that the δ-functions spawned by the PE derived using the FW transformation are associated with real physical effects rather than being unfortunate artifacts that compromise the PE.

Significantly, our study of the Lamb shift also exposes the role that these contact potentials can play specifically in the context of multiscale rough surface scattering. As discussed in Section 4.4, the Lamb shift phenomena associated with the hydrogen atom and a sound speed cusp — and from Eq. (103) apparently also that associated with a density jump — all include both a dominant contribution due to "smearing" (i.e., the "transverse Lamb shift proportional to $k_0^2 \left\langle f^2 \right\rangle$) and a vacuum polarization correction (i.e., the "downrange Lamb shift" proportional to $\left\langle \dot{f}^2 \right\rangle$). (In the hydrogen atom, there is also a third contribution associated with an anomalous magnetic moment, but this does not occur in acoustics.) The vacuum polarization effect in particular is a true "broad spectrum" rough surface effect (i.e., one that involves all scales from the largest down to the limits of the uncertainty principle — about 1/12 of a wavelength). Thus, our consideration of the Lamb shift, both atomic and acoustic, tells us that the δ-functions generated by the FW transformation play an indispensable role in bringing together the many scales involved in the full rough surface scattering problem. The techniques that accurately describe this effect can then be used with confidence to model more important aspects of the rough surface scattering problem. We will shortly see that introducing a density jump leads to new FW-generated δ-functions (i.e., boundary conditions) that are directly relevant to the problem of underwater propagation near rough ocean bottoms.

6. BRAGG-SCALE VORTICITY

This section addresses an important phenomenon associated with density jumps — Bragg-scale vorticity. This effect is much more important than the classical Lamb shift (let alone its small "vacuum polarization" component). In Section 6.1, the effect is defined, and then brought into the PE formalism. Although Bragg-scale vorticity enters the acoustic problem in a way that evokes no *direct* analogies from atomic physics, the mathematical formalism built up to this point imposes a specific procedure for incorporating this effect. The effects associated with Bragg-scale vorticity emerge naturally when the high-order PE generated by the FW procedure is applied to an interface where the density jumps. The second-order PE at the interface is analyzed below, and the subtle mechanics associated with the formalism are discussed. The result is then placed into the context of current PE techniques in Section 6.2. Section 7 adapts the formal approach developed for the acoustic field with varying density to the electromagnetic and elastodynamic problems.

6.1 The $\mathrm{O}\left(\lambda^2\right)$ Parabolic Equation at an Interface Where the Density Jumps

In Section 6.1.1, we consider the range-independent problem and identify a discontinuity in the transverse component of the energy flux that occurs when the density jumps along a horizontal interface, but is not included in the first-order theory developed in Sections 5.3.1 and 5.3.2. At the conclusion of this section, we note that higher orders of the theory must somehow account for this missing effect. This

is quite subtle, so Section 6.1.2 opens the discussion with an intuitive overview of how the formalism goes about constructing a solution. Section 6.1.3 supplements this with a discussion of the physical significance of our formal results. This section identifies the underlying physical effect, Bragg-scale vorticity. This has prepared us for Section 6.1.4, a systematic formal treatment of the second-order ($\mathrm{O}\left(\lambda^2\right)$) range-dependent problem where the density jumps. The resultant boundary conditions given in Eq. (120) are the most important results of this report. Section 6.1.4 also examines how the new physical effect, Bragg-scale vorticity, appears in the formalism. It also discusses how a step function in the downrange flux can gradually materialize as higher orders are added. This includes a discussion of the role played by noncommutivity relations that enable the migration of boundary conditions. Section 6.1.5 addresses the formal role that the "vacuum polarization" terms play in recreating the full wave problem, where the density jumps. Section 6.1.6 underlines the distinction between the two effects newly incorporated by the FW procedure: Bragg-scale vorticity and "vacuum polarization."

6.1.1 The Basic Issue

In Section 5.4, as our examination of the classical Lamb shift neared its conclusion, we touched upon a result that holds great significance for our primary goals. These goals were outlined in Section 2.3: first to understand why imperfect ad hoc solutions have until now proven to be the only way to apply the PE formalism to a range-dependent interface where the density jumps, and second to use this understanding to systematically improve upon the current standard PE techniques. The achievement of these goals is needed if we are to apply the PE to multiscale penetrable rough surfaces where the density jumps, which is the ultimate goal that is of the most immediate practical importance.

To be specific, new insights that advance these goals emerge from an expanded consideration of the new function briefly examined in Section 5.4: $w = \left(\sqrt{H}\right)^{-1/2}\chi$. As in that context, for the moment we consider the range-*in*dependent problem, and assume that the density jumps along a horizontal line (e.g., $z = 0$), but is (as always in our current study) constant in the half-spaces. Recall that $\sqrt{H}$ commutes with the Hamiltonian H, and so in the range-*in*dependent problem, w obeys the same wave equation, and consequently the same boundary conditions as χ itself. In simple $\mathrm{O}(\lambda)$ theory, we have continuity of χ and of $1/\rho \cdot \partial\chi/\partial z$ and the same for w and $1/\rho \cdot \partial w/\partial z$. As noted in Section 5.4, in the half-spaces, we have

$$\sqrt{\frac{\rho}{\rho_0}}\left(\sqrt{H}\right)^{-1}\chi = A = \sqrt{\frac{\rho}{\rho_0}}\cdot w$$

and with the usual choice $\rho_0 = \rho_{II}$, in Region I we have

$$\sqrt{\frac{\rho_I}{\rho_{II}}}\cdot w_I = A_I, \tag{106}$$

and in Region II, $w_{II} = A_{II}$. Substituting these results into the continuity condition for w gives us

$$\sqrt{\frac{\rho_{II}}{\rho_I}}A_I = A_{II}.$$

With $\sqrt{\rho_{II}/\rho_I}\cdot A_I - A_{II} = 0$ along the interface (i.e., the $z=0$ line), we have

$$\frac{\partial}{\partial x}\left(\sqrt{\frac{\rho_{II}}{\rho_I}}A_I - A_{II}\right) = 0 = \underbrace{\sqrt{\frac{\rho_{II}}{\rho_I}}\cdot\frac{\partial A_I}{\partial x} - \frac{\partial A_{II}}{\partial x}}_{\substack{\text{using the fact that } \sqrt{\rho_{II}/\rho_I} \\ \text{is simply a constant}}}$$

along the interface, and so continuity of $1/\sqrt{\rho}\cdot\partial A/\partial x$. Now consider the continuity condition on $1/\rho\cdot\partial w/\partial z$:

$$\frac{1}{\rho_I}\frac{\partial w_I}{\partial z} = \frac{1}{\rho_{II}}\frac{\partial w_{II}}{\partial z}. \tag{107}$$

Once again, since $\sqrt{\rho_{II}/\rho_I}$ is just a constant, we can use Eq. (106) to substitute $\sqrt{\rho_{II}/\rho_I}\cdot A_I$ for w_I in Eq. (107). Similarly, substitute A_{II} for w_{II}. This gives us

$$\frac{\rho_{II}^{1/2}}{\rho_I^{3/2}}\frac{\partial A_I}{\partial z} = \frac{1}{\rho_{II}}\frac{\partial A_{II}}{\partial z} \quad \text{or} \quad \frac{1}{\rho_I^{3/2}}\frac{\partial A_I}{\partial z} = \frac{1}{\rho_{II}^{3/2}}\frac{\partial A_{II}}{\partial z}.$$

Combining results, we have

$$\frac{A}{\sqrt{\rho}}, \frac{1}{\sqrt{\rho}}\frac{\partial A}{\partial x}, \frac{1}{\rho^{3/2}}\frac{\partial A}{\partial z} \quad \text{all continuous}. \tag{108}$$

In Appendix Q.2, these results are obtained using a variation on the above argument.

Now, let us consider the time-averaged energy flux vector [98, Eqs. (64.5 and 64.5)] and use a well known result for the time averaged product of the real parts of two complex fields; also see Eq. (C.12):

$$\vec{S}_{\text{ave}} = \frac{\text{Im}\left(A^*\vec{\nabla}A\right)}{2\rho\omega}. \tag{109}$$

Combining Eqs. (108) and (109), the PE gives us the boundary condition on the flux:

$$S_x \sim \frac{A}{\rho}\frac{\partial A}{\partial x}, \frac{S_z}{\rho} \sim \frac{A}{\rho^2}\frac{\partial A}{\partial z} \text{ all continuous}.$$

Now, let us compare this with the full wave result. In this case, we have

$$A, \frac{\partial A}{\partial x}, \frac{1}{\rho}\frac{\partial A}{\partial z} \quad \text{all continuous} \quad \Rightarrow \quad \rho S_x \sim A\frac{\partial A}{\partial x}, S_z \sim \frac{A}{\rho}\frac{\partial A}{\partial z} \text{ all continuous}.$$

Thus, although the $\text{O}(\lambda)$ (first order) PE conserves energy (the Hamiltonian is after all Hermitian), the horizontal and vertical fluxes appear to be redistributed relative to the full wave result. On the other hand, as discussed in Section 2.3, it should be possible to construct a downrange stepping algorithm that

generates a field that can be made arbitrarily close to the full-wave solution. Somehow, as we add higher orders, the correct behavior known from the full-wave result must reappear.

6.1.2 A Heuristic Approach

Let us now proceed to get a handle on how all this might fit into the formalism. First we will examine a heuristic presentation drawing in aspects of the structure suggested by the FW transformation as needed. Then Section 6.1.3 will supplement these new formal insights with a look at the underlying physical processes, and subsequently in Section 6.1.4 we will move on to a more systematic discussion that builds up directly from the formal structure generated by the FW transformation.

6.1.2.1 The Contact Potential Needed to Produce the Correct Jump in the Downrange Flux

The heuristic discussion echoes Appendix Q.2. To begin with, we follow the discussion surrounding form (Q.10) and (Q.11) in Appendix Q.2. To keep our heuristic discussion as clear as possible, let us maintain for one more section the assumption that the jump in the density occurs along the range-independent line $z = 0$. Then add to the first order Hamiltonian $H = k_0 - 2\gamma k_0 + \lambda$ an extra (energy conserving) term[eee]

$$\begin{aligned} &-\frac{1}{2k_0}\cdot\frac{\rho_0}{\rho}\gamma_I\delta'(z)\chi \\ &\gamma_I = \frac{\rho_{II}-\rho_I}{2\rho_{II}} = \frac{\delta\rho}{2\rho_{II}} \end{aligned} \quad . \tag{110}$$

(For the moment, take the expression for γ_I as a definition, but also keep in mind that the expression for γ_I given in Eq. (110) is the same as that obtained if we set the reference density to be the density in Region II — ρ_{II}, and then take the definition for γ first given in Eq. (87) (Section 5.1), and evaluate it in Region I where the local density ρ is the constant ρ_I. This result is, of course, anticipated when we use the label γ_I.)

Recall (again using the definition first given in Eq. (87))

$$\begin{aligned} \lambda &= \frac{\nabla_T \frac{\rho_0}{\rho}\nabla_T}{2k_0}\chi + \text{terms that have no } \delta\text{-functions} \\ &= \frac{\rho_0}{\rho}\frac{\nabla_T^2\chi}{2k_0} + \left[\nabla_T\left(\frac{\rho_0}{\rho}\right)\right]\frac{\nabla_T\chi}{2k_0} + \cdots \end{aligned} \quad .$$

The second term on the right-hand side of the second line contains a simple δ-function that will not survive an indefinite integration followed by an infinitesimal integration[eee]. Thus we drop this term as well as terms that contain no δ-functions. Now, we multiply through by $2k_0\cdot(\rho/\rho_0)$ and find that the key terms that generate the boundary condition on the wavefunction χ itself are

$$\nabla_T^2\chi - \gamma_I\delta'(z)\chi + \cdots .$$

[eee] Implicitly, we are again either truncating at first order or bifurcating δ-functions in order to make sense of terms that contain δ-functions times field quantities that are discontinuous.

Taking the infinitesimal integration across the interface, we have to first order

$$\chi_I - \chi_{II} - \gamma_I \chi = 0$$

or

$$\begin{aligned}
\chi_I &= \chi_{II}\left(1+\frac{\delta\rho}{2\rho_{II}}\right)+\mathrm{O}\left(\left[\frac{\delta\rho}{\rho}\right]^2\right) \\
&\approx \chi_{II}\left(1+\frac{\delta\rho}{2\rho_I}\right)+ \text{ 2nd order} \\
&\approx \chi_{II}\sqrt{1+\frac{\delta\rho}{\rho_I}} \\
&= \chi_{II}\sqrt{\frac{\rho_{II}}{\rho_I}}
\end{aligned}$$

or

$$\sqrt{\rho_I}\chi_I = \sqrt{\rho_{II}}\chi_{II} + \text{ 2nd order}, \tag{111}$$

which is indeed the boundary condition we would expect for a quantity χ that is roughly the square root of the component of the energy flux that is transverse to the interface.

Thus the term given by Eq. (110) will "fix" first-order theory. However, we cannot simply insert it into our formalism by hand. We have no control over what such a term does to the boundary condition on $\partial\chi/\partial z$ or on the other boundary conditions (i.e., conditions on $\nabla_T^n\chi; n \geq 2$ that are all implicit in first-order theory). We therefore want the term shown in Eq. (110) to *emerge naturally* from our theory. Since this term needs to be present even in the range-independent problem, it cannot emerge from a "vacuum polarization" term generated by the FW transformation such as $-\ddot{\lambda}/8k_0^2$. We must look for it in terms that are higher orders in λ, say in the term proportional to λ^2. However, note that in the context of $\mathrm{O}(\lambda^2)$ theory (with lead order term proportional to $\nabla_T^4\chi$), the term in Eq. (110) will have migrated from being a boundary condition on χ itself to being a boundary condition on $\partial^2\chi/\partial z^2$. This has an important side benefit. Actual jumps in the wavefunction cause problems, because then the x-derivative of χ would spawn a δ-function, and this in turn would lead to a very problematic feedback loop in our boundary conditions. This problem is eliminated when the term in Eq. (110) is intrinsically embedded in $\mathrm{O}(\lambda^2)$.

6.1.2.2 $\mathrm{O}(\lambda^2)$ Theory Generates the Needed Contact Potential

The term in Eq. (110) will need to emerge from cross-terms in λ^2. The $\mathrm{O}(\lambda^2)$ Hamiltonian is

$$H = k_0 - 2\gamma k_0 + \lambda - \frac{\lambda^2}{2k_0}.$$

Now, let us echo the analysis that begins with the discussion surrounding Eqs. (Q.20) and (Q.21), and continues to the end of Appendix Q.2. The leading-order derivative comes from $-\lambda^2/2k_0$:

$$-\lambda^2/2k_0 = -\left(\frac{1}{2k_0}\right)^2\left(\frac{1}{2k_0}\right)\nabla_T\left(\frac{\rho_0}{\rho}\right)\nabla_T^2\left(\frac{\rho_0}{\rho}\right)\nabla_T + \cdots .$$

Now, consider the two cross-terms in $-\lambda^2/2k_0$ that will generate δ' -functions:

$$(-1/2k_0)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}(k_0\gamma)\chi \tag{112}$$

and

$$(-1/2k_0)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}(-k_0\mu)\chi. \tag{113}$$

The term in Eq. (110) will have to emerge from these terms.

Let us examine the second term. With our usual conventions that $K_0 = K_I$ and $\rho_0 = \rho_{II}$ (useful if, for example, medium I is water and medium II is mud), we find

$$\mu \equiv \frac{1}{2}\left(1-\frac{K}{K_0}\right) = \frac{1}{2}\left(1-\frac{K}{K_I}\right),$$

and so in Region I, $\mu = 0$ and in Region II,

$$\mu = \frac{K_I - K_{II}}{2K_I} = -\frac{\delta K}{2K_I} = \mu_{II},$$

or

$$\mu_{II} = \frac{1}{2}\left(1-\frac{K_{II}\rho_{II}}{K_I\rho_{II}}\right) = \frac{1}{2}\left(1-\frac{c_0^2}{c_{II}^2}\right).$$

Thus, with the positive z -axis pointing into Region I:

$$\begin{aligned} -k_0\mu &= -\frac{k_0}{2}\Theta(-z)\left(1-\frac{c_0^2}{c_{II}^2}\right) \\ &= -\frac{k_0}{2}\Theta(-z)\left(1-\frac{c_I^2}{c_{II}^2}\frac{\rho_I}{\rho_{II}}\right), \\ &= -\frac{k_0}{2}\Theta(-z)\left(1-n_{\text{total}}^2\frac{\rho_I}{\rho_{II}}\right) \end{aligned} \tag{114}$$

where $n_{\text{total}} \equiv c_I / c_{II}$ is the perfectly standard index of refraction between the media and $\Theta(z)$ is the Heaviside step function. Now $n_{\text{total}}^2 = 1 - 2\mu_{\text{total}}$, where μ_{total} is the familiar parameter measuring the sound speed jump between the media, and

$$\frac{\rho_I}{\rho_{II}} = \frac{\rho_I}{\rho_I + \delta\rho} = \frac{1}{1 + \frac{\delta\rho}{\rho_I}} = 1 - \frac{\delta\rho}{\rho_I} + \cdots = 1 - \frac{\delta\rho}{\rho_{II}} + \cdots$$

to first order (recall our conventions $\rho_{II} - \rho_I = \delta\rho$). Thus

$$n_{\text{total}}^2 \frac{\rho_I}{\rho_{II}} = 1 - 2\mu_{\text{total}} - \frac{\delta\rho}{\rho_{II}}$$

to first order. Substituting into Eq. (114), this gives us

$$\begin{aligned} -k_0\mu &= -\frac{k_0}{2}\Theta(-z)\left(1 - \left(1 - 2\mu_{\text{total}} - \frac{\delta\rho}{\rho_{II}}\right)\right) \\ &= -\frac{k_0}{2}\Theta(-z)\left(2\mu_{\text{total}} + \frac{\delta\rho}{\rho_{II}}\right) \\ &= -k_0\Theta(-z)\left(\mu_{\text{total}} + \frac{\delta\rho}{2\rho_{II}}\right) \\ &= -k_0\Theta(-z)\left(\mu_{\text{total}} + \gamma_I\right) \end{aligned} \tag{115}$$

(where we also used the second part of Eq. (110) to obtain the last equality). We also have

$$\gamma \equiv \frac{1}{2}\left(1 - \frac{\rho}{\rho_0}\right) = \frac{\rho_{II} - \rho}{2\rho_{II}} = \begin{cases} \delta\rho/2\rho_{II} = \gamma_I & \text{in Region I} \\ 0 & \text{in Region II} \end{cases}$$

and so

$$\gamma = \gamma_I \Theta(z). \tag{116}$$

Combining Eqs. (115) and (116), we have

$$-k_0\mu + k_0\gamma = -k_0\Theta(-z)\mu_{\text{total}} + k_0\gamma_I\left[\Theta(z) - \Theta(-z)\right] \tag{117}$$

at first order for our standard example $K_0 = K_I$ and $\rho_0 = \rho_{II}$.

Next, we demonstrate that the second term in Eq. (117) will lead to the term Eq. (110). From Eqs. (112) and (113), we see that Eq. (117) gets operated on by

$$\left(-\frac{1}{2k_0}\right)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}$$

to form

$$\left(-\frac{1}{2k_0}\right)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}\left(-k_0\mu+k_0\gamma\right)=\left(-\frac{1}{2k_0}\right)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}\left(-k_0\Theta(-z)\mu_{\text{total}}\right)$$
$$+\left(-\frac{1}{2k_0}\right)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}\left(k_0\gamma_I\left[\Theta(z)-\Theta(-z)\right]\right). \tag{118}$$

Now it is the second term on the right-hand side of Eq. (118) that will reproduce the term shown in Eq. (110). This term becomes

$$-\frac{1}{2k_0}\frac{\rho_0}{\rho}\frac{1}{2k_0}\cdot k_0\gamma_I\left(\frac{\partial^2\Theta(z)}{\partial z^2}-\frac{\partial^2\Theta(-z)}{\partial z^2}\right)+\left[\begin{array}{l}\text{terms that will not survive a}\\ \text{double infinitesimal integration}\end{array}\right].$$

Note that ∇_T operating on $1/\rho$ generates a simple δ-function, which will not survive a double integration across an infinitesimal integral, and so this operation has been dropped from the present calculation. Finally use

$$\frac{\partial^2\Theta(z)}{\partial z^2}=\delta'(z)=-\delta'(-z)=-\frac{\partial^2\Theta(-z)}{\partial z^2}$$

to recover the term in Eq. (110):

$$-\frac{1}{2k_0}\cdot\frac{\rho_0}{\rho}\gamma_I\delta'(z)\chi.$$

Thus, the second cross-term given in Eq. (118) indeed generates the term in Eq. (110) associated with the discontinuity of χ. (For more on this, also see Appendix Q.2).

6.1.2.3 The Terms Introduced by $\mathrm{O}\left(\lambda^2\right)$ Theory That Are Not Associated with the Jump in the Energy Flux

The first term on the right-hand side of Eq. (118) represents the remaining contribution from the cross-terms of $-\lambda^2/2k_0$. It is quite straightforward to demonstrate that the contribution from this term recovers the implicit boundary conditions on χ that would be expected if Bragg-scale vorticity were not an issue. To be specific, in the absence of Bragg-scale vorticity, we would expect that in the range-independent problem we are considering here, the field χ would behave just like the pressure field A. It is not difficult to show that the contribution to the boundary condition generated by the first term in Eq. (118) would, if taken alone, indeed cause the boundary condition on $\nabla_T^2\chi$ to mimic the implicit boundary condition on $\nabla_T^2 A$.

Now that we have a handle on what is basically going on, Section 6.1.3 will outline the underlying physical processes responsible for all this mathematical subtlety. After this is accomplished, Section 6.1.3 will put all of this on a firmer foundation.

6.1.3 The Physical Significance

The physical significance of our findings is that the FW transformation generates a one-way stepping algorithm that incorporates bounded back and forth motion. In the case of the tilt-induced smearing associated with the new FW terms, the transformation refines out the average influence of virtual backscatter. When a density jump is introduced, the formalism contends with something new not found in the quantum problem. The velocity of the oscillating fluid is given by $\vec{\nabla}A/\rho$. Since the pressure A is continuous along the interface, so is $\left(1-\hat{n}\hat{n}\right)\cdot\vec{A}$, the component of $\vec{\nabla}\vec{A}$ tangent to the interface ($\hat{n}$ is as always the normal to the interface). Note that the component of the velocity tangent to the interface is given by

$$\vec{\mathrm{v}}_{\mathrm{tangent}} = \frac{e^{-i\omega t}}{-i\omega}\left(1-\hat{n}\hat{n}\right)\cdot\frac{\vec{\nabla}\vec{A}}{\rho}.$$

The period of oscillation $T = 2\pi/\omega$ is the same everywhere. Therefore, when ρ is discontinuous on the interface, the component of the velocity tangent to the interface must also be discontinuous. The material will move more rapidly on the side of the interface with the lower density. As the material slips along the interface, the material is displaced further on the side with the lower density[fff]. On a wavelength scale, the fluid thus picks up an oscillating twist, which is called here Bragg-scale vorticity (BSV). This vorticity is not associated with a circulation; it is just a bounded twisting oscillation. (However, the variability in ρ is enough to ensure that curl of the velocity vector is non-zero, and so this is indeed a bona fide vorticity.) Since the energy flux $\vec{S}$ is proportional to $\mathrm{Im}\left[\left(A^{*}\vec{\nabla}A\right)/\rho\right]$, Bragg-scale vorticity also forces a jump in its tangential component along the interface. This might lead us to expect that χ, a carrier of tangential or near-tangential flux along the quasi-planar interface, jumps as well.

The FW transformation takes both these bounded oscillations (i.e., virtual backscatter and Bragg-scale vorticity), refines out the average influence, and incorporates them in the forward-stepping equation. In particular, the fact that the new formalism allows us to bring the higher-order PE right up to the interface is closely tied to the fact that it incorporates Bragg-scale vorticity. At lowest order, the formalism forces the vorticity to be zero, but then it builds the vorticity order by order, intimately coupling it to the higher-order transverse derivatives. Boundary conditions on the carrier of flux χ (and on its lower order derivatives) migrate up to the boundary conditions on higher-order derivatives, where they "launch" the functions in a way that appropriately simulates the full-wave boundary conditions.

6.1.4 A Systematic Formal Discussion

6.1.4.1 The $\mathrm{O}\left(\lambda^{2}\right)$ Boundary Conditions Associated with a Sound Speed and Density Jump

Section 6.1.2 opened a window into the mechanism used by the PE to address the discontinuities associated with a density jump. Then, Section 6.1.3 provided an insight into the physical issues involved, and an argument outlining why the FW procedure addresses this physical process in a way that is in significant respects similar to the way it handles the classical equivalent of the "vacuum polarization" effect. Now, let us pull all of this together into a systematic formal discussion.

[fff] Note that the relative displacement becomes greater as the density jump increases or the frequency ω decreases. In this sense, the effect is similar to torsion in elastic solids.

Begin with the $\mathrm{O}\left(\lambda^2\right)$ PE generated by the FW transformation (this is obtained by truncating Eq. (92) of Section 5.3.1 or in this case, equivalently, Eq. (90) of Section 5.1):

$$-i\frac{\partial\chi}{\partial x}=k_0\left(1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}\right)\chi. \tag{119}$$

Once again, as we focus on the interface itself, consider the one-dimensional interface embedded in two-dimensional space (i.e., no y-dependence and $\partial/\partial z \leftrightarrow \nabla_T$). The interface is now once again allowed to be range-dependent (e.g., $z=f\left(x\right)$). In Appendix Section Q.1, it is shown that this Hamiltonian produces the boundary conditions

$$\begin{aligned}
&\tfrac{1}{2k_0}\left[\alpha_I^2\nabla_T^3\chi_I-\nabla_T^3\chi_{II}\right]+k_0\alpha_I\gamma_I\nabla_T\chi_I+k_0\mu_{II}\nabla_T\chi_{II}=0\\
&\tfrac{1}{2k_0}\left[\left(1+2\alpha_I\gamma_I\right)\nabla_T^2\chi_I-\nabla_T^2\chi_{II}\right]+k_0\left(\mu_{II}+\gamma_I\right)\chi=0\\
&\tfrac{1}{\rho_I}\nabla_T\chi_I=\tfrac{1}{\rho_I}\nabla_T\chi_{II}\\
&\chi_I=\chi_{II}.
\end{aligned} \tag{120}$$

As always, the reference density is on Region II and the reference compressibility is on Region I. (Thus, $\gamma_I=\left(\rho_{II}-\rho_I\right)/\left(2\rho_{II}\right)$, $\mu_{II}=-\left(K_{II}-K_I\right)/\left(2K_I\right)$ and $\gamma_{II}=\mu_I=0$. We also have $\alpha_I=\left[\rho_0/\rho\right]_I=\rho_{II}/\rho_I$. For a boundary between the water column and the sea bottom, Region I would typically be the water, and Region II would be the bottom.) Note that we do not include the $O\left(\dot{f}^2,\ddot{f}\right)$ (and higher order) "vacuum polarization" terms at this stage, since here we are considering them to be third order (and higher) with each *downrange* derivative of λ adding an order. Equation (120) is the most important result in this entire endeavor.

Let us take a quick look at how the result (Eq. (120)) comes about. We instantly see that the cross-terms in λ^2 will in principle generate δ- and δ'-functions, but not higher-order derivatives of the δ-function. Therefore, taking two and three improper integrations followed by a proper integration over an infinitesimal transverse interval straddling the interface, we immediately obtain the above continuity conditions on $\left(1/\rho\right)\cdot\nabla_T\chi=\left(1/\rho\right)\cdot\partial\chi/\partial z$ and χ, respectively. Take one improper integration and then integrate over the infinitesimal interval to obtain the boundary condition for $\nabla_T^2\chi$ $\left(=\partial^2\chi/\partial z^2\right)$. Take one integration over the infinitesimal interval to obtain the boundary condition on $\nabla_T^3\chi$. The leading order derivative $\nabla_T\left(1/\rho\right)\nabla_T^2\left(1/\rho\right)\nabla_T\chi$ as well as the cross-terms $\nabla_T\left(1/\rho\right)\nabla_T\mu\chi$ and $\nabla_T\left(1/\rho\right)\nabla_T\gamma\chi$ contribute to the last two results.

6.1.4.2 Relating the PE Boundary Conditions to the Full-wave Result

Looking at the boundary conditions on χ and $\nabla_T\chi$, one might conclude that χ simply mimics the full pressure field A in our PE formalism. This, of course, cannot be, because we know from our full-wave result that A should be continuous, while Bragg-scale vorticity should produce a discontinuity in χ. As illustrated in Section 6.1.2, the higher-order boundary conditions begin to correct this situation by introducing Bragg-scale vorticity. Let us examine this a little more closely. The first two boundary conditions in Eq. (120) above can be rewritten in the form

$$\begin{aligned}
&\tfrac{1}{2k_0}\left[\alpha_I^2\nabla_T^3\chi_I - \nabla_T^3\chi_{II}\right] - k_0\alpha_I\gamma_I\nabla_T\chi_I + k_0\mu_{II}\nabla_T\chi_{II}\boxed{+2k_0\alpha_I\gamma_I\nabla_T\chi_I} = 0\\
&\tfrac{1}{2k_0}\left[\nabla_T^2\chi_I - \nabla_T^2\chi_{II}\right] + k_0\left(\mu_{II} - \gamma_I\right)\chi\boxed{+2k_0\gamma_I\chi + \tfrac{\alpha_I\gamma_I}{k_0}\nabla_T^2\chi_I} = 0.
\end{aligned} \tag{121}$$

Here the $\nabla_T^2\chi$ and the $\nabla_T^3\chi$ boundary conditions are presented in a way to illustrate which part is needed to reproduce the full wave behavior, and which part comes from "extra" terms that reproduce Bragg-scale vorticity. As demonstrated in Appendix Subsection Q.2, boundary conditions containing only the terms outside the boxes are those that would hold if χ truly mimicked A. The terms in the boxes come from the δ- and δ'-functions formally generated by the cross-term $\nabla_T\left(1/\rho\right)\nabla_T\gamma\chi$ and from the part of $\nabla_T\left(1/\rho\right)\nabla_T\mu\chi$ that is not needed to generate the portion of the boundary conditions on $\nabla_T^3\chi$ and $\nabla_T^2\chi$ that mimic the (implicit) boundary conditions on $\nabla_T^3 A$ and $\nabla_T^2 A$.

If we take, for example, the δ'-function responsible to first order for the extra part of the $\nabla_T^2\chi$ boundary condition: $\left(-1/2k_0\right)\alpha\gamma_I\delta'\left(z - f(x)\right)$, and insert it by hand into the first-order Hamiltonian, the required first-order jump in the carrier of downrange flux χ is indeed generated (for details, recall Section 6.1.2 or see the last paragraph of Appendix Q.2). However, note when this same cross-term remains in O(λ^2) theory (where it truly belongs), this δ'-function modifies the $\nabla_T^2\chi$ boundary condition rather than the χ boundary condition. Thus, as predicted at the end of Section 6.1.3, the boundary condition on χ has indeed migrated to become a boundary condition on $\nabla_T^2\chi$. Thus, we once again encounter an interesting example of the topic of migrating boundary conditions first raised in Section 4.2.2[ggg]. This reminds us that the following result is very widely applicable: Quite generally, we must take seriously the notion that a boundary condition is really a δ-function-type term, and that the effects associated with such a term will migrate to boundary conditions associated with derivatives of different order as the leading order of the differential equation is changed.

This then tells us something about what the PE derived using the FW transformation is doing at an interface where the density jumps. Although higher-order theory introduces the effects of Bragg-scale vorticity, the boundary conditions will still force χ and $\left(1/\rho\right)\nabla_T\chi\left[=\left(1/\rho\right)\left(\partial\chi/\partial z\right)\right]$ to be continuous. The step is smoothed as the FW transformation builds it as a distribution. (Recall that in distribution theory, the step function is built up as a sequence of continuous functions that progressively approaches the profile of a step. A sequence of arctangent functions is typically employed in this manner.) The boundary conditions on the higher-order derivatives launch the field at the interface in such a way that a step function is built up. Effectively, the interface is allowed to expand to fill the space allowed by the uncertainty principle, and the bare interface is buffered (or "fuzzed out"). This type of smoothing imposed by a one-way (i.e., non-relativistic) theory has a precedent. For example, [99 (especially the first full paragraph of p. 948)]: A point charge in Dirac theory becomes in nonrelativistic theory a distribution of charge and current extending over a domain of linear dimensions $\hbar/mc$. The Darwin term and spin-

[ggg] It is worthwhile at this point to remind ourselves of examples of boundary condition migration that we have previously encountered. Recall from the discussion in Section 4.2.2 that, similarly, the contact potential associated with cusp-induced Lamb shift really corresponds to boundary conditions on the third derivative of the wave function, but when it is put into the lowest order PE (or Schrödinger equation), it nominally corresponds to a jump in the first derivative. The classical Lamb shift generated by an interface (e.g., for a fluid, where the sound speed and/or the density jump(s)) is ultimately to be associated with the Helmholtz-equation boundary conditions on $\nabla_T^2\chi$, but in $\mathrm{O}(\lambda)$ theory it generates a jump in χ.

orbit interaction are consequences of this "fuzzing out" or buffering of the bare particle. (In quantum mechanics, this is also sometimes known as "dressing" the singularity.)

However, this raises an interesting issue. As just noted, when we keep on increasing the order of our PE by repeatedly applying the FW procedure, the behavior of the field χ should approach that of a step function in much the same way that a series of arctangent functions approaches the Heaviside step function in generalized function theory (i.e., distribution theory). This implies that χ becomes rapidly varying near the interface, and consequently that the lower order derivatives of the wave function should become large. For example, at some point in the process of moving to ever-higher order, $\nabla_T^2 \chi$ and so also the expansion parameter λ would have to become quite large. Nevertheless, this type of "convergence in the generalized sense" to a step function can still be reconciled with the notion that both the generator of the FW transformation and the "left behind" off-diagonal elements are getting smaller as we move to higher and higher order. The reason is as follows. The expansion parameters λ^n and $\lambda^m \gamma^{n-m}$ are always small when they are actually being used to generate a FW transformation[hhh]. The higher orders left in the off-diagonal (odd) operator are small as well. After the diagonalizing FW procedure "has passed through" a given order n, then λ^n and $\lambda^m \gamma^{n-m}$ now operating on a new higher-order wave function $\tilde{\chi}$ may become large, but by this time they no longer function as expansion parameters.

6.1.4.3 The Role of Noncommutivity in Boundary Condition Migration

It is very interesting to note that the key structural condition that makes all of this possible is the fact that λ no longer commutes with the Hamiltonian:

$$[\lambda, H] \neq 0 .$$

When this is the case, there is nothing to tie the value, of say, $\lambda\tilde{\chi}$ to $\lambda^n\tilde{\chi}$ or of $\lambda\tilde{\chi}$ from an earlier iteration to $\lambda\tilde{\chi}$ from a later iteration. Thus, $\lambda\tilde{\chi}$ can be small in low-order theory, and then later become large at higher orders. Furthermore, at the higher order where $\lambda\tilde{\chi}$ is big, our formalism still allows $\lambda^n\tilde{\chi}$ to be small.

In fact, the noncommutivity of λ and H allows orders of the PE to change the behavior of χ in a number of fundamental ways. For example, it is a necessary condition for the boundary conditions to migrate. Indeed, in the case of the variable density acoustic PE, we have just found that boundary conditions are allowed to migrate even in the absence of range dependence. This follows from the fact that $[\lambda, \gamma] \neq 0$ and so $[\lambda, H] \neq 0$. Similarly, when we add the new "vacuum polarization" terms generated by the FW transformation (and associated with range dependence), here also we find that these new terms end the commutivity of λ with H since $\left[\lambda, \ddot{\lambda}\right] \neq 0$.

[hhh] I.e., when they are the actual expansion parameters embedded within the generator of the FW transformation S — see Section 3.1 and Eq. (12); and note that S is proportional to $\tilde{\mathcal{O}}$, the current odd operator in the Hamiltonian left after some given number of iterations of the FW procedure, and that $\tilde{\mathcal{O}}$ contains operators of the form λ^n and $\lambda^m \gamma^{n-m}$ as well as operators with higher overall powers of λ-γ. Note that for the moment, we are temporarily reverting to the tilde (~) notation to remind ourselves that the current wavefunction $\tilde{\chi}$ and the currently remaining odd operator $\tilde{\mathcal{O}}$ have emerged from repeated applications of the FW transformation, and not just from the original ansatz.

On the other hand, boundary conditions cannot migrate in the constant-density range-*in*dependent problem where the sole expansion parameter λ commutes with the Hamiltonian H. In this case, higher orders only add new explicit boundary conditions, but they cannot change the boundary conditions at lower orders. Let us examine why this is so. Since the commutator $[\lambda, H]$ is now zero and there is no range dependence, we could decompose the field χ into eigenvectors χ_j and replace the dimensionless operator λ/k_0 with the eigenvalues ε_j and then $(\lambda/k_0)^n$ with ε_j^n [iii]. Then if λ/k_0 and ε_j are small, so are $(\lambda/k_0)^n$ and ε_j^n. Thus, we can no longer have the behavior where high orders of λ/k_0 are small while low orders are large. Furthermore, δ-functions and other singularities *within each term* of the form $(\lambda/k_0)^n \chi_j = \varepsilon_j^n \chi_j$ must all cancel one another internally[jjj]. It follows that increasing the order of the PE can generate new boundary conditions, but it cannot modify boundary conditions previously obtained at a lower order. Recall that in Appendix K.1.1.2, this insight was used to verify that δ-function bifurcation employed in the $\mathrm{O}(\lambda^3)$ PE for a sound speed jump (and, of course, constant density) correctly reproduced the implicit boundary conditions on higher-order derivatives of the wave function. Also note that since boundary conditions obtained at low orders remain fixed, and higher orders only serve to supplement these conditions with new boundary conditions affecting higher-order derivatives, it follows that boundary conditions can no longer migrate in this case. In this sense, the boundary conditions generated by each order in λ decouple.

For weak range dependence, we would in general not expect large deviations from the conclusions based on the assumption that there is no range dependence. However, recall that, as noted above, for a sound speed jump where the density is the same everywhere ($\delta\rho = 0$), the only thing that allows boundary conditions to migrate is the fact that range dependence adds new terms via the FW transformation, and these force the crucial commutator to become non-zero: $[\lambda, H] \neq 0$. Thus, the new "vacuum polarization" terms have introduced a fundamental change in the nature of the Hamiltonian H.

6.1.5 Tying Together "Vacuum Polarization" with Bragg-scale Vorticity and a Look at Other Future Extensions of the Results

6.1.5.1 Understanding the $O(\ddot{\lambda})$ Terms Introduced by the Foldy-Wouthuysen Transformation

Only now that we have established the predominant factor involved in the boundary conditions, Bragg-scale vorticity, and the related $\mathrm{O}(\delta\rho)$ jump in the carrier of flux χ, are we truly ready to go back and generalize to the variable density (i.e., $\delta\rho \neq 0$) problem the discussion in Section 4.2.1, and establish the meaning of the $\mathrm{O}(\ddot{f}, \dot{f}^2)$ "vacuum polarization" terms contributed to the deterministic problem by FW transformation.

[iii] By switching to the dimensionless operator λ/k_0, we ensure that the corresponding eigenvalues ε_j are also dimensionless. This allows us to unambiguously label the eigenvalues ε_j as small.

[jjj] This is ultimately the reason why contact potentials are allowed in the context of the PE. Similarly, it is also why we can have a $1/r$ potential in the atomic Schrödinger equation and still have the overall operator $-\nabla_T^2/2m + V$ remain small.

The tilt-induced terms proportional to $\dot{f}^2\left(\delta K/K_0 - \delta\rho/\rho_0\right)$ play a role that is essentially the same as that played by the $\dot{f}^2\mu$-term in the constant density discussion of Section 4.2.1; they are related to the boundary conditions for $\nabla_T^2 A$ (where A is as always the pressure field).

The "new" term proportional to $\delta\rho\cdot\dot{f}^2\cdot\delta'(z-f)$ is related to the jump in χ, which in turn is related to the jump in downrange flux, recalling that χ is roughly speaking a carrier of downrange flux in the sense that to within a integration by parts, $|\chi|^2$ is proportional to $\frac{1}{\rho}\mathrm{Im}\left(A^*\cdot\partial A/\partial x\right)$, which is in turn also proportional to the downrange flux. The effects of this term can already be seen in first-order theory. On the other hand, the other "new" term proportional to $\delta\rho\cdot\dot{f}^2\cdot\delta''(z-f)$ only kicks in at $\mathrm{O}\left(\lambda^2\right)$, and this one is related to corrections to the $(1/\rho)\cdot\partial A/\partial z$ boundary condition.

As before in Section 4.2.1, the terms proportional to the curvature $\ddot{f}$ lead to local curvature-induced boundary phenomena such as boundary waves (cf. polaritons in electromagnetic waves).

6.1.5.2 A Term in the Full-wave Problem that is Implicit in the PE Formulation

The $\mathrm{O}\left(\dot{f}\cdot\delta\rho\right)$ contribution to the downrange flux that exists in the full-wave problem apparently does not enter the PE via an explicit term contributed by the FW transformation. Instead, the $\mathrm{O}\left(\dot{f}\cdot\delta\rho\right)$ contribution intrinsically migrates up to the highest order derivative of χ (e.g., in quasi-first-order theory of the sort considered throughout Section 3, the $\nabla_T^2\chi$ term), where it is introduced via the implicit boundary condition on $H\chi$. Note that the tendency of the $\mathrm{O}\left(\dot{f}\cdot\delta\rho\right)$ term to migrate to higher order is not very different from the behavior of the $\mathrm{O}(\delta\rho)$ terms introduced by Bragg-scale vorticity. Both cases reflect the tendency of the PE to force the auxiliary field χ to remain continuous.

6.1.5.3 Future Extensions Beyond $\mathrm{O}\left(\lambda^2\right)$ or $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$ Theories

As before in the constant density case of Section 4.2.1, we have just now seen that also when the density jumps (i.e., $\delta\rho\neq 0$), we will need at least $\mathrm{O}\left(\lambda^2,\ddot{\lambda}\right)$ theory to fully understand all the "vacuum polarization" (i.e., $\propto\dot{f}^2,\ddot{f}$) terms. In fact, for the variable density case (i.e., $\delta\rho\neq 0$), we even have a term proportional to $\delta''(z-f)$ that does not contribute at all to quasi-first-order (i.e., $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$) theory. Therefore, future $\mathrm{O}\left(\lambda^2,\ddot{\lambda}\right)$ or even $\mathrm{O}\left(\lambda^3,\ddot{\lambda}\right)$ theories in both their deterministic and stochastic versions will be interesting and worthwhile, but we will leave this synthesis to future work. Furthermore, we will even defer for future work a consideration of the stochastic version of the basic $\mathrm{O}\left(\lambda^2\right)$ theory of Bragg-scale vorticity (which would of course include diffuse (Bragg) scattering). For the near term, we will concentrate on the acoustic Lamb shift based on stochastic quasi-first-order $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$ theory (minus diffuse scattering) separately and in isolation from the Bragg-scale vorticity based on deterministic second-order $\mathrm{O}\left(\lambda^2\right)$ theory (which implicitly includes diffuse scattering).

Furthermore, recall that we have all along assumed that ρ does not vary in the half spaces. Thus, we have not yet allowed for the possibility that there may be steps in $\nabla_T \rho$ and in $\nabla_T^2 \rho$ at the interface. Such singularities will lead to new Lamb-shift-type stochastic effects on the coherent field even in basic first-order (i.e., $O(\lambda)$) theory. In the future, this possibility will need to be examined as well. Finally, all these versions of the theory will have to be thoroughly compared to data.

6.1.6 The Distinction Between Bragg-scale Vorticity and the Lamb Shift

It is appropriate to close our examination of Bragg-scale vorticity by clearly reviewing the distinctions between this effect and the classical Lamb shift. The latter already occurs for first-order (i.e., $O(\lambda)$) theory, or if we want to include the classical equivalent of the vacuum polarization correction, quasi-first-order (i.e., $O(\lambda, \ddot{\lambda})$) theory. It modifies the coherent field near stochastic quasi-planar surfaces, where the sound speed, sound speed gradient, and/or density jump. The effect takes the form of contact potentials, which modify the boundary conditions, and there is a close analogy to the Lamb shift problem of atomic physics. The validity of the new physics predicted by the FW transformation is confirmed by the relationship between the new FW term for a scalar field and the phenomenon of vacuum polarization known from atomic physics. It is relatively easy to incorporate the acoustic Lamb shift into existing codes, and so this has been the first (and so far only) aspect of the new theory to be numerically implemented (see Section 5.4).

Bragg-scale vorticity occurs at a density jump, and it is associated with second-order (i.e., $O(\lambda^2)$) and higher theory. It applies most dramatically to diffuse (Bragg) scatter and to the deterministic problem. The proper incorporation of Bragg-scale vorticity involves a basic restructuring of existing PE codes, and there is no immediate quantum analogy. On the other hand, Bragg-scale vorticity is of greater importance than the classical Lamb shift for modeling acoustic fields since it addresses the problem that has ultimately motivated this effort: that of properly applying the PE to a tilted interface where the density jumps (see Section 2.3 for a discussion of why this is so important). Furthermore, as we see in Section 7, jumps in electric and magnetic permeability (in electromagnetic theory) and in the second Lamé parameter (in the theory of elastic waves) involve similar issues. The development of new PE codes that include Bragg-scale vorticity will thus have a high priority in the future. However, since they will have to be developed from scratch, the development of these codes will not be pursued in the current effort, but will instead be deferred to follow-on work.

6.2 Comparison to the Currently Popular Parabolic Equation Techniques of Tappert and Collins

This section uses the new formalism developed in this report to reexamine the two PE methods first mentioned in Section 2.2. These are currently the preferred techniques for describing range-dependent interfaces with density jumps. In Section 6.2.1, the new formalism is used to examine Tappert's technique of changing the variable and smearing out the interface, and in Section 6.2.2, Collins' stair step technique is examined in light of the new formalism. Section 6.2.3 summarizes the relative merits of these approaches and serves to guide the modeler toward the optimal method in a given context.

6.2.1 Tappert's Change of Variable Formalism

The change of variable (COV) method by Tappert briefly described in Section 2.2 (see also Ref. 15, pp. 262-264) rests on the observation that in the full-wave Eq. (1), one can change the wavefunction to $u = A/\sqrt{\rho}$ (i.e., make a change of variables from $A \rightarrow A = \sqrt{\rho} \cdot u$). This leads to a standard Helmholtz equation for u with a new effective index of refraction. Now, one can proceed as before to

create a new PE. The discussion surrounding Eq. (19) demonstrates that this, like any other PE, will actually propagate an auxiliary wave χ:

$$\chi \propto \sqrt{H}\cdot u = \sqrt{H}\cdot\frac{A}{\sqrt{\rho}} = \sqrt{-i\frac{\partial}{\partial x}}\cdot\frac{A}{\sqrt{\rho}}.$$

χ is immediately recognizable as a carrier of flux (if this is not clear, see Eq. (97) and the related discussion). The Hamiltonian that propagates this field is a Hermitian (i.e., magnitude-conserving or "stable") Hamiltonian, and so $|\chi|^2$ and consequently the downrange flux are conserved quantities, and it follows so is the energy.

The result obtained using the COV technique anticipates that obtained using the FW transformation, but with a key difference that becomes important in the interface limit. For the substitution $A \to \sqrt{\rho}\cdot u$, the expansion parameter $\mu_{\text{effective}} = \left(1-n_{\text{effective}}^2\right)\big/2$ picks up δ-functions in the interface limit. The COV formalism therefore becomes too singular in this limit. The FW approach effectively differs from the COV approach in that it takes the factor of $1\big/\sqrt{\rho}$ in the auxiliary wave function $u = A\big/\sqrt{\rho}$ and expands it in $2\gamma = \left(\rho_0-\rho\right)\big/\rho_0 = -\Delta\rho/\rho_0$. This slows down convergence enough so that δ-function bifurcation can be used to evaluate those previously troublesome terms that involve products of distributions at interfaces. More specifically, the Helmholtz equation generated by the COV substitution can be properly interpreted even at an interface, provided that one properly expands in $2\gamma = -\Delta\rho/\rho_0$ and then uses δ-function bifurcation to evaluate the result (Appendix K.2.1.2 shows how things begin to work out). Proceeding along these lines, a PE similar to that generated by the FW transformation could then in principle be obtained from the Helmoltz equation containing δ-function potentials. Such a PE would effectively buffer the density jump[kkk]. In summary, the COV substitution becomes too singular in the interface limit, while the FW procedure smoothes out the discontinuity in the density ρ by interjecting an extra expansion in $\Delta\rho/\rho_0$. In principle, the COV technique could be applied to an interface by introducing this expansion by hand.

On the other hand, if the COV formalism is to be applied directly to an interface without such additional modifications that bring it into line with the FW formalism, then the interface must be *artificially* smoothed. Tappert originally adopted this ad hoc approach and it has been used since. Since the formalism generated by the FW transformation effectively smoothes the surface in a manner precisely determined by field theory, it is clearly the proper way to handle a true interface. On the other hand, there are many instances in nature where the transition from one medium to another is very gradual on the order of a wavelength, and in such instances, there is no advantage to slowing down convergence by interjecting an extra expansion. The substitution proposed and developed by Tappert would then work very well, and indeed it would likely be the better approach.

Finally, note that Tappert's COV technique shares an important physical insight with the result predicted by the FW transformation. A central result of the procedure based on the FW transformation is that the density discontinuity is buffered. The COV technique reconciles the PE with a density jump by smoothing out the interface. At least at low orders, the two pictures are quite similar, implying that the

[kkk] I.e., as discussed in Section 6.1.4, the PE would replace the (discontinuous) step in the downrange flux with a distribution (i.e., a sequence of continuous functions) that only approaches the step function (at least to within the tolerance of the uncertainty principle) in the limit as the PE goes to ∞ order. This is similar to the effect that would be produced by "fuzzing out" the density jump.

COV technique was based on a very profound physical insight: that the key to reconciling the PE with the issues associated with a density jump lies in buffering the interface. The new technique generated by the FW transformation represents an advance since it automatically introduces this smoothing in a manner dictated by a precise physical theory, rather than by fiat.

6.2.2 Collins' Stair Step PE

6.2.2.1 The Stair Step PE Exploits Several Attributes of the Range-independent Problem

The current state of the art PE (Stair Step PE) developed primarily by Collins and Westwood [18] builds on a very clean solution to the truly range-independent problem. As long as an interface is *completely flat* (i.e., range-independent), designing an appropriate PE is perfectly straightforward — even when the density jumps ($\delta\rho \neq 0$). In the range-independent environment, this PE can be written by taking the square root of the wave equation:

$$\left[\frac{\partial^2}{\partial x^2} + \rho\nabla_T \tfrac{1}{\rho}\nabla_T + k^2\right] A = 0 \Rightarrow$$

$$-i\frac{\partial A}{\partial x} = \sqrt{k_0^2 + \rho\nabla_T \tfrac{1}{\rho}\nabla_T - k_0^2\left(1-n^2\right)}\cdot A,$$

$$= k_0\sqrt{1+\tfrac{2\lambda}{k_0}}\cdot A$$

where

$$\lambda \equiv \frac{\rho\nabla_T \frac{1}{\rho}\nabla_T}{2k_0} - k_0\frac{1-n^2}{2},$$

and A is the pressure field. Note that this operator λ is not quite the same as the one we have been using in the context of the FW procedure — in fact, it is not strictly speaking Hermitian. However, energy is nevertheless conserved for this PE. We can see this as follows: first, note that the operator $\sqrt{H}$ commutes with H and $\partial/\partial x$, and so in this range-independent scenario we can use the same Hamiltonian to propagate the auxiliary field defined by

$$v \equiv \sqrt{H}\cdot A = \sqrt{-i\,\partial/\partial x}\cdot A.$$

At all finite orders of the expansion in λ, this Hamiltonian is Hermitian *with respect to* the metric $\int \frac{dR_T}{\rho}$ (recall that dR_T is a differential element in transverse space: $dR_T = dydz$). Thus,

$$\frac{\partial}{\partial x}\int \frac{dR_T}{\rho}|v|^2 = \int \frac{dR_T}{\rho}\left[\underbrace{\frac{\partial v^*}{\partial x}}_{\left(\partial v/\partial x\right)^*}\cdot v\right] + \int \frac{dR_T}{\rho}\left[v^*\cdot\frac{\partial v}{\partial x}\right]$$

$$= \int \frac{dR_T}{\rho}\left[\left(iHv\right)^*\cdot v\right] + \int \frac{dR_T}{\rho}\left[v^*\cdot iHv\right]$$

$$= i\int \frac{dR_T}{\rho}\left[-\left(Hv\right)^* v + v^* Hv\right] \underbrace{=}_{\text{Use Hermiticity under the metric}} 0$$

Thus, the total downrange flux (which is to within one integration by parts proportional to $\int \frac{dR_T}{\rho}|v|^2$), is conserved, as is the energy.

In a typical implementation of the stair step PE, one only uses the lowest order boundary conditions: continuity of A and of $(1/\rho)(\partial A/\partial z)$. One could in principle use higher-order boundary conditions by explicitly imposing the boundary conditions that are implicit in full-wave theory. Such an approach would use the technique developed earlier in Section 3.3.2 (i.e., force the grid to fall on the interface, and then use the boundary conditions to generate the derivatives that go into the Hamiltonian needed for downrange stepping). However, this approach is not used in the standard implementation of the Stair Step PE. Instead, as discussed in footnote kk and Ref. 69, one instead places the interface in between two grid points, then overlaps the upper and lower half-spaces by extending each out beyond the interface by one extra grid point, and then uses the two boundary conditions of $O(\lambda)$-theory to solve for the field at the extra (nonphysical) points. The extra points are used to calculate the second transverse derivative in the first-order Hamiltonian, which is the one used to generate downrange stepping right at the surface. Unfortunately, this method does not readily generalize to higher-order theory, and so higher-order theory has not typically been used in conjunction with the stair step PE. In a typical implementation, one converts from the higher-order PE to first-order theory in a narrow band surrounding the interface.

The Stair Step PE has one clear advantage over the PE generated by the FW transformation. It exploits the fact that when the problem is truly range-independent[lll], it is possible to take the square root of the wave equation and propagate the pressure A directly. Now the continuity condition is applied to A and not to the auxiliary field χ, so *Bragg-scale vorticity is present from the beginning and the Stair Step formalism does not need to work to generate it.* Furthermore, keep in mind that although it has not been done in the past, there is no a priori reason why boundary conditions that are implicit in full-wave theory could not be made explicit to generate a higher-order version of the range-*in*dependent Stair Step PE. Thus, Collins' Stair Step PE is clearly the method of choice when the interface is completely range-independent.

6.2.2.2 Range-dependence in the Context of the Stair Step PE

Let us now examine how this picture changes when range-dependence is introduced (i.e., when the interface acquires tilt and curvature). As always, energy conservation is maintained by conserving the downrange flux S_x. Conservation of the downrange flux S_x is achieved by conserving $\sqrt{S_x} \propto \sqrt{1/\rho \cdot (\partial/\partial x)} \cdot A \propto \sqrt{H/\rho} \cdot A$. This conservation rule must be explicitly applied globally along the entire transverse space and not just in the immediate vicinity of the interface. This procedure has the same effect as applying the endpoint transformation to go from the pressure field A to the carrier of flux χ, then applying the first boundary condition generated by the FW theory (continuity of χ), and then transforming back to A.

As noted in Section 2.2, forcing downrange-energy-flux conservation at a vertical interface leads to a discontinuity of the pressure field, while the boundary conditions imposed along the horizontal interface demand pressure continuity. This leads to an unphysical discontinuity in the pressure at the corners of the stair step, which in turn spawns Gibbs oscillations. The Gibbs oscillations are buffered by introducing waves that are evanescent in the downrange direction (i.e., k_x is imaginary). As noted towards the end of Appendix B, evanescent waves cannot be propagated using the finite-order PE expansions of the sort

[lll] An environment is truly range-independent if the sound speed and density profiles are independent of the range *r* and all interfaces are flat (i.e., have zero slope).

generated by the FW transformation since the expansion parameter $k_z/k_0 > 1$. However, the exact square-root operator can be inserted into the Hamiltonian by hand, and this is indeed what is done by introducing complex Padé coefficients into the Hamiltonian. The evanescent waves do not harm energy conservation, because they have no downrange flux, but they contribute to the total field and participate in the boundary conditions along the horizontal interface for some distance behind a step (until they decay to insignificance). For example, while they restore continuity of the field A at the step, as in the method based on the FW transformation, the *actual physical (propagating) waves* remain *discontinuous* near a range-dependent interface. In other words, the *propagating component of the field* — as opposed to the total field consisting of both the propagating component and the evanescent waves — continues to obey the same first boundary condition as that imposed by the FW procedure. The evanescent waves also carry vertical flux and contribute the second boundary condition (i.e., that on the derivative of the field $\partial A/\partial z$). Among other things, this has the effect of modifying the effective boundary condition on the derivative of the *downrange propagating component* of the field. In fact, the set of evanescent waves can be chosen so that at a step the *propagating field* precisely obeys the second boundary condition demanded by FW theory as well as the first boundary condition.

Note that once again as with the PE generated by the FW transformation and with an implementation of the change of variable technique near an interface, the density discontinuity is effectively buffered in the context of the Stair Step PE — this time by evanescent waves. Thus we see that by employing physical intuition and by addressing practical considerations imposed on them, both Tappert and Collins anticipated the key philosophical insight that emerges from the technique based on the FW transformation.

6.2.2.3 Comparing the Stair Step PE with that Generated by the FW Transformation

We have just established that the Stair Step PE effectively goes over to first-order FW theory at the vertical interface, and then gradually fades back to the range-independent theory as the evanescent waves decay. Thus, the Stair Step PE is in essence a hybrid that combines lowest-order FW theory with the range-independent theory. It is ideally suited for cases where the range dependence is modest (i.e., where there is relatively little wavelength-scale roughness). Indeed, as already noted above, along a truly range-independent (horizontal) interface, the Stair Step PE correctly generates jumps in the downrange flux already at first order, and so if the interface is flat or very nearly so, the Stair Step PE should be *better* than the one generated by the FW procedure[mmm]. Whenever the interface is locally flat and the evanescent waves have all died out, the Stair Step method could be improved even further by imposing the implicit boundary conditions on the higher-order derivatives, and then using the procedure outlined in Section 3.3.2 to evaluate higher-order Hamiltonians.

For a multiscale rough surface (especially one that induces Bragg scattering), the PE crosses the interface very frequently. If the interface increments to a new level frequently enough, then the evanescent waves never die off, and the Stair Step PE essentially remains first-order of the theory generated by the FW transformation[nnn]. Under such a scenario, the theory generated by the FW transformation has several advantages:

- It is only necessary to perform the transformations from $A \to \chi$ and back again from $\chi \to A$ once at the endpoints rather than at each step.

[mmm] To be specific, in this case it would take fairly high orders of the PE generated by the FW transformation to match the accuracy of the Stair Step PE.

[nnn] Note that changing the vertical and horizontal step size will not change this analysis. The decay range of the evanescent range is determined by the size of the vertical step, but not that of the horizontal step. On the other hand, if we reduce the size of the vertical step, then we have to step more often and generate evanescent waves more often.

- It is not necessary to insert the evanescent waves by hand; their presence is inferred by the nature of the boundary conditions on χ.
- The second boundary condition of FW theory effectively selects out an optimal subset of allowable evanescent solutions.
- In the FW theory, it is possible to obtain higher orders[ooo]. At higher orders, the "on-shell" unphysical evanescent waves are replaced by "off-shell" virtual particles ("off-shell" solutions do not have to follow the Helmholtz equation, just the higher-order PE)[ppp]. These produce a field that eventually agrees with the full wave result to within the tolerance of the uncertainty principle.

Note that the first two bullets imply that the approach based on the FW transformation is more efficient. Furthermore, taken as a whole, these four advantages suggest that the theory based on the FW transformation is the best method for modeling the scattering from multiscale rough surfaces (e.g., diffuse (Bragg) scatter).

A potentially useful hybrid theory would employ Stair Step PE (Collins' method) along relatively smooth surfaces until the surfaces become so rough that steps in the interface become frequent; at that point, the algorithm would go over to the theory based on the FW transformation. This should be developed in future research.

6.2.3 Overview of Available Methods

It is now possible to examine the range of validity of the various approaches to modeling propagation in a duct with rough quasi-planar interfaces[qqq]. The COV approach by Tappert (Section 6.2.1) is best when changes to the density really are gradual (on the scale of a wavelength), even in the vertical direction. The Stair Step PE by Collins (Section 6.2.2) is the best theory to use when the interface is range independent (i.e., without tilt or curvature), and it continues to be the method of choice if the range dependence is modest (i.e., the interface is slowly varying on the order of a wavelength). When quasi-planar rough surfaces (with features of a wavelength and less) are present, then the theory based on the FW transformation is the best one to use. This is also a good general theory that can credibly be applied to the previous two scenarios as well as to the rough-interface problem for which it was designed. Since the FW approach is systematic, it includes higher orders, and so it can be adjusted to deal with larger density jumps than can alternatives that do not have this capability.

For completeness, it is also appropriate that we briefly note two other methods used to model ducted acoustic propagation: double sweep methods and the method of coupled modes. These are used, for example, if vertical interfaces are present and/or there is an interest in calculating backscatter. Coupled modes are also particularly useful in considering scenarios such as the fluid elastic interface where the

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[ooo] Some of the evanescent waves are not physical (since, for example, they do not appear in the full-wave solution where a plane wave hits a tilted interface without curvature). The correct higher-order theory should make the non-physical evanescent waves disappear as the higher orders are added. Thus, nothing would be gained, for example, by simply imposing the higher-order implicit boundary conditions for the full wave on the combined evanescent wave/propagating wave solution. It follows that although Collins' technique can be extended to higher orders along a truly range-independent interface, there is no way to introduce the higher-order boundary conditions at the stair steps. The new theory based on the FW transformation must then be used.

[ppp] For "off-shell" waves, the magnitude of the wave vector does not need to equal $k = \omega/c$ as demanded by the Helmholtz equation (or its generalization for the variable density problem). Such solutions are allowed, because the higher-order PE has many extra derivatives (compared with the Helmholtz equation), and it ceases to operate precisely like the standard wave equation. By contrast, an "on-shell" wave has a wave vector with a magnitude that is compatible with the given Helmholtz equation.

[qqq] In this report, the terms "waveguide" and "duct" are more or less used interchangeably. For some authors, waveguides are associated with an arrangement of impenetrable interfaces that confine and direct the propagation of a wave and ducts with environmental profiles that achieve a similar effect without the presence of interfaces.

(zero) speed of secondary waves in the fluid create a (dimensionless) PE expansion parameter of one (see Section 7.2).

For an overview and comparison of available methods for propagating classical fields propagating through a ducted environment in the presence of rough interfaces, see Table 3. Tappert's and Collins' approaches are discussed in Sections 2.2, 6.2.1, and 6.2.2. Bremmer's approach is discussed in Ref. 20. Modes with rough boundaries have been extensively discussed by Kuperman, Schmidt, and collaborators [65, 100-104]. The approach used is a hybrid between mode theory and perturbative rough surface scattering theory. The use of impedance boundary conditions to characterize propagation through waveguides with rough boundaries has been examined by Berman [105, 106].

Table 3 — The Optimal Use of the Various Approaches for Modeling Downrange Propagation in a Ducted Environment

<table>
<tr><th>Underlying Approach</th><th>Method</th><th colspan="2">Optimal Use</th></tr>
<tr><td rowspan="8">Parabolic Equation</td><td>Tappert's approach
(uses new field variable $u = A/\sqrt{\rho}$)</td><td colspan="2">Density changes as a function of the range and depth really are gradual</td></tr>
<tr><td rowspan="2">Stair Step PE (Collins [1991])
(use range independent theory + conserve energy at interface steps; use evanescent solutions to eliminate Gibbs oscillations)</td><td colspan="2">Interface is allowed to vary but there is little wavelength-scale roughness (density jumps allowed)</td></tr>
<tr><td colspan="2">May be adequate for wavelength-scale roughness</td></tr>
<tr><td rowspan="4">Theory based on the Foldy-Wouthuysen transformation
(developed systematically using canonical transformations; can be extended to higher orders)</td><td colspan="2">A good general theory that can credibly be applied to both the scenarios above</td></tr>
<tr><td colspan="2">Stochastic Problem</td></tr>
<tr><td colspan="2">If 2nd order correction is needed</td></tr>
<tr><td colspan="2">Quasi-planar penetrable rough interfaces (Bragg scattering and density jumps allowed)</td></tr>
<tr><td>Double Sweep
(Bremmer Series: uses full wave solution locally at the interface; uses PE to propagate between vertical interfaces)</td><td>⇑
We are interested in backscatter</td><td>⇑
Vertical interfaces</td></tr>
<tr><td rowspan="2">Full Wave</td><td rowspan="2">Coupled Modes
These become numerically expensive unless the range dependence is very modest
For aspects of the stochastic rough surface component of the approach, see Kuperman, Schmidt.</td><td>⇓</td><td>⇓</td></tr>
<tr><td colspan="2">Very large jumps in the physical parameters
[rough surfaces are treated by stochastic theory and this component of the range-dependence effectively goes away; other range dependence (e.g., from deterministic large scale features) is modest – otherwise the approach becomes very expensive]</td></tr>
<tr><td>Impedance boundary conditions
(Berman)</td><td colspan="2">Range-dependence is stochastic
Applies to backscatter</td></tr>
</table>

7. SIMILAR EFFECTS IN THE ELECTROMAGNETIC AND ELASTODYNAMIC PROBLEMS

This section adapts the formal approach developed for the acoustic field with varying density to electromagnetic and elastodynamic (i.e., elastic) wave propagation. These results will be very useful since there are currently unresolved issues in applying such vector field PEs to tilted interfaces, and the results have many possible applications, including fiber optics, radio/radar (these involve electromagnetic fields), and seismology (which involves elastic waves). Electromagnetic fields are considered in Section 7.1 and elastic waves are examined in Section 7.2.

The discussion below sets up the problem by deriving the state space equation and taking a brief look at the transformations connecting the familiar full-wave fields with the associated auxiliary fields that are propagated by the PE. Full development of the theory for the sake of practical implementations will not be pursued below. However, beginning with the state space equation and the transformation between the two fields (i.e., between PE and full-wave fields), it should be a strictly mechanical procedure to fully develop the theory. Indeed, the first-order PE can be immediately read off: it is simply the even part of the state space equation.

It turns out that jumps in electric and magnetic permeability (in electromagnetic theory) and in the second Lamé parameter (in the theory of elastic waves) will involve issues that are similar to those associated with density jumps in the acoustic problem (i.e., the issues associated with Bragg-scale vorticity).

7.1 The Electromagnetic Field

7.1.1 The Foldy-Wouthuysen Ansatz for the Electromagnetic Field

The discussion at the beginning of Appendix I provides general guidelines for constructing an ansatz that will lead to a state space equation that is a suitable starting point for the FW transformation. Following these guidelines, the FW ansatz for the electromagnetic field is (in MKS units):

$$\underset{\sim}{\Phi} = \begin{pmatrix} \vec{\theta}_T \\ \vec{\chi}_T \end{pmatrix} = \frac{1}{2}\left(\vec{H}_T \pm \sqrt{\tfrac{\varepsilon_0}{\mu_0}}\hat{x} \times \vec{E} \right), \tag{122}$$

where ε_0 is the reference electric permittivity and μ_0 is the reference magnetic permeability. As always, the x-axis denotes the downrange direction. The subscript T indicates that the given vector only includes components in the transverse (i.e., y-z) dimensions. $\vec{H}_T$ is the projection in (transverse) y-z space of the magnetic field $\vec{H}$ and $\vec{E}$ is the electric field. The underlying tilde in $\underset{\sim}{\Phi}$ serves to remind us that this quantity now has four rather than two components. To within a constant, $\underset{\sim}{\Phi}$ is indeed a carrier of the flux:

$$\underset{\sim}{\Phi}^{\dagger}\underset{\sim}{\Phi} = \vec{\theta}_T^{\,*} \cdot \vec{\theta}_T - \vec{\chi}_T^{\,*} \cdot \vec{\chi}_T = 2\left(\tfrac{\varepsilon_0}{\mu_0}\right)^{1/2} \vec{S}_{\text{ave}} \cdot \hat{x}\,, \tag{123}$$

where, as before, $\vec{S}$ is the time-averaged energy flux associated with the field, and $S_x \equiv \vec{S} \cdot \hat{x}$ is its downrange component.

7.1.2 The State Space Equation for the Electromagnetic Field

This ansatz is used to generate the state space equation. This equation involves the following operators:

$$\begin{aligned} \lambda^{jk} &\equiv \begin{Bmatrix} \frac{1}{2k_0}\vec{\nabla}_T^i\left(\frac{\varepsilon_0}{\varepsilon}\right)\vec{\nabla}_T^i\delta^{jk} - \frac{1}{2k_0}\vec{\nabla}_T^k\left(\frac{\varepsilon_0}{\varepsilon}\right)\vec{\nabla}_T^j \\ -\frac{1}{2k_0}\vec{\nabla}_T^j\left(\frac{\mu_0}{\mu}\right)\vec{\nabla}_T^k + \frac{k_0}{2}\left(\frac{\delta\mu}{\mu_0} - \frac{\delta\varepsilon}{\varepsilon_0}\right)\delta^{jk} \end{Bmatrix}, \\ \gamma^{jk} &\equiv -\frac{1}{2k_0^2}\vec{\nabla}_T^j\left(\frac{\mu_0}{\mu}\right)\vec{\nabla}_T^k - \frac{1}{2}\frac{\delta\varepsilon}{\varepsilon_0}\delta^{jk} \end{aligned} \tag{124}$$

where $k, j \in (1,2)$ label the transverse directions y and z, δ^{jk} is the Kronecker delta, and

$$\begin{aligned} \delta\varepsilon &= \varepsilon - \varepsilon_0 \\ \delta\mu &= \mu - \mu_0 \\ k_0 &= \frac{\omega}{c_0} = \omega\sqrt{\varepsilon_0\mu_0} \end{aligned} \quad .$$

$\underline{\lambda}$ and $\underline{\gamma}$ are 2×2 matrix operators. To remind us that they are no longer scalars, they are underlined.

As derived in Appendix R.1, the state space equation for the electromagnetic field is

$$i\begin{pmatrix} \partial\vec{\theta}_T^{\,j}/\partial x \\ \partial\vec{\chi}_T^{\,j}/\partial x \end{pmatrix} = \left[\lambda^{jk} \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\xi} + \left(\lambda^{jk} - 2k_0\gamma^{jk}\right) \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta} + k_0\delta^{jk} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta} \right] \begin{pmatrix} \vec{\theta}_T^{\,k} \\ \vec{\chi}_T^{\,k} \end{pmatrix}. \tag{125}$$

This result assumes that the free current $\vec{J}_f$ is zero (i.e., the material is nonconducting). It would not be difficult to incorporate the correction for a linear isotropic conductor such that $\vec{J}_f = \sigma\vec{E}$.

Note that in Eq. (125) we have included the definitions for ξ and η (Eqs. (8) and (11)). The odd and even operators are now 4×4 matrices defined by the outer products

$$\begin{aligned} \underset{\sim}{\mathcal{O}} &= \underline{\lambda} \otimes \xi \\ \underset{\sim}{\mathcal{E}} &= \left(\underline{\lambda} - 2\underline{\gamma}\right) \otimes \eta \end{aligned} .$$

To remind ourselves that the odd and even operators are now 4×4 rather than 2×2 matrices, these operators are now underlined with a tilde $\sim$. Recalling that $\underset{\sim}{\Phi}$ is a 4-component vector, the state equation can be written in the standard form (cf. Eq. (9))

$$i\frac{\partial\underset{\sim}{\Phi}}{\partial x} = \left(\underset{\sim}{\mathcal{O}} + \underset{\sim}{\mathcal{E}} + k_0 1 \otimes \eta\right)\underset{\sim}{\Phi} .$$

Just as for the Dirac equation (and harking back to the discussion just above Eq. (16) in Section 3.1), the even and odd properties of $\underset{\sim}{\mathcal{O}}$ and $\underset{\sim}{\mathcal{E}}$ are defined by their commutation properties vis-à-vis the block diagonal

$$\begin{pmatrix} 1_{2\times 2} & 0 \\ 0 & -1_{2\times 2} \end{pmatrix}. \tag{126}$$

To avoid confusion, the corresponding one-way Hamiltonian will not be denoted by H, but by the underlined 2×2 matrix operator $\underline{\mathbb{H}}$ (its matrix character is denoted by the underline and the font is used to clearly distinguish the Hamiltonian $\underline{\mathbb{H}}$ from the magnetic field $\vec{H}$). Although it is now a 4×4 matrix operator, the 2-way Hamiltonian will still be denoted by $\mathcal{H}$.

7.1.3 The Transformation Between the Auxiliary Field $\vec{\theta}_T$ and the Magnetic Field $\vec{H}_T$

Next, we examine the approximate transformation connecting the transverse component of the familiar full-wave magnetic field $\vec{H}_T$ with the corresponding auxiliary field $\vec{\theta}_T$ that is associated with downrange propagation by the PE. As shown in Appendix R.2, the two fields are approximately connected by the equation

$$\vec{\theta}_T = \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} \frac{1}{\sqrt{\varepsilon_0\left(1+\frac{\delta\varepsilon}{\varepsilon_0}\right)\omega}} \left[k_0\sqrt{1+\frac{2\hat{\lambda}}{k_0}} - \vec{\nabla}_T \frac{1}{k_0\sqrt{1+\frac{2\hat{\lambda}}{k_0}}} \vec{\nabla}_T \right]^{1/2} \cdot \vec{H}_T , \tag{127}$$

where

$$\hat{\lambda} \equiv \frac{\nabla_T^2}{2k_0} + \frac{k_0}{2}\left(\frac{\delta\varepsilon}{\varepsilon_0}\frac{\delta\mu}{\mu_0} + \frac{\delta\varepsilon}{\varepsilon_0} + \frac{\delta\mu}{\mu_0}\right). \tag{128}$$

Note that $\hat{\lambda}$ is similar to other scalar λ's defined above, but does not precisely match any of them. To properly use Eq. (127), expand in $\delta\varepsilon/\varepsilon_0$ and $\hat{\lambda}$ to get a finite-order transformation. The downrange component of the magnetic field H_x and the electric field $\vec{E}$ can be deduced from $\vec{\theta}_T$ (or more generally $\vec{\theta}_T - \vec{\chi}_T$ if the uprange field $\vec{\chi}_T$ is non-zero) and $\vec{H}$, respectively, using Maxwell's equations[rrr].

Equation (127) (with definition in Eq. (128)) neglects the range- and transverse- (e.g., vertical) dependence of ε and μ *locally in the immediate vicinity of the point in space where the transformation is performed.* We usually only need to transform between the physical field $\vec{H}_T$ and the PE field $\vec{\theta}_T$ at the endpoints of the propagation. The endpoints of the propagation are at the values of the range and transverse coordinates, where the source and receiver are located. Elsewhere, the field is only "passing through," and only the auxiliary field $\vec{\theta}_T$ is needed. In other words, Eq. (127) (with definition in Eq (128)) applies in a typical implementation, where we only transform between $\vec{H}_T$ and $\vec{\theta}_T$ at a source or receiver, and additionally have ε and μ slowly varying in the immediate neighborhood of the source and receiver. Equation (127) also assumes that the material is a linear and isotropic such that $\mu\vec{H} = \vec{B}$, where $\vec{B}$ is the magnetic induction. As with the PE (Eq. (125)), it is assumed that the free current $\vec{J}_f$ is zero (i.e., the material does not conduct).

Note that this transformation does not involve near-eigenvalues, so it will have to evaluated even in the range-independent case. In fact, the behavior of the field $\vec{\theta}_T$ can be quite different from that of $\vec{H}_T$. However, as shown at the end of Appendix R.2, if we have very shallow grazing angles such that $\vec{\nabla}_T$ is effectively "small," then we have a "minimal correction":

$$\vec{\theta}_T = (\mu/\varepsilon)^{1/4}\vec{H}_T + \mathrm{O}\left(\frac{\nabla_T^2}{k_0^2}\right). \tag{129}$$

[rrr] E.g., Eq. (R.6) (derived using Maxwell's equations) gives $H_x \propto \vec{\nabla}_T \cdot \left(\vec{\theta}_T - \vec{\chi}_T\right)$, and we also have $\vec{\nabla}\times\vec{H}/i\omega\varepsilon = \vec{E}$ (assuming that the conductivity is zero); see Eq. (R.1) for a list of Maxwell's equations.

For almost all materials $\mu \approx \mu_0$, and so $\mu^{1/4}$ effectively acts like a constant that cancels at the endpoints. In this case, the minimal correction is $\vec{\theta}_T = (1/\varepsilon)^{1/4} \vec{H}_T$.

7.2 The Elastodynamic Field

7.2.1 The Foldy-Wouthuysen Ansatz for the Elastic Field

The basic environmental parameters that will appear in this treatment of the elastodynamic problem are[sss]

$$\begin{aligned}
&\vec{u} = \text{displacement vector} \quad \omega = \text{frequency} \quad \rho = \text{density} \\
&\lambda, \mu \text{ are Lamé parameters} \\
&c^s = \sqrt{\tfrac{\mu}{\rho}} = \text{ speed of shear waves} \quad c^p = \sqrt{\tfrac{\lambda+2\mu}{\rho}} = \text{ speed of pressure waves} \\
&\vec{\tau}^{ij} = \text{ stress tensor} = \lambda\left(\vec{\nabla}\cdot\vec{u}\right)\delta^{ij} + \mu\left(\nabla^i u^j + \nabla^j u^i\right) \\
&\lambda_0, \mu_0, \tilde{\mu}_0 \text{ are reference values for the Lamé parameters (usually } \mu_0 = \tilde{\mu}_0) \\
&\rho_0 \text{ is reference density} \\
&c_0^s = \sqrt{\tfrac{\mu_0}{\rho_0}} \quad c_0^p = \sqrt{\tfrac{\lambda_0+2\tilde{\mu}_0}{\rho_0}}.
\end{aligned} \tag{130}$$

Once again, we use the discussion at the beginning of Appendix I to guide us in constructing an ansatz that will lead to a state space equation that is a suitable starting point for the FW transformation. The appropriate ansatz for elastodynamic waves is

$$\begin{pmatrix} \vec{\theta} \\ \vec{\chi} \end{pmatrix} = \frac{1}{2}\left(\vec{u} \pm \frac{i}{\omega\rho_0 c_0^s} \hat{x}\cdot\vec{\tau} \right). \tag{131}$$

Equation (131) must be multiplied by $\sqrt{\omega\rho_0 c_0^s}$ to form a true carrier of the flux.

7.2.2 The State Space Equation

The state space equation for the elastodynamic field will also involve a number of additional parameters derived from the environmental parameters in Eq. (130):

$$\begin{aligned}
&n^s = \frac{c_0^s}{c^s}, \quad n^p = \frac{c_0^p}{c^p}, \quad n_0^{sp} = \frac{c_0^s}{c_0^p} \\
&k_0^s = \frac{\omega}{c_0^s} \\
&\left(n^s\right)^2 \frac{\rho_0}{\rho} = \frac{\mu_0}{\mu} \\
&\left(n^p\right)^2 \frac{\rho_0}{\rho} = \frac{\lambda_0 + 2\tilde{\mu}_0}{\lambda + 2\mu}
\end{aligned}$$

[sss] Note that dispersive effects take the form of complex components to environmental parameters such as the density and the Lamé parameters (i.e., the sound speeds).

These quantities are used to define a set of operators that appear in the state space equation. Some will play a familiar role and are labeled accordingly:

$$\lambda^{jk} \equiv \left\{ \begin{array}{c} \frac{1}{2\omega\rho_0 c_0^s}\left(\vec{\nabla}_T^{\,j}\left(\frac{2\lambda\mu}{\lambda+2\mu}\right)\vec{\nabla}_T^{\,k} + \vec{\nabla}_T^{\,i}\mu\vec{\nabla}_T^{\,i}\left(\delta^{jk}-\delta^{0j}\delta^{0k}\right) + \vec{\nabla}_T^{\,k}\mu\vec{\nabla}_T^{\,j}\right) \\ -\frac{k_0^s}{2}\left(1-\frac{\rho}{\rho_0}\right)\delta^{jk} + \frac{k_0^s}{2}\left(1-n_s^2\frac{\rho_0}{\rho}\right)\left(\delta^{jk}-\delta^{j0}\delta^{0k}\right) \\ +\frac{k_0^s}{2}\left(n_0^{sp}\right)^2\left(1-n_p^2\frac{\rho_0}{\rho}\right)\delta^{j0}\delta^{k0} + \frac{k_0^s}{2}\left(1-\left(n_0^{sp}\right)^2\right)\delta^{j0}\delta^{k0} \end{array} \right\}$$

$$\gamma^{jk} \equiv \left\{ \begin{array}{c} \frac{k_0^s}{2}\left(1-n_s^2\frac{\rho_0}{\rho}\right)\left(\delta^{jk}-\delta^{j0}\right) + \frac{k_0^s}{2}\left(1-\left(n_0^{sp}\right)^2\right)\delta^{j0}\delta^{k0} \\ +\frac{k_0^s}{2}\left(n_0^{sp}\right)^2\left(1-n_p^2\frac{\rho_0}{\rho}\right)\delta^{j0}\delta^{k0} \end{array} \right\}, \tag{132}$$

while others will play entirely new roles:

$$\kappa^{jk} \equiv \left\{ \begin{array}{c} \frac{1}{2}\left(-i\vec{\nabla}_T^{\,j}\delta^{k0} + i\vec{\nabla}_T^{\,k}\delta^{j0}\right) \\ +\frac{1}{2}\left(-i\left(\frac{\lambda}{\lambda+2\mu}\right)\vec{\nabla}_T^{\,k}\delta^{j0} + i\vec{\nabla}_T^{\,j}\left(\frac{\lambda}{\lambda+2\mu}\right)\delta^{k0}\right) \end{array} \right\}$$

$$\beta^{jk} \equiv \frac{i}{2}\vec{\nabla}_T^{\,k}\delta^{j0} + \frac{i}{2}\vec{\nabla}_T^{\,j}\left(\frac{\lambda}{\lambda+2\mu}\right)\delta^{k0} \tag{133}$$

Note that

$k, j \in (1,2)$ - label transverse directions y and z

$k, j = 0$ - labels downrange direction x

As discussed in Appendix S.1.2.1 to use straightforward δ-function bifurcation at an interface, we will need to make the change of variable:

$$K_1 = \frac{1}{\lambda} \quad ; \quad K_2 = \frac{1}{\mu}.$$

However, in the current treatment, we will stick with the familiar Lamé parameters λ and μ.

As derived in Appendix S.1.1, the state space equation for the elastodynamic field is

$$i\begin{pmatrix} \partial\vec{\theta}_T^{\,j}/\partial x \\ \partial\vec{\chi}_T^{\,j}/\partial x \end{pmatrix} = \begin{bmatrix} +\lambda^{jk}\underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\xi} + \left(\lambda^{jk}-2\gamma^{jk}\right)\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta} \\ +\kappa^{jk}\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\tau} + \left(\kappa^{jk}-2\beta^{jk}\right)\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{1} + k_0^s\delta^{jk}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta} \end{bmatrix}\begin{pmatrix} \vec{\theta}_T^{\,k} \\ \vec{\chi}_T^{\,k} \end{pmatrix}. \tag{134}$$

Note the familiar 2×2 matrices ξ, η and the unit matrix $\mathbf{1}$ have been labeled, as is the new matrix

$$\tau \equiv \eta\xi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

In outer-product notation (see the treatment of the electromagnetic field in Section 7.1), the odd and even operators are given by

$$\left.\begin{aligned} \underset{\sim}{\mathcal{O}} &= \lambda\otimes\xi + \kappa\otimes\tau \\ \underset{\sim}{\mathcal{E}} &= (\lambda - 2\gamma)\otimes\eta + (\kappa - 2\beta)\otimes 1 \end{aligned}\right\} \begin{array}{l}\text{outer product defines } 6\times 6 \text{ matrices} \\ \lambda,\gamma,\kappa \text{ and } \beta \text{ are } 3\times 3 \text{ matrices}\end{array}.$$

Now, the tilde reminds us that these are 6×6 matrices. "Even" and "odd" are defined as commutation and anti-commutation, respectively, vis-à-vis the block-diagonal

$$\begin{pmatrix} \mathbf{1}_{3\times 3} & 0 \\ 0 & \mathbf{-1}_{3\times 3} \end{pmatrix}.$$

Similarly, we have the six-component vector:

$$\underset{\sim}{\Phi} = \begin{pmatrix} \vec{\theta}^{\,k} \\ \vec{\chi}^{\,k} \end{pmatrix},$$

and, as always, we can write the result in standard form:

$$i\frac{\partial \underset{\sim}{\Phi}}{\partial x} = \left(\underset{\sim}{\mathcal{O}} + \underset{\sim}{\mathcal{E}} + k_0^s 1\otimes\eta\right)\underset{\sim}{\Phi}.$$

In Eq. (132), there appears a new kind of expansion parameter:

$$\left(1-\left(n_0^{sp}\right)^2\right) = \left(1-\left(\frac{c_0^s}{c_0^p}\right)^2\right). \tag{135}$$

To understand the meaning of this parameter, note that PEs not only select out a preferred axis (the downrange x-axis), but they also select a preferred wave number k_0 (i.e., the overall reference wave number). For the elastodynamic waves, it is convenient to choose as the preferred wave number k_0 the reference wave number for the shear waves k_0^s. The expansion parameter (Eq. (135)) is intrinsic to the elastic PE, and it reflects the discrepancy between the preferred wave number k_0^s and the reference wave number associated with the primary (or pressure or p-) waves: k_0^p. It has much in common with the expansion parameter associated with the acoustic (in this example constant density) PE $\mu \propto \left(1-n^2\right) = \left(1-\left(c_0/c\right)^2\right)$, which reflects the discrepancy between the local wave number k and the reference wave number k_0. However unlike μ, the expansion parameter (Eq. (135)) is even present for a downrange plane wave (i.e., one without any transverse (y,z)-dependence) embedded in a completely homogeneous medium. This is the first time we have encountered a PE parameter that does not vanish in this basic case. Such expansion parameters will occur whenever the PE is applied to a field that has more

than one characteristic wave number. Since the p-wave speed is generally around two times the s-wave speed, the presence of the term (Eq. (135)) suggests that the PE for the elastic solid will tend to require fairly high orders. Finally, it is worth noting that in the presence of a fluid-solid interface the expansion parameter (Eq. (135)) goes to 1 (with the usual conventions; other conventions will cause even more severe problems) and this limit is consequently quite problematical for the PE. The reasons for this are discussed in footnote yyyyy in Appendix S.1.2.2. (More generally, a number of subjects addressed in this paragraph are examined in further detail in Appendix S.1.2.2.)

7.2.3 The Transformation Connecting the PE Field $\vec{\chi}$ to the Displacement Vector $\vec{u}$

The endpoint correction for the elastic PE (tying the familiar full-wave displacement vector $\vec{u}$ to the corresponding auxiliary field $\vec{\chi}$ that is associated with downrange propagation by the PE) is quite difficult to obtain, and for the present purposes as well as for most conceivable future applications, the first-order (in $\vec{\nabla}_T$) is sufficient. This result is

$$\vec{\chi} = \frac{1}{\sqrt{\rho_0 \omega c_0^s}} \ddot{D} \cdot \vec{u} \tag{136}$$

where

$$\ddot{D} \equiv \sqrt{\rho\omega^2}\left(\frac{\ddot{1}}{k}\right)^{1/2} + \frac{\sqrt{\rho\omega^2}}{8}\left(k_s k_p\right)^{1/4}\left(\frac{1}{k_p^2} - \frac{1}{k_s^2}\right)\left(3 + \frac{k_p}{k_s}\right) i\left(\hat{x}\vec{\nabla}_T + \vec{\nabla}_T \hat{x}\right) + \mathrm{O}\left(\nabla_T^2\right) \tag{137}$$

and

$$\left(\frac{\ddot{1}}{k}\right)^{1/2} = \begin{pmatrix} 1/\sqrt{k_p} & 0 & 0 \\ 0 & 1/\sqrt{k_s} & 0 \\ 0 & 0 & 1/\sqrt{k_s} \end{pmatrix}. \tag{138}$$

This result is derived in Appendix S.2.

When λ, μ and ρ are only locally, *but not globally,* constant, then $\vec{\nabla}_T$ is no longer an observable (i.e., $\left[\vec{\nabla}_T, \mathcal{H}\right] \neq 0$) even in the range-independent case, so there is no cancellation of endpoint contributions in a range-independent environment, and of course no near-cancellation in a weakly range-dependent environment. This is similar to the electromagnetic case. However, since for shallow grazing angles $\vec{\nabla}_T$ is "small" and the endpoint contribution does not accumulate, it may be possible to get away using the 0th order, but use of the first order in $\vec{\nabla}_T$ is the safer practice. Note that the second order (i.e., $\mathrm{O}\left(\nabla_T^2\right)$) is the lowest order contribution in $\vec{\nabla}_T$ when one assumes that the medium parameters are locally constant for the electromagnetic and acoustic fields, so the first-order effect appearing in Eq. (137) is an unusually big endpoint effect associated with transverse differentiation. Note that in considering "minimal" endpoint corrections, we have generally kept first order in jumps in the medium parameters. Thus, it is best to consider the expression above as a "minimal" endpoint correction much like $\sqrt{\rho_0/\rho} \approx 1 - \Delta\rho/2\rho_0$ in the two-fluid acoustic problem.

This completes our examination of the PE for vector fields.

8. SUMMARY AND FUTURE TRENDS

In this section, the core findings of this report are summarized in Section 8.1, and finally, desirable future extensions of this research are explored (Section 8.2). The latter includes both plans to implement the new formalism and extensions of the theory.

From a practical point of view, the chief goal of the effort outlined in this work has been to tie the acoustic PE technique to rough surface scattering theory. As the surface roughness extends through the wavelength scale, it behaves like a diffraction grating and leads to what is called Bragg scattering. This is a nontrivial, phase-sensitive problem that involves theoretical and computational challenges that go beyond those found in problems to which the PE is most typically applied. Although there has in the past been some success in applying the PE to impenetrable rough surfaces, this record has until now not been matched for penetrable rough surfaces. In this report, the FW transformation has been used to design a PE that addresses this challenge. The paradigm employed is based on the nonrelativistic theory of the quantum Lamb shift, where a PE (the Schrödinger equation) was used to model a field near a rough surface (the world line of the hydrogen nucleus advected by vacuum fluctuations). The applicability of this technique to the acoustic problem was established by examining the direct classical analogy to the atomic Lamb shift. Then, the technique was extended to describe Bragg scattering from a rough interface where the density jumps (such as is common at the water-sediment interface). The PE derived in this way exploits higher-order boundary conditions to buffer the density discontinuity in a manner precisely dictated by the formalism.

The results of this work complement the current state-of-the-art PE, and suggest a promising new line of development. This approach is particularly well-suited for addressing a variety of important scattering problems–particularly those where the density, electric permittivity, magnetic permeability, or the Lamé parameters vary rapidly as a function of the transverse coordinates, while the range dependence involves spectral scales down to the Bragg wave number. This scenario includes rough interfaces where these parameters jump such as the ocean bottom.

8.1 Summary

The new PE applicable to a rough interface where the density jumps has the most immediate practical relevance to the field of underwater acoustics, and it therefore constitutes the core of this report. The key equations needed to implement this PE are presented by:

- Equation (95), the Hamiltonian in the half spaces (which can be resummed to give the familiar Hamiltonians in the half spaces, but the error terms will involve powers of the new expansion parameters λ and 2γ–these parameters are given by Eq. (87)),
- Equation (97), the transformation good in the half spaces that takes us from the auxiliary field associated with the PE χ to the physical pressure field A,
- and Eq. (120), the second order $\mathrm{O}\left(\lambda^2\right)$ boundary conditions applicable along a density/compressibility jump.

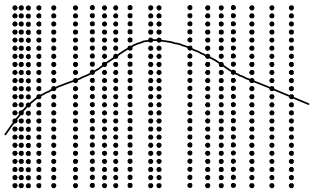
The method for evaluating derivatives at the interface described in

Fig. 10 is needed for a numerical implementation of the new deterministic theory.

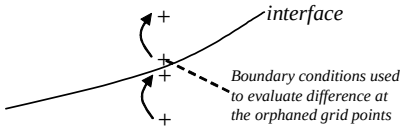
Figure 19 traces the development of this core result. These topics are covered in Sections 3.1, 3.3, 5.1, 5.3, and 6.1 of this report. The mechanics of discretizing the problem are discussed first, and it is

established that the downrange stepping procedure requires that boundary conditions be specified on the interface. The FW transformation is used to generate a PE for the auxiliary field that carriers the downrange flux, complete with the needed boundary conditions. When this approach is applied to an interface where the density jumps, the jump in energy flux becomes buffered in the PE. (In the full-wave equation, the tangential component of the flux jumps at an interface where the density jumps.)

The mechanics of stepping downrange, and the related need for boundary conditions (Section 2.3)



A. Using the PE to step downrange such that the interface always falls right on the grid.



B. Using boundary conditions in finite difference schemes to evaluate derivatives right on the interface and so get the Hamiltonian needed for downrange stepping.

Using the Foldy-Wouthuysen transformation to obtain boundary conditions

Ansatz:

$$field = \begin{pmatrix} \Leftarrow energy\ flux \\ \Rightarrow energy\ flux \end{pmatrix}$$

FW transformation:

$$\mathcal{H} = \begin{pmatrix} h_1 & h_2 \\ h_3 & h_4 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} H$$

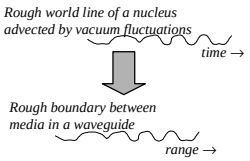
Result:

Scalar PE with scalar Hamiltonian H

A. Use a series of canonical transformations to generate the PE: i.e., the Foldy-Wouthuysen transformation adapted to acoustics (Sections 2.1 and 4.1).

$$\frac{\partial^n \chi_I}{\partial z^n} \Leftrightarrow \frac{\partial^n \chi_{II}}{\partial z^n}$$

B. The Foldy-Wouthuysen transformation generates boundary conditions along discontinuities (Sections 2.2, 4.3 and 5.1).



C. Validate the approach by considering the classical field phenomenon analogous to the atomic Lamb shift (Sections 2.2, 3.3 and 4.3).

A new suite of boundary conditions along a density jump for the higher order PE. These effectively buffer the density jump much like an electron cloud buffers an atomic nucleus (Section 5.1). (*Key result*)

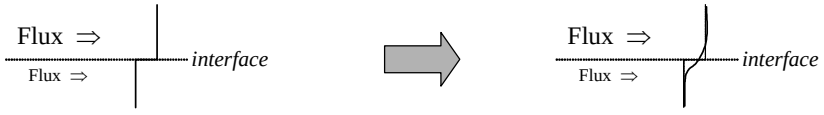


Fig. 19 — A schematic summary of the most important and results introduced in this report

As noted in Fig. 19, the classical Lamb shift places our formal efforts into context and enhances the credibility of the results (Sections 3.2, 4.1, 4.2, 4.3, and 4.4). The key result is the classical Lamb shift induced by the combined effect of sound speed cusps and sound speed/density jumps (Eq. (105) complemented by Eqs. (95) and (97)). The quasi-first-order stochastic boundary conditions for (separately) a sound speed cusp (Eq. (40)), the sound speed jump (Eq. (82)) and a sound speed/density jump (Eq. (103)) provide examples of the classical Lamb shift, and when compared to the deterministic

quasi-first-order boundary conditions (Eqs. (31), (72) and (99), respectively), they indicate that the new FW term, which is identified with "vacuum polarization" in Section 4.2.1, indeed involves a kind of smearing associated with (imaginary – i.e., $\propto i$) displacements in the uprange/downrange direction. Thus, the examination of the classical Lamb shift reinforces the notion that the FW transformation can smear a singularity – even in the deterministic problem. In addition to the field-theoretic interpretation, the new FW term can also be explained in geometrical terms by tracing it back to the effects of tilt on the normal derivative in the full-field boundary conditions (Section 4.2.1).

The discussion of the classical Lamb shift is further reinforced when, in the formalism for the acoustic problem, it is used to create a toy model of the atomic Lamb shift (Section 3.2.4). The classical Lamb shift is connected to boundary waves (Section 4.4.4). Curvature-induced boundary waves are induced by the new FW term (Sections 5.3.3.4 and 5.3.3.5). There is a connection between these boundary waves and Biot-Tolstoy boundary waves (Section 5.3.3.5).

Going beyond topics mentioned in Fig. 19, Section 5.2 addresses the important technical question of what to do when the formalism seems to multiply distributions, Section 6.2 places the results into the context of other work in the field (e.g., see Table 3 for an overview), and Section 7 extends the basic approach to electromagnetic and elastic fields.

8.2 Future Trends

Now that the underlying formalism has been developed, a number of interesting extensions are possible.

8.2.1 Direct Applications of Results in this Report

A researcher applying this formalism to acoustic modeling could begin by directly applying the results developed in this report.

Acoustic Lamb shift. An initial examination of this effect associated with cusps in the sound speed and/or jumps in the density and sound speed would be based on the stochastic quasi-first-order $\mathrm{O}\left(\lambda, \ddot{\lambda}\right)$ theory reflected in boundary conditions (Eq. (105)). Such an effort would build on the preliminary modeling results presented in Section 5.4.2. These results could be expanded to include the effects of classical vacuum polarization. An extensive parameter study would reveal scenarios where the classical Lamb shift could play a significant role in shallow water propagation. Specifically, a closer study of localization induced by sound speed cusps would be very worthwhile, since it could suggest ways to exploit signals trapped by this effect to deploy sonar more effectively.

Acoustic "vacuum polarization" within the water column. Previously, quasi-first-order $\mathrm{O}\left(\lambda, \ddot{\lambda}\right)$ theory was used to evaluate the effects of classical "vacuum polarization" in (deterministic) long-range propagation in deep water. It was assumed that range dependence is induced as the sound speed profile is advected by internal waves. Wurmser et al. assumed single-scale internal waves, but Frank Henyey (APL-UW) has pointed out that a power law is much more realistic and the effect should be larger for such a power law [107]. Furthermore, Henyey has also suggested that classical "vacuum polarization" might be significant in the context of bubble clouds, since the scales of the bubbly medium and acoustic wavelength are closely matched [107]. These hypotheses should be examined in the future.

Bragg scattering. Initially, second-order $\mathrm{O}\left(\lambda^2\right)$ theory could be used to model scattering from a deterministic rough interface characterized by a density and compressibility jump. This study would be

based on boundary conditions (Eq. (120)), and it will proceed with the problem of scattering from the ocean bottom in mind. It would be useful to benchmark the results against finite difference solutions and/or against controlled experiments (perhaps using scale models). Since the ratio of the jump in the density relative to the reference density is an expansion parameter and the theory has initially been restricted to low orders, initial studies should begin by considering density jumps that are somewhat smaller than the factor of two jump typical for a water-sand bottom. This will allow a preliminary, qualitative investigation of subcritical-angle penetration into the ocean bottom. The theory could also be used to examine the effects of layered bottoms on the acoustic field.

8.2.2 Extensions of the Results in this Report

Straightforward extensions of the formalism derived in this result can lead to several promising new avenues of research.

Higher-order theories. Once the second-order $O(\lambda^2)$ version of the theory is fully implemented and understood, then the higher-order theory (e.g., third-order $O(\lambda^3)$ theory) can also be developed and used in a more definitive study of subcritical angle penetration into the ocean bottom. At some point in the future, the formalism could also be extended to include two-dimensional surfaces embedded in the full three-dimensional space.

As noted in the final two paragraphs of Section 6.1.5, second/third-order hybrid $O(\lambda^2, \ddot{\lambda})$ and the pure third-order $O(\lambda^3, \ddot{\lambda})$ theories in both their deterministic and stochastic versions will be interesting and worthwhile, as will consideration of the stochastic version of the basic $O(\lambda^2)$ theory. The stochastic theories will involve both "losses" due to Bragg scattering and Lamb shift-type effects. The $O(\ddot{\lambda})$ terms introduce the classical equivalent of the vacuum polarization effect known in atomic physics.

Variable densities. At some point in the future, the possibility that ρ varies in the half spaces should be allowed, and consideration given to the possibility that there may be steps in $\nabla_T \rho$ and in $\nabla_T^2 \rho$ at the interface. Such singularities will lead to new stochastic effects similar to the classical Lamb shifts discussed above.

Other fields. The new approach based on the FW transformation has also been extended to elastic and electromagnetic fields. It would be best to use these results at first to consider media without interfaces, and then expand the approach to consider interfaces. The elastic-wave theory can be developed with an eye toward seismic and seismo-acoustic applications. It remains to be seen whether this theory can be applied to a fluid-elastic boundary such as appears along an ocean bottom consisting of an interface between water and solid rock (e.g., see footnote yyyy in Appendix S.1.2.2).

Data. Finally, all of these versions of the theory will have to be thoroughly compared to data.

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discussions that provided valuable understanding without which this work would never have been completed.

This work is dedicated to Roger Dashen's memory. He left the author with scientific direction, truly valuable clues, and faith that if I pursued his intuitions, things would work out. Ideas and suggestions inherited from Roger Dashen include:

- Use the FW transformation to derive the range-dependent PE.
- Only apply the FW transformation at the endpoints and propagate the auxiliary field. Furthermore, it is by and large okay to drop the endpoint transformation altogether since it does not accumulate.
- Perform an extra transformation to make the new FW terms manifestly reciprocal under range reversal.
- Apply the FW terms to an interface, and do not fret about the δ-functions because such terms commonly appear in quantum mechanics.
- Apply the findings to the problem of a range-dependent (i.e., sloping) interface where the density jumps (recalling that it is fairly trivial to obtain a PE that propagates across a range-*in*dependent interface (i.e., a flat interface without tilt or curvature)).

This work is also dedicated to Fred Tappert, who taught me many important things about the PE. He was the father of this field, and his work was characterized by integrity, creativity, and vision. He will be missed.

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A Appendix: χ as a carrier of downrange flux

It is shown in [1] that the FW procedure by design ties the conservation rule for $\int dR_T \left|\chi\right|^2$ to the conservation of the downrange flux, and so to the conservation of energy. This connection also helps us understand the relationship between the auxiliary field χ and the pressure field A. Here we examine the case of constant density. It can be shown that $\chi = \sqrt{H/k_0} \cdot A$ (see the second to the last paragraph of Section 2.1, the discussion around equation (3.14) in Section 3.1 and most of all Appendix D.1), which can be rewritten in the suggestive form $\chi = \sqrt{\left(-i/k_0\right)\partial/\partial x} \cdot A$ (where recall functions of operators are understood as expansions). To further illuminate the interpretation of χ as a kind of carrier of flux, take $\left|\chi\right|^2 = \chi^* \chi \propto \left(H^{1/2}A\right)^* \left(H^{1/2}A\right)$, split it in halves, integrate over transverse space, and integrate the halves by parts each in the opposite direction from the other to get

$$\int dR_T \left|\chi\right|^2 \propto \int dR_T \left[\tfrac{1}{2}(HA)^* A + \tfrac{1}{2} A^* (HA)\right] = \int dR_T \,\mathrm{Im}\left[A^* \cdot (\partial A/\partial x)\right] \propto \int dR_T S_x \qquad \text{(A.1)}$$

(S_x is the downrange flux). In the eigenvalue problem (i.e., when the duct is range independent), the eigenfunctions χ_n form a basis for the solution set: $\chi = \sum_n c_n \chi_n$ (c_n are constants), and each eigenfunction is (to within a phase) the actual square root of the corresponding (downrange) flux. (The basis can be made orthogonal using the Graham-Schmidt orthogonalization procedure; see, for example, reference [108].) For weak range dependence, we can decompose the field A into its corresponding set of eigenfunctions and replace the operator H with eigenvalues k_x; and similarly we can substitute $\sqrt{k_x}$ for $\sqrt{H}$. If there is no range dependence, there is no mode coupling and the endpoint transformations from A to χ at the beginning and χ back to A at the end precisely cancel. If the coupling is weak in the sense that most of the coupling is between nearby eigenfunctions (nearby means the eigenvalues are close), the endpoint transformations will involve factors of $\sqrt{k_x/k_x'}$ (unprime is from the $A \to \chi$ transformation, prime is from the $\chi \to A$ transformation) and the transformations nearly cancel. In such typical cases, reasonably good answers can be obtained using the PE to directly propagate A. Although this is often done, it is good practice to keep in mind that this is an approximation, and that the PE really propagates an auxiliary field χ.

B Appendix: The place of backscatter in the PE formalism

The parabolic equation converges to the full wave solution asymptotically. Although the expansion is of ever-higher order, there remains a small but finite probability of backscatter. A complete description of propagation through a range-dependent sound speed profile must take this into account. There is a precedent from quantum field theory[109]. A charged particle field in a constant uniform electric field has a finite probability of initiating particle-antiparticle pair production. The probability of pair production goes as the negative exponential of the reciprocal of the field, and it is therefore non-perturbative. Backscatter for the acoustic field corresponds to pair production in a quantum field[110,111,112].

We now follow the procedure starting on p. 193 of reference [109]. Unlike the electric field, the sound speed variation is automatically decoupled from the range momentum component, and a transformation to a pure time-dependent gauge is unnecessary (see equation 4-113 of reference [109]). Therefore, $e^2E^2X_0^2$ is replaced with $k_0^2\mu$. Now, locally expand μ through second order (note: for very strong range dependence, this becomes a poor approximation). We now have an equation mathematically very similar to the quantum harmonic oscillator (see reference [109], equation 4-115), but there is now an extra term linear in the canonical coordinate. This term comes from the first order of the Taylor expansion. The effect of a linear term added to the Hamiltonian of a harmonic oscillator is simply to shift the zero point of the oscillator. This is not physically significant, and it can be eliminated by redefining the zero point of the range. Finally, we arrive at the result for bosons undergoing pair production (equation 4-119 in reference [109]) with eE replaced by $k_0\sqrt{\ddot{\mu}/2}$:

$$\frac{\text{Probability}}{\text{unit volume}} = \frac{k_0^2\ddot{\mu}}{16\pi^3}\sum_{s=1}^{\infty}\frac{(-1)^{s+1}}{s^2}\exp\left(\frac{-s\pi k_0}{\sqrt{\frac{1}{2}|\ddot{\mu}|}}\right). \qquad \text{(B.1)}$$

Note that the crucial quantity is the second range derivative of $\mu = \frac{1-n^2}{2}$. Also note that in the limit as the range dependence disappears (i.e., $\ddot{\mu} \to 0$), the quantity on the right hand side of equation (B.1) goes to zero faster than any integer power of $\ddot{\mu}$. In other words, it is an essential singularity at $\ddot{\mu} = 0$, and backscatter lies at a higher order than any finite order of the parabolic equation. Equation (B.1) also suggests a technique for calculating the backscatter. The intensity of the (incoherent) scattered field would be omni-directional and proportional to the probability density given in (B.1) above.

Solutions evanescent in the downrange direction play a prominent role when there is ducting in the direction transverse to the original downrange direction (for example, in geoacoustics, when a downward propagating field can hit a salt dome that is elongated in the transverse direction and so acts as a transverse duct), or as transients near a spherical

wave source[ttt]. These waves do not produce an energy flux in the downrange direction. Since the expansion parameter $k_z/k_0 > 1$, these solutions are not compatible with the usual Taylor series expansion of the PE square root operator (as pursued in this paper). Indeed, these solutions along with other more conventional near-transverse modes will render the expansion techniques discussed in this paper ineffective. Like backscatter, evanescent modes only have weak curvature-induced coupling to downrange-propagating waves, and this coupling goes to zero faster than any finite order of the PE expansion. In fact, pair production, the mechanism that gives rise to backscatter, is also responsible for coupling propagating waves to evanescent pairs. Once again, we see that these effects can be neglected in many problems of physical interest, including many typical ducted propagation problems. In Sections 2.2 and 6.2.2, it is noted that Michael Collins exploits the existence of non-physical evanescent solutions in order to eliminate Gibbs' oscillations. Issues related to evanescent waves are fully discussed in the work of Fishman *et al.* in reference [25] and in their subsequent work currently under preparation.

Note that like the PE, the pair-production calculation selects a preferred direction and specifically postulates weak *range* dependence. Perturbation theory, which leads to the Born series, begins with a fundamentally different assumption. It is based on an iterative procedure that already at the 1st order of the iteration intrinsically generates solutions that involve the full Fourier transform space of the spatial dependence of the environmental parameters. The full Fourier transform space automatically incorporates backward propagating causality, and so in the context of the Born series, backscatter becomes a 1st order effect. The different properties of these expansions arise because we are expanding about fundamentally different limits.

Finally, recalling the qualitative discussion in Section 2.3, we can see how the basic insights in this appendix generalize to the interface problem. There, it was noted that when a surface is single valued, has small slope, and furthermore, the incoming field consists of spectral components with shallow grazing angles, then backscatter is a subtle effect related to the surface curvature ($\ddot{f}$ for an interface given by $z = f(x)$). In other words, $\ddot{f}$ roughly takes the role of $\ddot{\mu}$ when we go from the volume scattering to the interface scattering problem. Backscatter goes to zero faster than any finite order PE as $\ddot{f} \to 0$.

[ttt] Reflecting the fact that the Klein-Gordon equation is a hyperbolic partial differential equation (rather than an elliptic one), the equivalent quantum mechanical solution must decay in at least one spatial (i.e., transverse) dimension in addition to being evanescent in the downrange (i.e., temporal) direction.

C Appendix: Using the Foldy-Wouthuysen transformation to derive the basic (constant density) acoustic parabolic equation

This appendix provides the key features of reference [1]. These are reproduced here for completeness. The Foldy-Wouthuysen transformation is used to derive a parabolic in a fluid, where the density is everywhere the same (such as the water column in the ocean). This is the most basic application of the Foldy-Wouthuysen transformation to a classical field, and it establishes the paradigm to be used in all the subsequent formal development in this paper.

Section C.1 recasts the problem so that uprange and downrange propagation are clearly identified. The 2nd-order scalar Helmholtz equation is converted to a 1st-order "state-space" equation involving 2-dimensional vectors operated on by 2×2 matrices (Section C.1.1). The components of the 2-dimensional vectors represent uprange and downrange propagation. A basic attribute of the matrix operator and its connection to energy conservation is then discussed (Section C.1.2).

In Section C.2, the Foldy-Wouthuysen transformation is used to decouple uprange and downrange propagation. The canonical nature of the transformation is discussed (Section C.2.1) and then a form of the transformation is derived for the range-independent problem (Section C.2.2). This result is good to infinite order. Next, a number of issues related to the range-dependent problem are examined (Section C.2.3). Most significantly, a general iterative procedure for implementing the Foldy-Wouthuysen transformation is derived. This basic procedure generates a perturbative expansion, and it will be used again later as the formalism is extended to other problems, such as acoustics where the density varies, electomagnetics and elastic solid waves. The Foldy-Wouthuysen procedure is then explicitly applied to the range-dependent (constant density) acoustic problem (Section C.2.4). The proper symmetry properties are made manifest (Section C.2.5) and then the physical meaning of the results are discussed (Section C.2.6).

C.1 The vector formulation of the Helmholtz equation

In Subsection C.1.1 we develop the ansatz of the procedure developed by Foldy-Wouthuysen, and then in Subsection C.1.2 examine an important attribute of the structure of the equation generated by the ansatz: the pseudo-Hermiticity of the matrix Hamiltonian.

C.1.1 Converting a 2nd order differential equation to 1st order

The acoustic pressure field is assumed to propagate according to the (constant density) wave equation through a time-independent environment:

$$\nabla^2 P - -\frac{1}{c^2}\frac{\partial^2}{\partial t^2} P = 0 .$$

Note that $\nabla^2 = \vec{\nabla}\cdot\vec{\nabla}$ where once again as in Section 2.1, $\vec{\nabla} \equiv \left(\partial/\partial x, \underline{\nabla}_T\right)$ with

$\underline{\nabla}_T = \left(\partial/\partial y, \partial/\partial z\right)$ the gradient in the transverse direction.

Each frequency ω can be considered separately, and so the pressure is given by

$$\begin{aligned} P\left(x, \underline{R}_T, t\right) &= \int_{-\infty}^{\infty} P_\omega\left(x, \underline{R}_T, t\right) d\omega \\ P_\omega\left(x, \underline{R}_T, t\right) &= \mathrm{Re}\left[A\left(x, \underline{R}_T\right) e^{-i\omega t} \right] \end{aligned} \tag{C.1}$$

where the complex field $A\left(x, \underline{R}_T\right)$ solves the Helmholtz equation.

$$\frac{\partial^2 A}{\partial x^2} + \underline{\nabla}_T^2 A + k_0^2 n^2 A = 0 . \tag{C.2}$$

As in Section 2.1 $k_0 = \omega/c_0$, c_0 is a reference sound speed, and $n\left(x, \underline{R}_T\right)$ is the index of refraction.

In solving second or higher-order differential equations, it is common practice to reduce the order of the derivatives by adding degrees of freedom. Here, we go from a second order differential equation for a scalar A to a first order equation for a vector Φ. The components of the vector Φ must be linear combinations of A and its first derivative $\partial A/\partial x$. Following [57] (pp. 199-207), we make the usual choice (e.g., see Section 3.1)

$$\Phi \equiv \begin{pmatrix} \theta \\ \chi \end{pmatrix},$$

where

$$\begin{aligned}\theta &\equiv \frac{1}{2}\left(A + \frac{i}{k_0}\frac{\partial A}{\partial x}\right) \\ \chi &\equiv \frac{1}{2}\left(A - \frac{i}{k_0}\frac{\partial A}{\partial x}\right)\end{aligned}. \tag{C.3}$$

This is an ansatz, which has been used previously for the acoustic problem (see, for example, [113],[114]). Later in Subsection C.1.2, we will see that Φ is closely related to the downrange energy flux.

The Helmholtz equation can be rewritten as

$$ik_0\left(\dot{\theta} - \dot{\chi}\right) = \underline{\nabla}_T^2\left(\theta + \chi\right) + k_0^2 n^2\left(\theta + \chi\right), \tag{C.4}$$

where as always $\dot{a}$ denotes $\partial a/\partial x$. Manipulating the definitions, we also have the equation of constraint

$$ik_0\left(\dot{\theta} + \dot{\chi}\right) = k_0^2\left(\theta - \chi\right). \tag{C.5}$$

Adding and subtracting (C.4) and (C.5), expressing the answers in matrix form, and we have

$$i\dot{\Phi} = \left[k_0\eta + \lambda\eta + \lambda\xi\right]\Phi,$$

where as in Section 2.1,

$$\begin{aligned}\lambda &\equiv \frac{\nabla_T^2}{2k_0} - \mu k_0 \\ \mu &\equiv \frac{1}{2}\left(1 - n^2\right)\end{aligned},$$

and as always

$$\eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad ; \quad \xi = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{C.6}$$

The "odd" operator $\mathcal{O} \equiv \lambda\xi$ is off-diagonal and couples the components of Φ while the "even" operator $\mathcal{E} \equiv \lambda\eta$ is diagonal and does not couple θ and χ.
We now have (cf. equation (3.4))

$$i\frac{\partial\Phi}{\partial x} = \mathcal{H}\Phi \tag{C.7}$$

where

$$\mathcal{H}(\lambda) \equiv \mathcal{O} + \mathcal{E} + k_0 \eta \tag{C.8}$$

This formal result is the same as the quantum mechanical analog with the reference wave number k_0 replacing the mass. This equation determines the behavior of Φ as a function of the range.

Note that (C.7) is nothing more than the Helmholtz equation rewritten in vector form. It has previously been derived in references [114] and [115], where it is written in slightly different form. This result is exact[uuu].

Taking equations (C.7) and (C.8) as a starting point, the Foldy-Wouthuysen transformation of Section 4.3 in reference [57] can now be used to solve the problem.

C.1.2 Energy conservation and pseudo-Hermiticity

Before proceeding to a solution of the problem, we digress to further examine the structure developed up to this point. This will serve to provide a physical intuition for the formal results above as well as motivate what comes later. It will be shown that Φ is related to the energy flux and that a simple mathematical property of the Hamiltonian $\mathcal{H}$ known as "pseudo-Hermiticity" guarantees that the energy is conserved for all values of the range.

To introduce the concept of pseudo-Hermiticity, it is first necessary to define Hermiticity. The Hermitian conjugate of the wave function Φ is its transpose and complex conjugate:

[uuu] Also note that there are a number of other ways to recast the Helmholtz equation as a first order matrix equation; i.e. there are a number of "branches" for taking the square root of the operator. As pointed out in reference [115], the Dirac operator would be another choice. However, unlike equation (C.7), the Dirac equation introduces a superfluous non-physical degree of freedom (corresponding to quantum mechanical spin). There are a number of other choices, including those corresponding to other spin states. These introduce extra degrees of freedom, which are not present in the acoustic propagation problem. Equation (C.7) is appropriate for spinless particles such as pions and K-mesons, as well as for the acoustic field, which of course also has no quantum mechanical spin. (Incidentally, we will see later that classical electromagnetic and elastic fields will automatically introduce vector properties into the Hamiltonian, but the resulting vector behavior comes in addition to the spins being discussed here and the two classes of phenomena should not be confused.)

$$\Phi^\dagger = \left(\Phi^*\right)^T .$$

To extend the concept of Hermiticity to an operator α it is necessary to assume the sturcture

$$\int \left(\Phi^\dagger \alpha \Phi\right) d^2 R_T . \tag{C.9}$$

The Hermitian conjugate $\alpha^\dagger$ is defined by the equation

$$\int \left(\Phi^\dagger \alpha^\dagger \Phi\right) d^2 R_T = \int \left(\left(\alpha\Phi\right)^\dagger \Phi\right) d^2 R_T .$$

The Hermitian conjugate of a matrix operator turns out to be the transpose and complex conjugate of the matrix, while for operators containing powers of the differential operator $\nabla^n_{\underline{R}_T}$ it is necessary to integrate by parts, picking up a minus sign for every power – i.e., after the necessary n integrations by parts we pick up a factor of $(-1)^n$. It follows from these definitions that the Hermitian conjugate of a product is the product of the Hermitian conjugates in reverse order (i.e. $(\alpha\beta)^\dagger = \beta^\dagger \alpha^\dagger$). (Note that it is here where we implicitly assume that the field is zero at the boundaries.)

Note that the structure (C.9) is required specifically so that the concept of Hermiticity can be extended to the differential operator $\underline{\nabla}_T$. In quantum mechanics, the integral would be over full 3-dimensional space, but for the PE, it becomes the 2-dimensional transverse space given by $\underline{R}_T$. This is consistent with the notion that the range x takes the place of the time. Continuing the analogy to quantum mechanics, $\underline{R}_T$ is the coordinate vector and the operator $-i\underline{\nabla}_T$ is the corresponding momentum $\underline{P}_T$.

An operator α is Hermitian if $\alpha^\dagger = \alpha$. The definition of pseudo-Hermiticity is similar: α is pseudo-Hermitian if $(\eta\alpha)^\dagger = \eta\alpha$ where η is defined in equation (C.6). (Note that pseudo-Hermiticity is Hermiticity with the unit matrix replaced by the metric η. As will be shown below, the physical significance of this metric lies in the fact that the energy associated with the two components of Φ propagates in different directions.) Since λ and η are Hermitian, ξ anti-Hermitian (i.e. $\xi^\dagger = -\xi$) and $\eta\xi = -\xi\eta$, it follows that $\mathcal{H}$ defined in (C.8) is pseudo-Hermitian.

This implies that

$$\begin{aligned} i\int\left[\Phi^\dagger \eta \frac{\partial\Phi}{\partial x}\right] d^2 R_T &= \int\left[\Phi^\dagger \eta\mathcal{H}\Phi\right] d^2 R_T \\ &= \int\left[\left(\eta\mathcal{H}\Phi\right)^\dagger \Phi\right] d^2 R_T , \\ &= -i\int\left[\left(\frac{\partial\Phi}{\partial x}\right)^\dagger \eta\Phi\right] d^2 R_T \end{aligned} \tag{C.10}$$

which in turn leads to the result

$$\frac{\partial}{\partial x}\left(\int\left[\Phi^{\dagger}\eta\Phi\right]d^2R_T\right)=0\,. \tag{C.11}$$

It will now be shown that this equation is an expression of total energy conservation. (By *total* energy, it is meant that the forward and backward propagating components of the field are both included.)

Consider

$$\begin{aligned}\int\left[\Phi^{\dagger}\eta\Phi\right]d^2R_T &= \int\left(\theta^*\theta-\chi^*\chi\right)d^2R_T\\ &= \frac{i}{2k_0}\int\left(A^*\partial_x A-\left(\partial_x A\right)^* A\right)d^2R_T\\ &= -2\rho c_0\int\left(\frac{\mathrm{Im}\left(A*\vec{\nabla}A\right)}{2\rho\omega}\cdot\hat{x}\right)d^2R_T\\ &= -2\rho c_0\int\left(\vec{S}_{\mathrm{ave}}\cdot\hat{x}\right)d^2R_T\end{aligned}, \tag{C.12}$$

where $\vec{S}_{\mathrm{ave}}$ is the time-averaged energy flux and ρ is, as always, the density (begin with reference [98] (equations 64.6 and 65.4), and then use a well known result for the time-averaged product of the real parts of two complex fields). It follows that $\int\left[\Phi^{\dagger}\eta\Phi\right]d^2R_T$ is proportional to the total down-range flow of energy. Since it is the same for all values of the range, there are no energy sources or sinks, and we have shown that the pseudo-Hermiticity of $\mathcal{H}$ guarantees energy conservation. Furthermore, the physical significance of the quantity $\Phi^{\dagger}\eta\Phi$, taken as a function of the position $\left(x,\underline{R}_T\right)$, has been established. It is the time-averaged energy density flux in the direction of the range $\hat{x}$.

C.2 The basic acoustic ($\delta\rho=0$) Foldy-Wouthuysen transformation

Here we examine the actual Foldy-Wouthuysen transformation. The canonical nature of the transformation is discussed (Section C.2.1) and then a form of the transformation is derived for the range-independent problem (Section C.2.2). Next a general procedure for implementing the transformation is derived (Section C.2.3), and then applied to the range-dependent acoustic problem (Section C.2.4). The equation is made manifestly symmetric under range reversal (Section C.2.5) and physical interpretation of the results are discussed (Section C.2.6).

C.2.1 The use of canonical transformation to solve a problem

At its core, the Foldy-Wouthuysen technique exploits a procedure familiar from classical mechanics (e.g., see references [116] and [117]). A canonical transformation is used to simplify the problem, in this case to decouple the forward and backward propagating solutions. The canonical problem is solved in the transformed space, and the final answer is transformed back into the original space. In the present context, an additional step is added. The Foldy-Wouthuysen ansatz recasts the scalar field in vector form (and the scalar operator of the wave equation into a matrix Hamiltonian operator). The approach is shown diagrammatically in Figure C.1.

The transformation $\Phi \to \tilde{\Phi}$ and $\mathcal{H} \to \tilde{\mathcal{H}}$ is canonical if the form of the equation is preserved, i.e.:

$$i\frac{\partial \Phi}{\partial x} = \mathcal{H}\Phi \to i\frac{\partial \tilde{\Phi}}{\partial x} = \tilde{\mathcal{H}}\tilde{\Phi}.$$

The Foldy-Wouthuysen transformation is a canonical transformation where $\tilde{\mathcal{H}}$ is diagonalized, and the components of $\tilde{\Phi}$, $\tilde{\theta}$ and $\tilde{\chi}$, represent decoupled backward and forward propagating solutions respectively.

Physical systems tend to be amenable to numerical simulations largely because they obey physical conservation rules (e.g., energy conservation), which in turn force the related mathematical equations to enjoy numerical stability. To maintain this source of numerical stability, we also demand that our new canonical equation maintain the conservation rule on $\Phi^{\dagger}\eta\Phi$. This implies that the transformation must be pseudo-unitary (i.e. if $\Phi = U\tilde{\Phi}$ then $U^{\dagger}\eta U = \eta$), which in turn guarantees that the total energy flux remains equal to $-\left(2\rho c_0\right)^{-1}\int\left(\tilde{\Phi}\eta\tilde{\Phi}\right)d^2R_T$. As demonstrated by the argument in Subsection C.1.2, the fact that this quantity remains conserved even after downrange propagation implies that $\tilde{\mathcal{H}}$ must be pseudo-Hermitian. (It also turns out that $\tilde{\mathcal{H}}$ is Hermitian. This can be seen as follows. Recall that $\tilde{\mathcal{H}}$ is diagonal, and so the equations for the components of $\tilde{\Phi}$ are decoupled, and each must independently conserve energy. The corresponding components of the diagonal matrix $\tilde{\mathcal{H}}$ must then be Hermitian, and so is $\tilde{\mathcal{H}}$ itself. See also the results (3.11), and the Hamiltonians (C.31) and (C.35) below in this appendix to see this principle explicitly at work.)

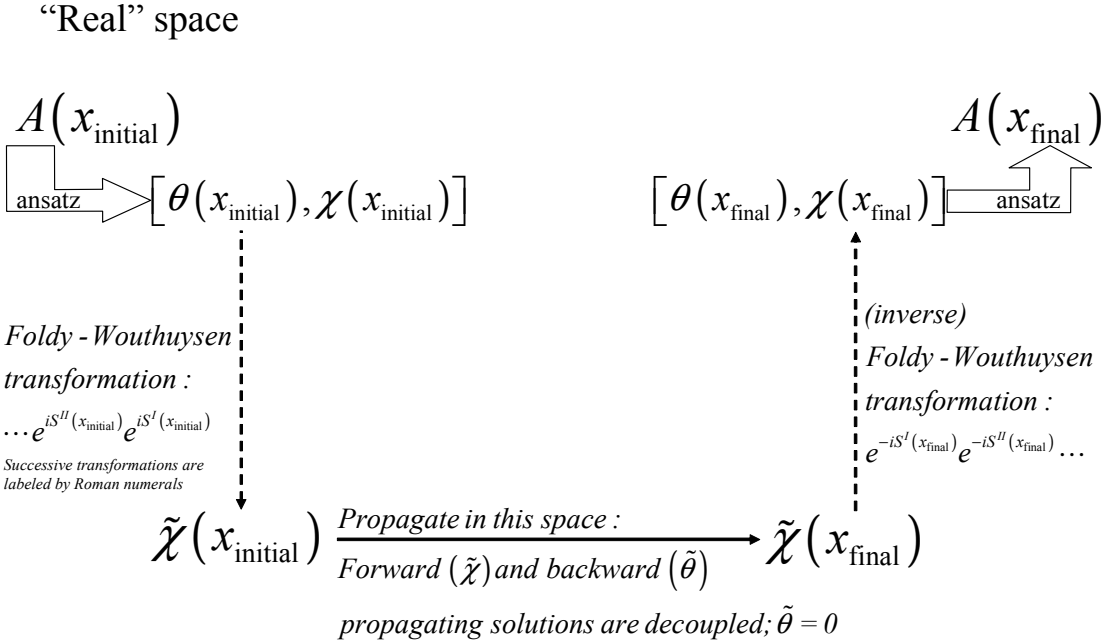

Figure C.1 - The strategy to be employed is diagrammed above. The ansatz is used to convert the scalar field into a 2-dimensional vector whose components are, roughly speaking, carriers of the uprange and downrange flux. The Foldy-Wouthuysen transformation is used to reformulate the problem such that forward and backward propagating solutions are decoupled. The problem is solved in transformed space. After propagation, the physical field is recovered. For many applications, propagation effects dominate, and it is possible to drop the contribution from the transformations at the endpoints.

C.2.2 Example: the range-independent sound speed profile

We now illustrate the Foldy-Wouthuysen technique by examining the case where there is no range dependence in the sound speed profile (i.e. μ can depend on the transverse coordinate $\underline{R}_T$, but it is independent of the range x). With the formal substitutions

$$\frac{\pi^2}{2m} \to \lambda \quad , \quad m \to k_0$$

the PE problem is identical to the non-relativistic reduction of the Klein-Gordon equation in the absence of an external field. The latter is solved in reference [57] (p. 200). The corresponding Foldy-Wouthuysen transformation is

$$\tilde{\Phi} = e^{iS}\Phi$$

where

$$S = \eta\xi\Theta(\lambda) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\Theta(\lambda)$$
$$\Theta(\lambda) \equiv -\frac{i}{2}\tanh^{-1}\frac{\lambda}{k_0+\lambda} \quad . \tag{C.13}$$

(This particular form follows the notation of reference [57]; however, in Appendix D.1 below, when we examine the relation connecting χ and A for the downrange problem (i.e., the transformation at the endpoints), the result will be recast in a form more conducive to the calculations to be pursued there [see equation (D.5)].)

The form of S was obtained heuristically by invoking an analogy to rotations about coordinate axes commonly used in quantum mechanics, while the value of Θ given in equation (C.13) comes from the requirement that off-diagonal elements of $\tilde{\mathcal{H}}$ must be zero. Note that S is pseudo-Hermitian and e^{iS} is pseudo-unitary.

The relation $\partial\lambda/\partial x$ implies that $\tilde{\mathcal{H}} = e^{iS}\mathcal{H}e^{-iS}$ and, from the definition of $\mathcal{H}$ given in (C.8), it follows that $e^{iS}\mathcal{H} = \mathcal{H}e^{-iS}$. Finally, this leads to

$$\tilde{\mathcal{H}} = \mathcal{H}e^{-2iS} = \eta k_0\sqrt{1+\frac{2\lambda}{k_0}}\,. \tag{C.14}$$

(The factor of 2 in the exponential cancels the factor of ½ in Θ.) The exponential reduces to

$$e^{-2iS} = \cosh\left[\tanh^{-1}\left(\frac{\lambda}{\lambda+k_0}\right)\right] + \sinh\left[\tanh^{-1}\left(\frac{\lambda}{\lambda+k_0}\right)\right],$$

which is easily reduced (e.g., using the symbolic manipulation program like Maple).

For a forward propagating wave, we have

$$\tilde{\Phi} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\tilde{\chi}\,,$$

where

$$-i\frac{\partial\tilde{\chi}}{\partial x} = k_0\sqrt{1+\frac{2\lambda}{k_0}}\,\tilde{\chi}\,. \tag{C.15}$$

Since the operator on the right hand side of equation (C.15) is (in this case) independent of x, this is an eigenvalue equation, and it follows that $\tilde{\chi}$ must be expressible as a sum of eigenvectors of λ ($\tilde{\chi} = \sum_n c_n\tilde{\chi}_{\lambda_n}$). Therefore, the transformation at the endpoints

$$A = \theta + \chi = \begin{bmatrix}1 & 1\end{bmatrix}e^{-iS(\lambda)}\begin{bmatrix}0 \\ 1\end{bmatrix}\tilde{\chi} = \sum_n c_n\begin{bmatrix}1 & 1\end{bmatrix}e^{-iS(\lambda_n)}\begin{bmatrix}0 \\ 1\end{bmatrix}\tilde{\chi}_{\lambda_n} \tag{C.16}$$

simply involves rescaling each eigenvector by a constant, and so A also satisfies equation (C.15). This is the standard PE for a range-independent sound speed profile (first introduced in equation 3.24 of [15]). Finally, expanding in $2\lambda/k_0$, we have

$$-i\frac{\partial A}{\partial x} = \frac{\nabla_T^2}{2k_0}A + k_0\left(1-\mu\right)A, \tag{C.17}$$

and with $A = \Psi e^{ik_0 x}$, we recover the basic, lowest order PE, as it appears, for example, in [15] (equation 1.21). It has been recognized previously in [118] that this equation can be obtained using the Foldy-Wouthuysen transformation. (Also note that to obtain this range-*in*dependent result, it was *not* necessary to drop the contribution from the endpoints.)

Thus for a range-*in*dependent sound speed profile, the Foldy-Wouthuysen transformation recovers the various well known forms of the parabolic equation. Assuming μ to be slowly varying, $\partial\mu/\partial x$ is a 2nd order correction, and the 1st order result, equation (C.17), is also applicable to the more general case of a range-dependent sound speed profile.

C.2.3 The general range-dependent problem

C.2.3.1 The expansion parameter

A perturbative solution to the range-dependent problem will now be obtained by repeated applications of the Foldy-Wouthuysen transformation. The formal expansion parameter is the dimensionless operator $\Lambda \equiv \lambda/k_0$. Note that if we take the operator $\Lambda = \nabla_T^2/2k_0^2 - \mu$, and operate it on eigensolutions (i.e., modes), we find that the first operator $\nabla_T^2/2k_0^2$ roughly corresponds to the square of the grazing angle and the second $-\mu$ measures the deviation of the local sound speed from the reference value. A sufficient, but strictly speaking not necessary, condition for the operator Λ to be small is that the grazing angles and sound speed deviation both be small. (The pathological case where both are large, but cancel will be discussed near the beginning of Appendix K.1.1.2.)

The range dependence is assumed to be small and slowly varying, and so the dimensionless operator $k_0^{-1}\partial\Lambda/\partial x = -k_0^{-1}\partial\mu/\partial x$ is formally 2nd order. In general, either the operator Λ or the operator $k_0^{-1}\partial/\partial x$ contributes an order.

Some of what follows can also be found in [57], but the full calculation is reproduced here for completeness. Looking at the definitions $\mathcal{O} = \lambda\xi$ and $\mathcal{E} = \lambda\eta$, we see that, unlike for the calculation in the reference, these operators are now of the same order, and, even on a formal level, some care must be taken in transferring the previous results. In particular, when the calculation is carried through 4th order, it will be necessary to add terms which did not appear previously.

Before proceeding with the calculation, let us examine the source of these differences. Consider the expansion parameter

$$\Lambda = \frac{\nabla_T^2}{2k_0^2} - \mu .$$

For comparison to the quantum problem, make the usual identification of the transverse derivative $i\underline{\nabla}_T$ with the momentum p, $k_0\mu$ with a scalar potential ϕ, k_0 with the mass m, and explicitly display the speed of light c which was set equal to unity in the notation of [57] (as was $\hbar$). The result is

$$\Lambda \to -\left(\frac{p^2}{2m^2c^2} + \frac{\phi}{mc^2} \right).$$

With $p \sim mv + \mathrm{O}(v/c)$ (note that v is the velocity of the particle), the expansion parameter becomes

$$\Lambda \to -\left(\frac{v^2}{2c^2} + \frac{\phi}{mc^2} \right).$$

This would mean that the expansion is in v/c and in the ratio of the potential energy to the rest energy of the particle. Thus, following the practice appropriate for the acoustic calculation, the kinetic and potential energies should be placed on an equal footing.

While such an expansion would be very reasonable from a *formal* relativistic point of view, it is not followed in many practical quantum mechanical applications. Of the calculations performed in reference [57], the one most closely analogous to the acoustic problem (because it is spinless; i.e., has no non-physical degrees of freedom) is given in chapter 9. However in that particular calculation ϕ is not small compared to the rest energy, and it is therefore not treated as an expansion parameter. On the other hand for the calculation involving the hydrogen atom (chapter 4), ϕ is considered to be of smaller order than the kinetic energy term.

C.2.3.2 The iterative procedure

To generate the expansion, a succession of transformations is used, each having the form $\tilde{\Phi} = e^{iS}\Phi$. With each iteration, S is of increasing order in Λ, and the transformation is designed to diagonalize $\tilde{\mathcal{H}}$ to that order. Henceforth, Roman numeral superscripts will denote the order of S and of the diagonalized part of $\tilde{\mathcal{H}}$. The corresponding $\tilde{\Phi}$, $\mathcal{O}$ and $\mathcal{E}$ will also be labeled in this way. For example, $\tilde{\Phi}^I = e^{iS^I}\Phi$ obeys the equation

$$i\frac{\partial \tilde{\Phi}^I}{\partial x} = \tilde{\mathcal{H}}^I \tilde{\Phi}^I , \qquad \text{(C.18)}$$

where $\tilde{\mathcal{H}}^I = k_0\eta + \mathcal{E}^I + \mathcal{O}^I$ to $\mathrm{O}(\Lambda)$.

Substituting $e^{-iS^I}\tilde{\Phi}^I$ for Φ in the original equation of motion (C.7), we have the result

$$0 = e^{iS^I}\left(\mathcal{H} - i\frac{\partial}{\partial x}\right)e^{-iS^I}\tilde{\Phi}^I . \tag{C.19}$$

From a theorem given in reference [57] (p. 49), and using $\mathcal{H} = \mathrm{O}(\Lambda^0)$ and $S^I = \mathrm{O}(\Lambda)$, we have

$$\begin{aligned} e^{iS^I}\mathcal{H}e^{-iS^I} \quad = \quad & \mathcal{H} + i\left[S^I,\mathcal{H}\right] - \frac{1}{2}\left[S^I,\left[S^I,\mathcal{H}\right]\right] - \frac{i}{3!}\left[S^I,\left[S^I,\left[S^I,\mathcal{H}\right]\right]\right] \\ & + \frac{1}{4!}\left[S^I,\left[S^I,\left[S^I,\left[S^I,\mathcal{H}\right]\right]\right]\right] + \mathrm{O}(\Lambda^5) \end{aligned} , \tag{C.20}$$

and, also using $\left[S^I,(\partial/\partial x)\right] = -\dot{S}^I = \mathrm{O}(\Lambda^2)$,

$$e^{iS^I}\frac{\partial}{\partial x}e^{-iS^I} = \frac{\partial}{\partial x} - i\dot{S}^I + \frac{1}{2}\left[S^I,\dot{S}^I\right] + \frac{i}{3!}\left[S^I,\left[S^I,\dot{S}^I\right]\right] + \mathrm{O}(\Lambda^5). \tag{C.21}$$

These results are substituted into (C.19) and the expression for $\tilde{\mathcal{H}}^I$ is obtained by comparison to (C.18). (Recall that the commutator $[,]$ is defined in footnote f.)

By analogy to the range-independent calculation, choose

$$S^I = -\frac{i\eta\mathcal{O}}{2k_0} \tag{C.22}$$

and evaluate the expression for $\tilde{\mathcal{H}}^I$ using $\eta\mathcal{O} = -\mathcal{O}\eta$, $\eta\mathcal{E} = \mathcal{E}\eta$, $\eta^2 = \mathbf{1}$, and equation (C.8).

Since $\mathcal{E}/k_0, \mathcal{O}/k_0 = \mathrm{O}(\Lambda)$, the anticommutation of $\mathcal{O}$ and η implies that $i\left[S^I,\mathcal{H}\right] = -\mathcal{O} + \mathrm{O}(\Lambda^2)$. All other new terms such as those proportional to $\left[S^I,\left[S^I,\mathcal{H}\right]\right]$ or $\dot{S}^I$ are second order or higher. Thus, by construction, the Foldy-Wouthuysen transformation cancels the odd 1st order terms, and replaces them with new terms of higher order.

Note that this result depends only on the definition of S and the anticommutation relation $\{\eta,\mathcal{O}\} = 0$. The procedure can be repeated order-by-order, with the order of the remaining odd terms increasing with each iteration. As can be seen from the following argument, the anticommutation relation will always be met.

Beginning with the Hamiltonian $\mathcal{H}$ and applying repeated transformations of the sort just discussed, the transformed Hamiltonian will consist of terms whose matrix part is

constructed from products of η's and ξ's. Since $\xi^{2n} = (-1)^n \mathbf{1}$, $\eta^{2n} = \mathbf{1}$ and $\{\xi, \eta\} = 0$, the matrix part of the odd operators will be either $\eta\xi$ or ξ while that of the even operators η or $\mathbf{1}$. It follows that the odd operators all anticommute with η.

The anticommutation relation, together with the iterative nature of the procedure also insures that energy will be conserved no matter how many times the procedure is repeated. Before iteration, $\mathcal{H}$ and therefore $\mathcal{O}$ are pseudo-Hermitian ($\mathcal{O}^\dagger \mathcal{H} = \mathcal{H}\mathcal{O}$), which, using the anticommutation relation, also implies that $S = -i\eta\mathcal{O}/2k_0$ is pseudo-Hermitian. Thus, e^{iS} is pseudo-unitary and the transformation preserves energy conservation. The new Hamiltonian and consequently the new $\mathcal{O}$ are therefore once again pseudo-Hermitian, and the process can start all over again.

In this way, we have provided an order-by-order prescription for diagonalizing the Hamiltonian. This implies that the "true" coupling between forward and backward modes (i.e. backscatter) is of higher order than any finite order of perturbation theory, and that the perturbative expansion constructed in this way must be asymptotic. We will return to this issue later.

C.2.4 Implementing the procedure

On page 50 of [57], the terms needed to implement the first Foldy-Wouthuysen transformation are evaluated. The results are included here for completeness. Note that any odd operator to an even power is even. Terms of $\mathrm{O}(\Lambda^5)$ and higher are dropped. Recall that S^I is given by equation (C.22). The first iteration of the Foldy-Wouthuysen procedure yields the Hamiltonian $\tilde{\mathcal{H}}^I$. From equations (C.19) to (C.21), $\tilde{\mathcal{H}}^I$ is given by the original matrix Hamiltonian $\mathcal{H}$ followed by a sum over the following terms:

$$
\begin{aligned}
i\left[S^I, \mathcal{H}\right] &= -\mathcal{O} + \frac{\eta}{2k_0}\left[\mathcal{O}, \mathcal{E}\right] + \frac{1}{k_0}\eta\mathcal{O}^2 \\
-\frac{1}{2}\left[S^I, \left[S^I, \mathcal{H}\right]\right] &= -\frac{\eta\mathcal{O}^2}{2k_0} - \frac{1}{8k_0^2}\left[\mathcal{O}, \left[\mathcal{O}, \mathcal{E}\right]\right] - \frac{\mathcal{O}^3}{2k_0^2} \\
-\frac{i}{3!}\left[S^I, \left[S^I, \left[S^I, \mathcal{H}\right]\right]\right] &= \frac{\mathcal{O}^3}{6k_0^2} - \frac{\eta\mathcal{O}^4}{6k_0^3} \\
\frac{1}{4!}\left[S^I, \left[S^I, \left[S^I, \left[S^I, \mathcal{H}\right]\right]\right]\right] &= \frac{\eta\mathcal{O}^4}{24k_0^3} \\
-\dot{S}^I &= \frac{i\eta\dot{\mathcal{O}}}{2k_0} \\
-\frac{i}{2}\left[S^I, \dot{S}^I\right] &= -\frac{i}{8k_0^2}\left[\mathcal{O}, \dot{\mathcal{O}}\right].
\end{aligned}
$$

To the order that we are concerned with, it would at first appear that two terms are missing:

$$-\frac{\eta}{48k_0^2}\Big[\mathcal{O},\Big[\mathcal{O},[\mathcal{O},\mathcal{E}]\Big]\Big] \quad \text{in} \quad -\frac{i}{3!}\Big[S^I,\Big[S^I,\Big[S^I,\mathcal{H}\Big]\Big]\Big]$$

and

$$\frac{1}{6}\Big[S^I,\Big[S^I,\dot{S}^I\Big]\Big] \quad = \quad -\frac{i\eta}{24k_0^3}\Big[\mathcal{O},\Big[\mathcal{O},\dot{\mathcal{O}}\Big]\Big]$$

However, these terms are 4th order and odd. The next Foldy-Wouthuysen transformation will remove these odd terms, replacing them with terms of 5th order and higher, which is of higher order than concerns us here. Therefore, to obtain the diagonalized Hamiltonian to $\mathrm{O}\left(\Lambda^4\right)$, we can use the results from [57] without modification. However, we have to be careful to make sure we include all relevant terms during the next stages of the diagonalization procedure. As mentioned already, the order counting in the reference is different from that which must be used for the parabolic equation.

Combining the terms calculated above, we have the result

$$\begin{aligned}
\tilde{\mathcal{H}}^I &= k_0\eta + \mathcal{E}^I + \mathcal{O}^I + \mathrm{O}\left(\Lambda^5\right) \\
\mathcal{E}^I &= \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\Big[\mathcal{O},[\mathcal{O},\mathcal{E}]\Big] - \frac{i}{8k_0^2}\Big[\mathcal{O},\dot{\mathcal{O}}\Big] \qquad \text{(C.23)} \\
\mathcal{O}^I &= \frac{\eta}{2k_0}[\mathcal{O},\mathcal{E}] - \frac{\mathcal{O}^3}{2k_0^2} + \frac{i\eta\dot{\mathcal{O}}}{2k_0} = \mathrm{O}\left(\Lambda^2\right).
\end{aligned}$$

So far, these results are the same as for the relativistic reduction problem in quantum mechanics.

Now, the procedure is iterated to eliminate odd terms, which are 2nd order in Λ. The second Foldy-Wouthuysen transformation is:

$$\begin{aligned}
S^{II} &= -\frac{i\eta\mathcal{O}^I}{2k_0} = \mathrm{O}\left(\Lambda^2\right) \\
\tilde{\mathcal{H}}^{II} &= \tilde{\mathcal{H}}^I + i\Big[S^{II},\tilde{\mathcal{H}}^I\Big] - \frac{1}{2}\Big[S^{II},\Big[S^{II},\tilde{\mathcal{H}}^I\Big]\Big] - \dot{S}^{II} + \mathrm{O}\left(\Lambda^5\right) \qquad \text{(C.24)} \\
&= k_0\eta + \mathcal{E}^I + i\Big[S^{II},\mathcal{E}^I\Big] + \frac{i}{2}\Big[S^{II},\mathcal{O}^I\Big] + \frac{i\eta\dot{\mathcal{O}}^I}{2k_0} + \mathrm{O}\left(\Lambda^5\right),
\end{aligned}$$

where the result $\Big[S^{II},k_0\eta\Big] = i\mathcal{O}^I$ was used to simplify $\tilde{\mathcal{H}}^{II}$. Simplifying the commutators, we now have

$$\begin{aligned}\tilde{\mathcal{H}}^{II} &= k_0\eta + \mathcal{E}^{II} + \mathcal{O}^{II} + \mathrm{O}\left(\Lambda^5\right) \\ \mathcal{E}^{II} &= \mathcal{E}^{I} + \eta\frac{\left(\mathcal{O}^{I}\right)^2}{2k_0} \\ \mathcal{O}^{II} &= \frac{\eta}{2k_0}\left[\mathcal{O}^{I},\mathcal{E}^{I}\right] + \frac{i\eta\dot{\mathcal{O}}^{I}}{2k_0} = \mathrm{O}\left(\Lambda^3\right)\end{aligned} \quad . \tag{C.25}$$

Note that the second term in $\mathcal{E}^{II}$ is new; this term did not appear in the calculation of reference [57] (see paragraph below equation (C.29)). Now, we apply the Foldy-Wouthuysen transformation yet again

$$S^{III} = -\frac{i\eta\mathcal{O}^{II}}{2k_0} = \mathrm{O}\left(\Lambda^3\right) \tag{C.26}$$

and obtain

$$\tilde{\mathcal{H}}^{III} = k_0\eta + \mathcal{E}^{II} + i\left[S^{III},\mathcal{E}^{II}\right] - \dot{S}^{III} + \mathrm{O}\left(\Lambda^5\right). \tag{C.27}$$

The last two terms of $\tilde{\mathcal{H}}^{III}$ are 4th order odd terms. Once again, note that the only effect of the fourth Foldy-Wouthuysen transformation will be to push such odd 4th order terms up to higher order, so we finally have

$$\tilde{\mathcal{H}}^{IV} = k_0\eta + \mathcal{E}^{II}, \tag{C.28}$$

where

$$\begin{aligned}\mathcal{E}^{II} = {} & \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right] - \frac{i}{8k_0^2}\left[\mathcal{O},\dot{\mathcal{O}}\right] \\ & + \frac{\eta}{8k_0^3}\left(-\left[\mathcal{O},\mathcal{E}\right]^2 - i\left\{\dot{\mathcal{O}},\left[\mathcal{O},\mathcal{E}\right]\right\} + \dot{\mathcal{O}}^2\right) + \text{ 5th order}\end{aligned} \quad . \tag{C.29}$$

(This recovers equation (3.10).) Recall that $\{,\}$ denotes the anticommutator. The last term is the expansion of $\eta\left(\mathcal{O}^{I}\right)^2 \Big/ 2k_0$.

Note that even on this formal level, we now have extra 4th order terms, which do not appear in the results of [57]. This is because powers of the expansion need to be tabulated differently in that problem. On the other hand, note that this is the only difference so far between the quantum mechanical and acoustic problems. Indeed, the only assumption that went into obtaining equation (C.29) was that the Hamiltonian $\mathcal{H}$ have the basic form (C.7), and that its constituents $\mathcal{O}$ and $\mathcal{E}$ obey the commutation relations described at the end of Subsection C.2.3.2 above. Equation (C.29) is therefore quite general, and will apply to the acoustic problem where the density varies, and even to vector fields (e.g., electromagnetic and elastodynamic fields).

Now substitute $\mathcal{E} = \lambda\eta$ and $\mathcal{O} = \lambda\xi$ into (C.29). This gives

$$\begin{aligned}\left[\mathcal{O},\mathcal{E}\right]^2 &= 4\lambda^4 \\ -i\left\{\dot{\mathcal{O}},\left[\mathcal{O},\mathcal{E}\right]\right\} &= 2\eta\left[\lambda^2,\dot{\lambda}\right] \\ \dot{\mathcal{O}}^2 &= -\dot{\lambda}^2\end{aligned} \qquad \text{(C.30)}$$

Combining results, we have

$$\begin{aligned}\tilde{\mathcal{H}}^{IV} &= \eta k_0\left(1+\frac{\lambda}{k_0}-\frac{\lambda^2}{k_0^2}+\frac{\lambda^3}{2k_0^3}-\frac{5\lambda^4}{8k_0^4}-\frac{\dot{\lambda}^2}{8k_0^4}\right) \\ &\quad +\frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right]-\frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right]+\mathrm{O}\left(\Lambda^5\right) \\ &= \eta k_0\left(\sqrt{1+\frac{2\lambda}{k_0}}-\frac{\dot{\lambda}^2}{8k_0^4}\right)+\frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right]-\frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right]+\mathrm{O}\left(\Lambda^5\right)\end{aligned} \quad , \qquad \text{(C.31)}$$

where recall $\lambda \equiv \nabla_T^2/2k_0 - \mu k_0$ and there is an implicit unit matrix $\mathbf{1}$ in the last two terms. In the last line, we have formally replaced the terms $1+\lambda/k_0-\lambda^2/2k_0^2+\lambda^3/2k_0^3-5\lambda^4/8k_0^4$ with $\sqrt{1+2\lambda/k_0}$, as always following the common practice of defining the function of an operator by the Taylor-Series expansion (the classic example of this being identification of the formal expression $\exp\left(a\frac{d}{dx}\right)$ with translation by a). As was assumed in deriving equation (C.31) and everywhere else this paper, this implicitly assumes that the operator $2\lambda/k_0$ is small in some sense.

Note that in the limit $\dot{\lambda}\to 0$ (i.e., no range dependence) we recover the expansion of $\tilde{\mathcal{H}} = \eta k_0\sqrt{1+2\lambda/k_0}$, which is indeed the result for a range-independent sound speed profile. Also note that if there is no transverse dependence in μ, then the commutator terms disappear as well. Thus the commutator terms are associated with the simultaneous presence of both range and transverse dependence.

For the diagonal Hamiltonian $\tilde{\mathcal{H}}$, the pure forward and backward propagating solutions,

$$\tilde{\Phi}\propto\begin{pmatrix}0\\1\end{pmatrix} \quad \text{and} \quad \tilde{\Phi}\propto\begin{pmatrix}1\\0\end{pmatrix} \quad \text{respectively},$$

remain of the same vector form as they propagate. For these solutions, η can be replaced by $\mp\mathbf{1}$, so that the energy flux is proportional to $\tilde{\Phi}^\dagger\tilde{\Phi}$. Following the same reasoning as before, it follows that the range propagation operator must be unitary and $\tilde{\mathcal{H}}$ must be Hermitian. Being diagonal and Hermitian, it remains pseudo-Hermitian as well. Using the expression for $\tilde{\mathcal{H}}^{IV}$ given in equation (C.31), Hermiticity can also be verified directly by inspection. Note that the forward and backward propagating solutions independently conserve energy, the perturbative formalism making no allowance for energy loss due to backscatter.

The explicit appearance of the complex number i as a coefficient in equation (C.31) creates the illusion that the propagation may be diffusive. However, note the term is actually Hermitian, and so overall energy is conserved, and there is be no diffusion here. It will shortly be shown that it is possible to further transform the result (C.31), among other things, removing these complex coefficients.

C.2.5 Manifestly range-reciprocal form

It is possible to apply a variation of the Foldy-Wouthuysen transformation to rearrange terms without changing the order of the diagonalized part of the Hamiltonian. For the Hamiltonian (C.31), choose

$$S^{IV.1} = \frac{\eta}{8k_0^2}\frac{\partial\lambda}{\partial x} = \frac{\eta\dot{\lambda}}{8k_0^2} = \mathrm{O}\left(\Lambda^2\right). \tag{C.32}$$

(There is here a slight labeling change here. The Roman numeral on S still corresponds to the order to which the Hamiltonian is diagonal, but not to that of S itself any more. The "1" after the Roman numeral identifies $S^{IV.1}$ as the generator of the *first* order-preserving variant of the Foldy-Wouthuysen transformation.) Note that $S^{IV.1}$ is diagonal and Hermitian, so the transformation $e^{iS^{IV.1}}$ is unitary, diagonal and pseudo-unitary, so energy conservation considerations discussed in the previous section will not be affected by the transformation.

Now, we have

$$\begin{aligned}
\tilde{\mathcal{H}}^{IV.1} &= \tilde{\mathcal{H}}^{IV} + i\left[S^{IV.1}, \eta\left(k_0 + \lambda - \frac{\lambda^2}{2k_0}\right)\right] - \frac{1}{2}\left[S^{IV.1}, \left[S^{IV.1}, \eta k_0\right]\right] - \dot{S}^{IV.1} + O\left(\Lambda^5\right) \\
&= \eta k_0\left(\left[1 + \frac{\lambda}{k_0} - \frac{\lambda^2}{k_0^2} + \frac{\lambda^3}{2k_0^3} - \frac{5\lambda^5}{8k_0^4}\right] - \frac{\ddot{\lambda}}{8k_0^3} - \frac{\dot{\lambda}^2}{8k_0^4}\right) - \frac{3i}{16k_0^3}\left[\lambda^2, \dot{\lambda}\right] + \mathrm{O}\left(\Lambda^5\right) \\
&= \eta k_0\left(\sqrt{1 + \frac{2\lambda}{k_0}} - \frac{\ddot{\lambda}}{8k_0^3} - \frac{\dot{\lambda}^2}{8k_0^4}\right) - \frac{3i}{16k_0^3}\left[\lambda^2, \dot{\lambda}\right] + \mathrm{O}\left(\Lambda^5\right).
\end{aligned} \tag{C.33}$$

Perform a second such transformation;

$$S^{IV.2} = \frac{-3\eta}{16k_0^3}\frac{\partial\left(\lambda^2\right)}{\partial x} = \frac{-3\eta}{16k_0^3}\left\{\lambda, \dot{\lambda}\right\} = \mathrm{O}\left(\Lambda^3\right), \tag{C.34}$$

where recall $\left\{\lambda, \dot{\lambda}\right\} = \lambda\dot{\lambda} + \dot{\lambda}\lambda$. Now,

$$\begin{aligned}\tilde{\mathcal{H}}^{IV.2} &= \tilde{\mathcal{H}}^{IV.1} + i\left[S^{IV.2}, \eta\left(k_0+\lambda\right)\right] - \dot{S}^{IV.2} + O\left(\Lambda^5\right) \\ &= \eta k_0\left(\left[1+\frac{\lambda}{k_0}-\frac{\lambda^2}{k_0^2}+\frac{\lambda^3}{2k_0^3}-\frac{5\lambda^5}{8k_0^4}\right]-\frac{\ddot{\lambda}}{8k_0^3}+\frac{\dot{\lambda}^2}{4k_0^4}+\frac{3\left\{\lambda,\ddot{\lambda}\right\}}{16k_0^4}\right)+\mathrm{O}\left(\Lambda^5\right) \\ &= \eta k_0\left(\sqrt{1+\frac{2\lambda}{k_0}}-\frac{\ddot{\lambda}}{8k_0^3}+\frac{\dot{\lambda}^2}{4k_0^4}+\frac{3\left\{\lambda,\ddot{\lambda}\right\}}{16k_0^4}\right)+\mathrm{O}\left(\Lambda^5\right).\end{aligned} \tag{C.35}$$

Equation (C.35) is the most important result of this appendix and it corresponds to equation (3.11) in the main body of the text. Once again, note that the square root operator above is essentially a placeholder for its Taylor Series expansion. The distinction is important, when the expansion parameter $2\lambda/k_0 > 1$, but this is outside the purview of this work (see the discussion in the third-to-last paragraph of Appendix B).

Thus, $\tilde{\mathcal{H}} = \eta H$ where

$$H = k_0\left(\sqrt{1+\frac{2\lambda}{k_0}}-\frac{\ddot{\lambda}}{8k_0^3}+\ldots\right), \tag{C.36}$$

and so

$$\begin{aligned} i\dot{\Phi} &= \eta H \Phi \\ i\begin{pmatrix}\dot{\theta}\\ \dot{\chi}\end{pmatrix} &= \eta H \begin{pmatrix}\theta\\ \chi\end{pmatrix}.\end{aligned}$$

For one-way (downrange) propagation, $\tilde{\theta} = 0$ and dropping the tilde on $\tilde{\chi}$, we have

$$-i\dot{\chi} = H\chi.$$

Note that the new terms manifestly exhibit range reciprocity. This means that the substitution $x \to -x$ will not change the form of the scalar Hamiltonian at all, and in the overall matrix equation it only flips the uprange and downrange labels. The original wave equation obeys this symmetry, and it is good to get a form of the PE that also manifestly maintains this symmetry. For this reason, the form given in equation (C.36) (and its higher-order versions) above will always be used in preference to the scalar version of the form given in equation (C.31).

Recall that modern wide angle PE's based on the so-called Padé approximation do not necessarily reproduce the series expansion in the appropriate limit (see footnote m), and so adaptation of results such as equation (C.36) to these approaches will be non-trivial.

It can also be shown that, to the order obtained here, the result is independent of the choice of k_0.

Also note that to 3rd order, we have the straightforward substitution $\mu \to \mu - \ddot{\mu}/\left(8k_0^2\right)$ (recall that $\lambda = \nabla_T^2/2k_0 - k_0\mu$ and $\ddot{\mu} = \partial^2\mu/\partial x^2$ refers to the second derivative with respect to the *range*). To this order, this is equivalent to rescaling the sound speed $c \to c - \ddot{c}/\left(8k_0^2\right)$.

The results may seem somewhat surprising at first. For example, the transformation $S^{IV.1}$, roughly speaking, substitutes a dependence on $\partial\left(\nabla_T^2\mu\right)/\partial x$ for one on $\ddot{\mu} = \partial^2\mu/\partial x^2$. These terms can be zero at different times, but this apparent discrepancy disappears after closer scrutiny. If $\ddot{\mu} = 0$, then $[H, \dot{\mu}] \propto d\mu/dx$, and the commutator terms simply contribute to the transformation at the endpoints. The contribution is only a phase change, since the term is Hermitian. In fact, since we always assume the range dependence is locally zero at the endpoints, this contribution is zero, and the commutator terms do not contribute at all to the final answer. Now, lets consider the opposite scenario: if $\left[\lambda.\dot{\lambda}\right] = 0$, then $\ddot{\mu} = d\dot{\mu}/dx$ and $\ddot{\mu}$ is a perfect derivative, and again we are left with a trivial endpoint (phase) change, which goes away entirely if we neglect the range dependence at the endpoints.

In this way, we can begin to see how these two very different representations of the same problem still lead to the same solution. The notion that very different looking Hamiltonians yield the same range propagation results is not unique to this problem. Canonical transformations often have this attribute. This is most easily seen when the problem is formulated in terms of the Lagrangian. The equations of motion are not changed by the addition of a total time derivative of a function of the coordinates and the time ($df\left(q,t\right)/dt$). However, after returning to the Hamiltonian picture, the connection between the corresponding Hamiltonians may be quite obscure.

C.2.6 A physically intuitive picture of the results

We are now in a position to develop physical interpretations of the Foldy-Wouthuysen procedure. The transformations used to diagonalize the Hamiltonian seek out the effects which accumulate during propagation, and separate them from effects which cancel everywhere except at the endpoints. The former come from "virtual" oscillations between forward and backward propagating modes. This concept can be developed as follows. Recall the prescription $\mu \to \mu - \ddot{\mu}/\left(8k_0^2\right)$. Consider a coordinate shift $x \to x + \delta x$ and expand $\mu\left(x + \delta x\right)$. We have

$$\mu\left(x + \delta x\right) = \mu\left(x\right) + \dot{\mu}\left(x\right)\delta x + \frac{1}{2}\ddot{\mu}\left(x\right)\delta x^2,$$

and treating δx as a random fluctuation to be averaged, we have

$$\left\langle \mu(x+\delta x)\right\rangle = \mu(x) + \dot{\mu}(x)\left\langle \delta x\right\rangle + \frac{1}{2}\ddot{\mu}(x)\left\langle \delta x^2\right\rangle .$$

Comparing the prescription $\mu \to \mu - \ddot{\mu}/\left(8k_0^2\right)$, we conclude that the fluctuation has average $\left\langle \delta x\right\rangle = 0$ (this is perfectly reasonable; most random fluctuations have this property) and root mean square displacement

$$\left\langle \delta x^2\right\rangle = -\frac{1}{4k_0^2}.$$

Note that this corresponds to fluctuations on the order $\delta x \sim i/\left(2k_0\right)$. The quantity is imaginary because it is associated with an evanescent wave phenomenon. As alluded to in Section 2.1, the 1st-order boundary term is sometimes moved from the endpoint transformation into the Hamiltonian, where it becomes $i\dot{\mu}/2$ (e.g., see Schurman *et al.*[19], and also Appendix B of reference [1]). It was pointed out in Section 2.1 that this is not usually a good practice, but here it is instructive. Including both the new Foldy-Wouhuysen term and this term in the Hamlitonian, we are left with the simple prescription $\mu(x) \to \mu\left(x + i/2k_0\right)$; i.e., a small shift of x into the complex plane.

Note that when averaged over any scale resolvable by the wavelengths of the field involved, no energy flows from the forward into the backward propagating modes (or vice versa). This is what is meant by a virtual oscillation between the modes. Higher-order terms correspond to virtual fluctuations into multiple backward propagating modes. (This can be deduced by once again appealing to the analogy to quantum field theory. The Feynman diagram picture identifies the order of a term in the perturbative expansion with the number of virtual particles [or modes] created.) The diagonalization procedure also serves to push "true" (as opposed to virtual) backscatter to its "natural" place at infinite order in perturbation theory.

The oscillations between forward and backward propagating modes have the attributes of a harmonic oscillator. The transformations used to simplify the diagonal representations of the Hamiltonian can be understood as translations of the zero point of the harmonic oscillator. The crucial quantity characterizing both the virtual fluctuations and the "true" backscatter is $\ddot{\mu}$, which corresponds to the spring constant of the oscillator. For "true" backscatter, the oscillator is not bound, and the spring constant is negative. Once again, we are reminded that "true" backscatter is not a process that lends itself to this kind of a perturbative approach. For virtual oscillations, on the other hand, the analogous oscillator is bound, the spring constant positive, small fluctuations remain small, and perturbation theory is appropriate.

D Appendix: The transformation between the pressure and the PE field

The goal here is to establish the relationship between the auxiliary field $\tilde{\chi}$ that propagates according to the PE (equation (3.13); in this appendix we put tildes on $\tilde{\chi}$ and $\tilde{H}$ to clearly distinguish between the ansatz (no tildes) and the transformed problem where the matrix Hamiltonian is diagonal (tildes)), and the actual pressure field A that propagates according to the Helmholtz equation (equation (2.2)).

D.1 The transformation when the density is everywhere the same

From the Foldy-Wouthuysen ansatz (equation (3.2); the definition of the 2-dimensional vector Φ) we have immediately the equation

$$\begin{pmatrix}1 & 1\end{pmatrix}\Phi = A\,. \tag{D.1}$$

We also need to be able to go from the 2-dimensional field vector that propagates according to the diagonalized Hamiltonian $\tilde{\Phi}$ back to the ansatz vector Φ. Recall from reference [1] (or equivalently Appendix C.2.3.2) that the Foldy-Wouthuysen procedure is iterative. If $\tilde{\Phi}_{n-1}$ obeys a matrix equation of motion that is diagonalized to order $n-1$, then one more Foldy-Wouthuysen transformation

$$\tilde{\Phi}_n = e^{iS_{n-1}}\tilde{\Phi}_{n-1} \tag{D.2}$$

will produce a field Φ_n that propagates according to a matrix equation of motion that is diagonalized to order n. So, we can write in general

$$\Phi = e^{-iS_I}e^{-iS_{II}}e^{-iS_{III}}\cdots\tilde{\Phi}$$

and

$$A = \begin{pmatrix}1 & 1\end{pmatrix}\Phi = \begin{pmatrix}1 & 1\end{pmatrix}e^{-iS_I}e^{-iS_{II}}e^{-iS_{III}}\cdots\tilde{\Phi}\,. \tag{D.3}$$

The Foldy-Wouthuysen (FW) procedure precisely determines $S_I, S_{II}, S_{III}\cdots$, and we can substitute for these operators to calculate product $e^{-iS_I}e^{-iS_{II}}e^{-iS_{III}}\cdots$ order by order. (Note that in this context, Roman numerals enumerate successive FW transformations, and do not refer to sides of an interface.) In Appendix D.2, we will employ precisely this strategy to obtain the $\chi \leftrightarrow A$ transformation good to O($\lambda^2, \lambda\gamma$) for the case when $\gamma \equiv (\rho_0 - \rho)/2\rho_0$ is non-zero (i.e., the density is not uniformly constant). However, here where the density is held uniformly constant, let us do something a little different. If we assume that there is no local range dependence (e.g., those extra Lamb-shift terms are all zero), we can take advantage of the fact that we already know how to calculate

$e^{-iS_I}e^{-iS_{II}}e^{-iS_{III}}\cdots$ to ∞-order. To do so, we follow Section II.B in reference [1], Section [9.7] in reference [57], and the treatment above in Appendix C.2.2. Rather than iterative infinite series, only a single Foldy-Wouthuysen transformation is needed to fully diagonalize the matrix Hamiltonian $\mathcal{H}$. In particular, we have

$$i\frac{\partial\tilde{\Phi}}{\partial x} = k_0\eta\sqrt{1+\frac{2\lambda}{k_0}}\tilde{\Phi}\,, \tag{D.4}$$

where (see, for example, equation 25 in reference [1] or equation (C.13) above)

$$\begin{aligned}\tilde{\Phi} &= e^{iS}\Phi \\ S &= \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\left(\frac{-i}{2}\right)\varphi \\ \varphi &\equiv \tanh^{-1}\left[\frac{\lambda}{\lambda+k_0}\right].\end{aligned} \tag{D.5}$$

The equations have been slightly recast into a form more conducive to the calculations to be pursued below.

Thus we have

$$\tilde{\Phi} = e^{iS}\Phi = e^{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{\varphi}{2}}\Phi$$

and we need to evaluate the exponential. Using the symbolic manipulation package Maple™, we have

$$e^{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{\varphi}{2}} = \begin{pmatrix}\dfrac{e^{\varphi/2}+e^{-\varphi/2}}{2} & \dfrac{e^{\varphi/2}-e^{-\varphi/2}}{2}\\ \dfrac{e^{\varphi/2}-e^{-\varphi/2}}{2} & \dfrac{e^{\varphi/2}+e^{-\varphi/2}}{2}\end{pmatrix}$$

or

$$e^{iS} = e^{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{\varphi}{2}} = \frac{1}{2\sqrt{e^{\varphi}}}\begin{pmatrix}1+e^{\varphi} & -1+e^{\varphi}\\ -1+e^{\varphi} & 1+e^{\varphi}\end{pmatrix}.$$

Thus, we have

$$\tilde{\Phi} = \begin{pmatrix}\tilde{\theta}\\ \tilde{\chi}\end{pmatrix} = e^{iS}\Phi = e^{iS}\begin{pmatrix}\theta\\ \chi\end{pmatrix} = \frac{1}{2\sqrt{e^{\varphi}}}\begin{pmatrix}1+e^{\varphi} & -1+e^{\varphi}\\ -1+e^{\varphi} & 1+e^{\varphi}\end{pmatrix}\begin{pmatrix}\theta\\ \chi\end{pmatrix},$$

and multiplying by $\begin{pmatrix}1 & 1\end{pmatrix}$, we get

$$\tilde{\theta}+\tilde{\chi} = \frac{1}{2\sqrt{e^{\varphi}}}\begin{pmatrix}2e^{\varphi} & 2e^{\varphi}\end{pmatrix}\begin{pmatrix}\theta\\ \chi\end{pmatrix} = \sqrt{e^{\varphi}}\,(\theta+\chi)\,.$$

Now, we need to evaluate

$$e^{\varphi} = \cosh\varphi + \sinh\varphi = \cosh\left[\tanh^{-1}(x)\right] + \sinh\left[\tanh^{-1}(x)\right],$$

where

$$x \equiv \frac{\lambda}{\lambda + k_0}.$$

Using standard identities (or Maple™), we now have

$$e^{\varphi} = \frac{x+1}{\sqrt{1-x^2}} = \frac{\dfrac{\lambda}{\lambda+k_0}+1}{\sqrt{1-\left(\dfrac{\lambda}{\lambda+k_0}\right)^2}}.$$

In all cases where the PE expansion (i.e., in $2\lambda/k_0$) would also apply, $\lambda + k_0 > 0$ and so we can multiply through by this operator and replace it with the square root of its square in the denominator to get

$$e^{\varphi} = \frac{\lambda+\lambda+k_0}{\sqrt{(\lambda+k_0)^2-\lambda^2}} = \sqrt{1+\frac{2\lambda}{k_0}}.$$

Thus, we have

$$\sqrt{e^{\varphi}} = \left(1+\frac{2\lambda}{k_0}\right)^{1/4} \tag{D.6}$$

and

$$\tilde{\theta}+\tilde{\chi} = \sqrt{e^{\varphi}}\,(\theta+\chi) = \left(1+\frac{2\lambda}{k_0}\right)^{1/4} A. \tag{D.7}$$

Finally, restricting ourselves to the case of right (downrange) propagation only, we have $\tilde{\theta} = 0$ and the final result

$$\tilde{\chi} = \left(1+\frac{2\lambda}{k_0}\right)^{1/4} A. \tag{D.8}$$

D.2 The transformation when the density is only constant in the half-space

In this case, we are only interested in the answer to second order (i.e., O($\lambda^2, \lambda\gamma$)). Thus we begin with equation (D.3) adjusted to this requirement:

$$A = \begin{pmatrix} 1 & 1 \end{pmatrix} e^{-iS_I} e^{-iS_{II}} \tilde{\Phi} \tag{D.9}$$

and calculate S_I and S_{II} to the required order.

The Foldy-Wouthuysen procedure (see reference [1], equation (35); or equivalently equation (C.22) above) gives us

$$S_I = \frac{-i\eta\mathcal{O}}{2k_0} = \frac{-i(\eta\xi)\lambda}{2k_0} = \frac{-i\lambda}{2k_0}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{D.10}$$

and so

$$e^{-iS_I} = e^{-\left(\frac{\lambda}{2k_0}\right)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}. \tag{D.11}$$

Substituting equation (39c) from reference [1] (or equivalently the third part of equation (C.23) above) into equation (40a) from reference [1] (or equivalently the first part of equation (C.24) above), and dropping the term that goes away if there is no local range dependence as well as the term proportional to $\mathcal{O}^3$, which is higher order than concerns us here, we have

$$\begin{aligned} S_{II} = \frac{-i\eta\mathcal{O}}{2k_0} &= \frac{-i\eta}{2k_0}\cdot\frac{\eta}{2k_0}[\mathcal{O},\mathcal{E}]+\cdots \\ &= \frac{-i}{(2k_0)^2}\left[\lambda\xi,(\lambda-2k_0\gamma)\eta\right] \\ &= \frac{-i}{(2k_0)^2}\left(2\lambda^2-2k_0\{\gamma,\lambda\}\right)\xi\eta \\ &= \frac{i}{(2k_0)^2}\left(2\lambda^2-2k_0\{\gamma,\lambda\}\right)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned} \tag{D.12}$$

and

$$e^{-iS_{II}} = e^{\frac{1}{(2k_0)^2}\left[2\lambda^2-2k_0\{\gamma,\lambda\}\right]\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}. \tag{D.13}$$

Expanding the exponentials to O($\lambda^2, \lambda\gamma$), we have

$$e^{-iS_I}e^{-iS_{II}} = 1+\left[-\frac{\lambda}{2k_0}+\frac{\lambda^2}{2k_0^2}-\frac{\{\gamma,\lambda\}}{2k_0}\right]\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}+\frac{1}{2}\cdot\frac{\lambda^2}{4k_0^2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}+\mathrm{O}\left(\lambda^3,\gamma\lambda^2,\gamma^2\lambda\right), \tag{D.14}$$

and (using equation (C.8))

$$A = \begin{pmatrix} 1 & 1 \end{pmatrix} e^{-iS_I} e^{-iS_{II}} \tilde{\Phi} = \left[1-\frac{\lambda}{2k_0}+\frac{5\lambda^2}{8k_0^2}-\frac{\{\gamma,\lambda\}}{2k_0}\right]\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} \tilde{\theta} \\ \tilde{\chi} \end{pmatrix}. \tag{D.15}$$

Only now do we need to invoke the fact that the density is locally constant in the half-spaces away from the interface so that $\{\gamma,\lambda\}=2\gamma\lambda$. Recalling from equation (5.13) that $\alpha\equiv\rho_0/\rho=1+2\gamma+\mathrm{O}\left(\gamma^2\right)$ we have to O($\lambda^2,\lambda\gamma$)

$$A=\left(1-\frac{\alpha\lambda}{2k_0}+\frac{5(\alpha\lambda)^2}{8k_0^2}+\cdots\right)\left(\tilde{\theta}+\tilde{\chi}\right)=\left(1+\frac{2\alpha\lambda}{k_0}\right)^{-1/4}\left(\tilde{\theta}+\tilde{\chi}\right), \tag{D.16}$$

and setting uprange propagation $\tilde{\theta}$ to zero, we have indeed verified to O($\lambda^2,\lambda\gamma$) that

$$\left(1+\frac{2\alpha\lambda}{k_0}\right)^{1/4}A=\tilde{\chi}. \tag{D.17}$$

E Appendix: A close look at volume fluctuations and the PE

This appendix closely examines volume fluctuations where the range dependence is generated by distorting the range-independent sound speed function $[\mu](z)$ by an arbitrary function of the range and depth $f(x,z)$[vvv]. This way of imposing range dependence is crudely illustrated in Figure E.1.

[vvv] Subject to the restriction that the range-derivatives of f are small. This restriction comes explicitly from the range-derivatives in the new terms generated from the Foldy-Wouthysen transformation (such as $-\ddot{\lambda}/8k_0^3$), and implicitly from the well-known PE requirement that fields are modestly inclined from the horizontal.

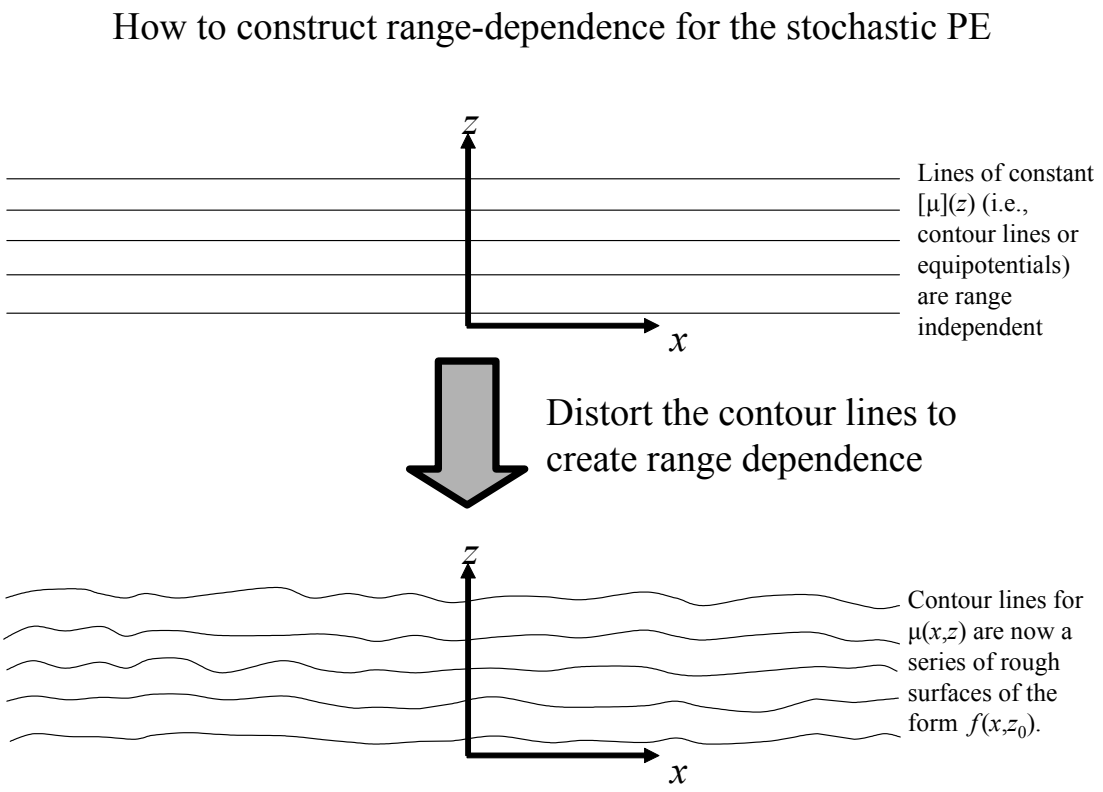

Figure E.1 – Range-dependent volume fluctuations of the sound speed function $\mu = \left(1 - c_0^2 / c^2\right)/2$ are generated by distorting contour lines in the range-independent problem.

The contour lines are now quasi-planar rough surfaces, and so the stochastic problem is obtained by range averaging functions of f (i.e., $\left\langle f^2 \right\rangle (z) = \frac{1}{L}\int_0^L f^2(x,z)\,dx$, etc.). The parabolic equation implicitly assumes that the range-dependent problem is derived from some range-independent problem by a distortion of this general form. This insight becomes crucial when we consider volume fluctuations adjacent to cusps and discontinuities. We will see below that this way of generating stochastic range dependence allows the averaging process used within the volume to dip down into the nooks and crannies adjacent to a rough line along which the sound speed has a cusp or a discontinuity. Thus, the stochastic results derived in this appendix will still apply everywhere except right on top of the singularity.

The basic geometry of a distorted contour line is shown in Figure E.2. The illustrated contour line was located at a depth z_0 in the original undistorted problem. After distortion, we have

$$\vec{\nabla}\mu = \left(\frac{\partial \mu}{\partial x}, \frac{\partial \mu}{\partial z} \right)$$
$$\hat{t} = \left(-\frac{\partial \mu}{\partial z}, \frac{\partial \mu}{\partial x} \right)$$

The slope of $\hat{t}$ (i.e., the slope of the tangent to the contour line) is given by

$$\dot{f} = \frac{\partial \mu / \partial x}{-\partial \mu / \partial z}$$

or

$$\frac{\partial \mu}{\partial x} = \alpha \frac{\partial \mu}{\partial z}. \qquad \text{(E.1)}$$

where $\alpha(x,z) \equiv -\dot{f}(x,z_0)$ is the negative of the slope of the tangent to the contour line passing through that point. It is a small random function of x, and it depends on z too.

The basic geometry of a contour line

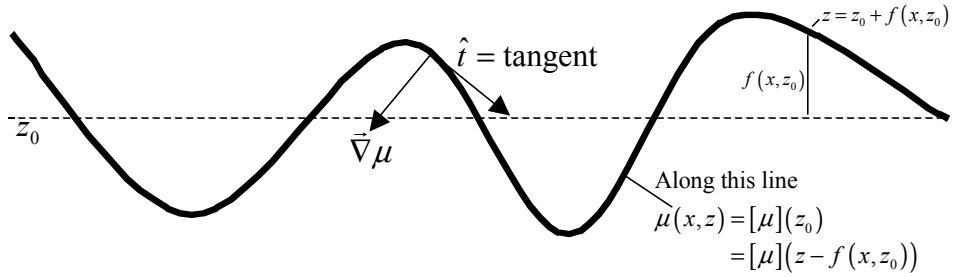

Figure E.2 - Contour lines are formed by deformation of the range-independent problem.

Recall that in this appendix, we are concerned with the new term $-\ddot{\lambda}/8k_0^3 = \ddot{\mu}/8k_0^2$. Let us drop the factor $1/8k_0^2$ and concentrate on $\ddot{\mu}$.

The starting point is formula (E.1). Taking the partial derivative with respect to the range x gives us

$$\frac{\partial^2 \mu}{\partial x^2} = \frac{\partial}{\partial x}\left(\alpha \frac{\partial \mu}{\partial z} \right) = \dot{\alpha} \frac{\partial \mu}{\partial z} + \alpha \frac{\partial^2 \mu}{\partial x \partial z}.$$

Now use

$$\frac{\partial^2 \mu}{\partial x \partial z} = \frac{\partial^2 \mu}{\partial z \partial x} = \frac{\partial}{\partial z}\left(\alpha \frac{\partial \mu}{\partial z} \right) = \frac{\partial \alpha}{\partial z} \frac{\partial \mu}{\partial z} + \alpha \frac{\partial^2 \mu}{\partial z^2}$$

to get

$$\frac{\partial^2 \mu}{\partial x^2} = \dot{\alpha}\frac{\partial \mu}{\partial z} + \alpha^2 \frac{\partial^2 \mu}{\partial z^2} + \alpha \frac{\partial \alpha}{\partial z}\frac{\partial \mu}{\partial z}. \tag{E.2}$$

Result (E.2) is quite general. In particular, along the line $z = z_0$, we have

$$\ddot{\mu}(x, z_0) = \dot{\alpha}(x, z_0)\frac{\partial \mu(x, z_0)}{\partial z_0} + \alpha^2(x, z_0)\frac{\partial^2 \mu(x, z_0)}{\partial z_0^2} + \alpha(x, z_0)\frac{\partial \alpha(x, z_0)}{\partial z_0}\frac{\partial \mu(x, z_0)}{\partial z_0}. \tag{E.3}$$

Now, let us use smoothness. From the geometry given in Figure E.2, we have $\mu(x, z_0 + f(x, z_0)) = [\mu](z_0)$. Performing a Taylor series expansion, this gives us

$$\mu(x, z_0) = [\mu](z_0) - f(x, z_0)\left.\frac{\partial \mu(x, z)}{\partial z}\right|_{z=z_0} + \mathrm{O}(f^2). \tag{E.4}$$

Truncating at 2nd order in f and its derivatives (including α), we see immediately that we can substitute $[\mu](z_0)$ for $\mu(x, z_0)$ in the second and third terms of (E.3). Similarly, in these two terms we can slide $\alpha(x, z_0)$ over to $\alpha(x, z_0 + f(x, z_0)) = -\dot{f}(x, z_0)$. However, we will have to use our knowledge of the distortion geometry to evaluate

$$\dot{\alpha}(x, z_0)\frac{\partial \mu(x, z_0)}{\partial z_0}.$$

Taylor series expansion gives us

$$-\dot{f}(x, z_0) = \alpha(x, z_0 + f(x, z_0)) = \alpha(x, z_0) + f(x, z_0)\frac{\partial \alpha(x, z_0)}{\partial z} + \mathrm{O}(f^3),$$

and taking a derivative

$$-\ddot{f}(x, z_0) = \frac{\partial \alpha(x, z_0 + f(x, z_0))}{\partial x} = \dot{\alpha}(x, z_0) + f(x, z_0)\frac{\partial \dot{\alpha}(x, z_0)}{\partial z} + \dot{f}(x, z_0)\frac{\partial \alpha(x, z_0)}{\partial z}$$

or

$$\dot{\alpha}(x, z_0) = -\ddot{f}(x, z_0) - f(x, z_0)\frac{\partial \dot{\alpha}(x, z_0)}{\partial z} - \dot{f}(x, z_0)\frac{\partial \alpha(x, z_0)}{\partial z} + \mathrm{O}(f^3). \tag{E.5}$$

From our Taylor series expansions above, to $O(f^3)$ in equation (E.5) we can again slide $\dot{\alpha}(x, z_0)$ and $\alpha(x, z_0)$ to $z_0 + f(x, z_0)$ where they become $-\ddot{f}(x, z_0)$ and $-\dot{f}(x, z_0)$ respectively. This leaves us with

$$\dot{\alpha}(x, z_0) = -\ddot{f}(x, z_0) + f(x, z_0)\frac{\partial \ddot{f}(x, z_0)}{\partial z} + \dot{f}(x, z_0)\frac{\partial \dot{f}(x, z_0)}{\partial z} + \mathrm{O}(f^3). \tag{E.6}$$

Finally, let us take $\partial/\partial z_0$ of equation (E.4) to get

$$\frac{\partial \mu(x,z_0)}{\partial z_0} = \frac{\partial [\mu](z_0)}{\partial z_0} - \frac{\partial f(x,z_0)}{\partial z_0}\frac{\partial \mu(x,z)}{\partial z}\bigg|_{z=z_0} - f(x,z_0)\frac{\partial^2 \mu(x,z)}{\partial z^2}\bigg|_{z=z_0} + \mathrm{O}\left(f^2\right). \quad \text{(E.7)}$$

From equation (E.4), we see to first order in f we can replace $\mu(x,z_0)$ with $[\mu](z_0)$ in equation (E.7), leaving us with

$$\frac{\partial \mu(x,z_0)}{\partial z_0} = \frac{\partial [\mu](z_0)}{\partial z_0} - \frac{\partial f(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} - f(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} + \mathrm{O}\left(f^2\right). \quad \text{(E.8)}$$

Thus we have

$$\begin{aligned}
&\dot{\alpha}(x,z_0)\frac{\partial \mu(x,z_0)}{\partial z_0} \\
&= \left(-\ddot{f}(x,z_0) + f(x,z_0)\frac{\partial \ddot{f}(x,z_0)}{\partial z} + \dot{f}(x,z_0)\frac{\partial \dot{f}(x,z_0)}{\partial z} \right) \\
&\qquad \cdot \left(\frac{\partial [\mu](z_0)}{\partial z_0} - \frac{\partial f(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} - f(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} \right) + \mathrm{O}\left(f^3\right) \qquad \text{(E.9)} \\
&= -\ddot{f}(x,z_0)\frac{\partial [\mu](z_0)}{\partial z_0} + f(x,z_0)\frac{\partial \ddot{f}(x,z_0)}{\partial z}\frac{\partial [\mu](z_0)}{\partial z_0} + \dot{f}(x,z_0)\frac{\partial \dot{f}(x,z_0)}{\partial z}\frac{\partial [\mu](z_0)}{\partial z_0} \\
&\qquad + \ddot{f}(x,z_0)\frac{\partial f(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} + \ddot{f}(x,z_0) f(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} + \mathrm{O}\left(f^3\right).
\end{aligned}$$

Now we substitute this back into equation (E.3). Recall that the last two terms are already 2nd order, so in these terms we are free to replace $\alpha(x,z_0)$ with $-\dot{f}(x,z_0)$ and $\mu(x,z_0)$ with $[\mu](z_0)$. This gives us:

$$\begin{aligned}
\ddot{\mu}(x,z_0) &= \dot{\alpha}(x,z_0)\frac{\partial \mu(x,z_0)}{\partial z_0} + \dot{f}^2(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} + \dot{f}(x,z_0)\frac{\partial \dot{f}(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} + \\
&= -\ddot{f}(x,z_0)\frac{\partial [\mu](z_0)}{\partial z_0} + f(x,z_0)\frac{\partial \ddot{f}(x,z_0)}{\partial z}\frac{\partial [\mu](z_0)}{\partial z_0} + \dot{f}(x,z_0)\frac{\partial \dot{f}(x,z_0)}{\partial z}\frac{\partial [\mu](z_0)}{\partial z_0} \\
&\qquad + \ddot{f}(x,z_0)\frac{\partial f(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} + \ddot{f}(x,z_0) f(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} \\
&\qquad + \dot{f}^2(x,z_0)\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} + \dot{f}(x,z_0)\frac{\partial \dot{f}(x,z_0)}{\partial z_0}\frac{\partial [\mu](z_0)}{\partial z_0} + \mathrm{O}\left(f^3\right) \qquad \text{(E.10)} \\
&= -\ddot{f}(x,z_0)\frac{\partial [\mu](z_0)}{\partial z_0} + \frac{\partial}{\partial z_0}\left\{ f(x,z_0)\ddot{f}(x,z_0) + \dot{f}^2(x,z_0) \right\}\frac{\partial [\mu](z_0)}{\partial z_0} \\
&\qquad + \left\{ f(x,z_0)\ddot{f}(x,z_0) + \dot{f}^2(x,z_0) \right\}\frac{\partial^2 [\mu](z_0)}{\partial z_0^2} + \mathrm{O}\left(f^3\right).
\end{aligned}$$

This equation holds for any x and any $z = z_0$. Note that $f(x, z_0)$ is the distance the point (x, z_0) has been displaced by the deformation (note the displacement is by construction vertical). It is also now the random variable characterizing $\ddot{\mu}$ (or μ for that matter) at that point. Note that $\ddot{\mu}$ now contains no information about any contour line other than the one that ran along the line $z = z_0$ in the *undistorted* problem. Thus, when we shortly average f to find $\langle \ddot{\mu} \rangle (z_0)$, we will not be slicing along contour lines; we will simply be measuring the amount the original contour line was distorted. In other words, we have effectively collapsed the distorted contour line back down to the original line at $z = z_0$, with now $f, \dot{f}, \ddot{f},$ etc. giving information about the distortion. For volume fluctuations near a rough interface along which our smoothness conditions are violated, this method of averaging indeed continues the volume problem in each given region down to where the undistorted interface used to be. This is true for all x regardless of where the interface may be at that particular moment. At the rough interface, we will proceed in a similar manner. We will convert the δ-functions to effective boundary conditions along the wavy interface, and then slide all necessary quantities down to the undistorted surface, in the process obtaining effective boundary conditions along the flattened undistorted surface. Again, the rough interface effectively collapses back to its original position. All this implies that our results for a fluctuating volume will be good right on down to the flattened interface, which then carries its own effective boundary conditions. It is all fully consistent, and we are now ready to consider the stochastic problem (which will be effectively range-independent).

When we take the stochastic average, we immediately use $\langle \ddot{f} \rangle = 0$ and

$$\langle f(x, z_0) \ddot{f}(x, z_0) \rangle + \langle \dot{f}^2(x, z_0) \rangle = 0$$

at all values of the height z to show that $\langle \ddot{\mu} \rangle = 0$ everywhere within the volume.

In closing, we note that volume fluctuations can in principle give non-zero contributions from the higher-order terms associated with range dependence. In this regard, note Exercise 7 in reference [63]. In equations (26) and (29) of the exercise, there is a higher-order term (in that context related primarily to the transverse smearing term rather than the downrange smearing term considered here) quite similar to the term $\dot{\lambda}^2 / 4k_0^4$ in equations (3.11) and (C.35) above. As shown in part *e* of Exercise 7, this provides a non-zero contribution to the expectation value of electron states that are excited relative to the s-state. These states are zero at the nucleus, and so will not see the contact potential there, and consequently do not see the lowest order Lamb shift.

F Appendix: Some idealizations inherent in the "toy model" of the hydrogen atom

In this appendix, we examine various aspects of the sequence of approximations that take us from a realistic hydrogen atom to our "toy model" (given by equation (3.37)). Issues related to Quantum Electrodynamics take us too far afield from our discussion here, and so the ramifications of replacing 2nd quantization with fluctuations in the underlying space will not be further discussed here. Issues related to the other approximations, however, are discussed below.

F.1 A fundamental distinction between the Foldy-Wouthuysen transformation for the Dirac equation and that for the Klein-Gordon/Helmholtz equation

Not only is the "toy model" crude vis à vis Quantum Electrodynamics, but it is even crude relative to a more realistic description of the hydrogen atom based on the Dirac equation instead of the Klein-Gordon equation. The distinction of most significance in the context of our study of the Foldy-Wouthuysen transformation centers on the fact that this transformation generates roughly twice as many terms for the Dirac equation as it does for the Klein-Gordon/Helmholtz equation. These extra terms introduce new physics into the Schrödinger equation.

To see how this occurs, consider the $\mathcal{O}^2$ term in the Foldy-Wouthuysen expansion of the Klein-Gordon/Helmholtz equation. Here, this term already gives the $\mathrm{O}\left(\nabla_T^4\right)$ contribution to the Schrödinger equation, while the same term in the context of the Dirac equation only provides an $\mathrm{O}\left(\nabla_T^2\right)$ contribution to the Schrödinger equation. Formally, we still have the same number of terms in the FW transformation as before, but now we are approaching the Schrödinger equation more slowly.

This leaves room for a greater variety of terms. For example, consider the term $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$. For the Klein-Gordon/Helmholtz equation, this term participates in recovering the expansion of the square-root operator associated in some general sense with the relativistic kinetic energy (e.g., $\sqrt{1+2\lambda/k_0}$ for the Helmholtz equation). In the context of the Dirac equation, it becomes an "intermediate" term whose sole effect is to introduce additional physical phenomena into the problem. This particular term leads to various spin related effects in the fine structure of hydrogen, and also to the Darwin term for the hydrogen atom (see page 51 or reference [57]). The new physics associated with the Darwin term is Zitterbewegung. We will see below (in Appendix F.2) that unlike the Helmholtz equation for a classical field, the Klein-Gordon equation for the pionic atom is modified in a way that a non-kinetic energy contribution from $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ still "sneaks

in" in the form of a Darwin term (of course there are no spin terms for this spinless field), but the appearance of this Darwin term does not herald a doubling of terms in the FW transformation as does $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ in the context of the expansion of the Dirac equation.

(Incidentally, the Darwin term is interesting because in some contexts it resembles the Lamb shift term even though it does not require time dependence, and so it is a product of 1st quantization rather than 2nd quantization. For further discussion concerning the distinction between the Lamb shift and a Darwin term and between 2nd quantization and 1st quantization, see Appendix F.3.)

The Foldy-Wouthuysen transformation for the Dirac equation also contains new explicitly time-dependent terms not found in the expansion of the Klein-Gordon/Helmholtz equation. In the context of the Dirac equation, the time dependent term $\left[\mathcal{O},\dot{\mathcal{O}}\right]$ in equation (C.29) goes roughly as $\vec{\nabla}\left(\partial\vec{A}/\partial t\right)$ (which in turn ends up in $\vec{\nabla}\cdot\vec{E}$), while the same term goes as $\nabla_T^2\left(\partial\mu/\partial x\right)$ in the case of the Helmholtz equation. Thus, for the FW expansion of the Dirac equation, we would not expect field-induced time-domain (i.e., downrange) virtual fluctuations to show up until the $\left\{\dot{\mathcal{O}},\left[\mathcal{O},\mathcal{E}\right]\right\}$ term from equation (C.29).

Thus, we see that replacing the Dirac equation for a spin ½ field with a Klein-Gordon equation for a spinless field results in a significant change in the structure of the Foldy-Wouthuysen transformation. This opens up room for a great deal of extra physics. Much of the fine structure of the hydrogen atom is ultimately derived from this additional physics. For more on this, see Chapter 4 of reference [57].

F.2 The impact of substituting a matrix scalar potential in state space with a bona fide scalar potential

The potential in pionic atom is not introduced in the scalar problem as was the case in our "toy model" (equation (3.37)). Instead, it is introduced as a diagonal matrix potential directly into the state space equation (see pp. 202-203 of reference [57]).

The diagonal matrix potential associated with the pionic atom also leads to a Darwin term that is absent from both the parabolic equation corresponding to the Helmholtz equation and from the Schrödinger equation for our "toy model". This Darwin term is emerges from the operator $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$, whose primary role in this context is to reproduce the 3rd order correction to the expansion of the operator $\sqrt{1+\pi^2/m^2}$ (where π^2 is the magnitude squared of the generalized 4-dimensional momentum vector in the presence of an electromagnetic 4-potential A_μ: $\pi_\mu = p_\mu - A_\mu$). In this sense, this is an incidental Darwin term associated with mixed products of odd and even operators, while the Darwin term for the Dirac operator illustrates a fundamental change in the symmetries of the

problem (i.e., an end to *independent* time- and range-reversal invariance), and as such it is a precursor of a larger class of extra terms (more or less doubling the number of terms at a given order of $\nabla_T \sim \vec{\nabla}$).

Let us fold our further exploration of the Darwin term for the pionic atom into an examination of the distinction between the downrange Lamb shift and the Darwin term. This is pursued in the next section.

F.3 The distinction between the downrange Lamb shift and the Darwin term

The Darwin term, vacuum polarization (i.e., the downrange Lamb shift), and stochastic smearing (i.e., the traditional or transverse Lamb shift) are sometimes confused with each other, and here we discuss the distinction. The key difference is that the Darwin term is a product of 1st quantization, while both flavors of the Lamb shift contribution are products of 2nd quantization.

The Darwin term comes out of the term $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ produced by the Foldy-Wouthuysen transformation. For a Helmholtz equation with a scalar potential, the potential gets folded into the operator λ and this term just leads to the standard λ^3 term. Note that in this case, the scalar potential is folded into both the odd part $\mathcal{O}$ and the even part $\mathcal{E}$ of the state space equation (i.e., the matrix representation of the wave equation).

On the other hand, if as for the pionic atom, the potential is a diagonal matrix (i.e., $\left(\text{a scalar function}\right)\cdot\mathbf{1} = V\left(\vec{r}\right)\cdot\mathbf{1}$) that is tacked on directly to the state space equation, then the potential is a part of the even operator $\mathcal{E}$ only. In fact, $\mathcal{O}$ is a scaled back version of the operator λ times ξ, while $\mathcal{E}$ is λ times the matrix η *plus* the potential term $V\cdot\mathbf{1}$. ξ and η are the same two odd and even 2×2 matrices as always, while the scaled back version of λ only includes a generalized kinetic energy term of the form $\pi^2/2m$ (where as above π^2 is the magnitude squared of the generalized 4-dimensional momentum vector in the presence of an electromagnetic 4-potential A_μ: $\pi_\mu = p_\mu - A_\mu$). Now $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ includes not only the λ^3 term familiar from the PE expansion of the Helmholtz equation, but also a term proportional to $\left[\lambda,\left[\lambda,V\right]\right] \propto \left[\pi^2,\left[\pi^2,V\right]\right]$. This extra term is a bona fide Darwin term provided that we use the following as our working definition of the Darwin term for a *scalar field* (as opposed to a field with spin such as the electron wave function, where other effects also emerge from the operator $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$): *the Darwin term for a scalar field is something that comes out of the* $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ *term other than some part of the omnipresent expansion of the square root operator* $\sqrt{1+2\lambda/k_0}$. In Section 6.1, when we consider density jumps, we will have

$\mathcal{E}=\lambda-2k_0\gamma$ and this again leads to something that we might technically call a Darwin term: a term proportional to $\left[\lambda,\left[\lambda,-2k_0\gamma\right]\right]$.

Note that the Darwin term for the Dirac equation also came from the operator $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$, but in this case, this operator is in no way connected to reproducing the basic Schrödinger equation (i.e., the expansion of the square root operator connected with relativistic kinetic energy). The term $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ instead contains a rich content associated with the spin. As noted above, $\left[\mathcal{O},\left[\mathcal{O},\mathcal{E}\right]\right]$ is the first example of a much larger class of terms in the context of the Dirac equation than it is in the context of the pionic atom. (In fact, for a given order of the transverse gradient, the number of terms in the FW transformation for a Dirac equation field is roughly doubled relative to the order for a scalar field.)

To contrast the Darwin term with the downrange Lamb shift term, note that the Darwin term is not proportional to a derivative with respect to time of the odd part of the Hamiltonian in the state space equation. Thus, the Darwin term can be non-zero even when it is assumed that all the parameters in the full wave equation do not vary with time. Implicit in this assumption is the assumption that the underlying fabric of space-time does not vary as a function of time. The Darwin terms, therefore, are a product of 1st quantization.

On the other hand, the term that produces the downrange Lamb shift is non-zero only if some parameter in the odd part of the state space equation fluctuates as a function of time (at least to the orders considered here; eventually at very high order, a time dependence in the even part could add terms as well). To induce time dependence in the odd component of the state space Hamiltonian $\mathcal{O}$, we need to introduce time dependence into the existing time-independent potentials by *imposing* (by hand) fluctuations of the underlying fabric of space-time (or equivalently introducing some time-dependent fluctuating external field). These fluctuations are called vacuum fluctuations. Since our theory is based on ordinary relativistic quantum mechanics (and its reduction down to its non-relativistic limit), the vacuum fluctuations must be imposed by hand, and do not emerge automatically from 1st principles as they would in quantum field theory. Nevertheless, the introduction of vacuum fluctuations by whatever means is called 2nd quantization. Thus, the downrange Lamb shift is a product of 2nd quantization. In the context of quantum field theory, the downrange Lamb shift is known as vacuum polarization.

Similarly, the well-known transverse (or traditional) Lamb shift also occurs when we impose fluctuations by hand to create a time-dependent potential. This time, contact potential associated with the transverse Lamb shift comes out of a stochastic averaging process, but it does not take the form of a specific term in the deterministic Hamiltonian. In this way, it is different from both the Darwin term and the downrange Lamb shift.

G Appendix: Generalizing the formalism to accommodate 2-dimensional interfaces embedded in 3-dimensional space

This appendix provides guidelines for constructing the stepping algorithm when a third dimension given by the unit vector $\hat{y}$ is present. Full examination of the 2-dimensional interface embedded in 3-dimensional space will be left to future research. This issue is not particularly urgent from a practical point of view, as most current work in the discipline is restricted to 1-dimensional interfaces embedded in 2-dimensional space. However, the treatment here is provided both for completeness, and even more importantly, because an understanding of this material provides a good feel for some fundamental issues that are glossed over in simpler problem that is examined in some detail in this paper (i.e., the 1-dimensional interface embedded in a 2-dimensional space).

G.1 The stepping procedure

In this subsection, we examine the generalization of the basic stepping procedure developed for the simpler 2-dimensional problem in Subsection 3.3.1. Now, we should also fix the step size Δy just as we previously fixed Δz, and begin by choosing the step size Δx so that the 2-dimensional $y-z$ grid slides downrange until it first hits the interface somewhere. The situation now becomes more complicated than it was before. At this new value of the range, it is very likely that elsewhere within the 2-dimensional $y-z$ grid, the interface will fall between grid points. Under such circumstances, it is best to step different $y=\text{constant}$ lines of grid points different downrange distances so that they always hit the interface. These steps should be performed in order of increasing downrange terminus.

Note that some supplementary downrange stepping would still have to be used to evaluate expressions that involve many points on the transverse grid at once. Such expressions are relevant, because evaluation of $H\chi$ in a discretized space inherently involves a neighborhood of nearby points in the (transverse) $y-z$-grid. In particular, $H\chi$ contains the operator $\nabla_T^{2n}\chi$ (n is some integer), which in turn contains the operator $\partial^{2n}\chi/\partial y^{2n}$. To calculate such a quantity at a given point on the grid, we need to make available at the current value of the range at least a few neighboring grid points that lie on other $y=\text{constant}$ lines. (As described in Subsection 3.3.2, these additional points appear in finite difference expressions for the y-derivatives.) The needed nearby $y=\text{constant}$ lines of grid points would thus be temporarily stepped the downrange distance needed to bring them to the same value of the range as the $y=\text{constant}$ line currently under consideration (i.e., the one that actually intersects the interface on a grid

point). The resultant values would be used only to evaluate the non-local function ($H\chi$ in our case) along the $y = \text{constant}$ line that is currently under consideration.

For points along this line that are near to but not directly on the interface (or directly on the interface, but near an extremum), this procedure will typically need to be supplemented by additional interpolation methods, because the interface might still pass between a nearby pair of points on the $z = \text{constant}$ line that emanates from the given grid point. Note that this is an issue, because the procedure for calculating derivatives using a discrete grid near an interface requires that we use the boundary conditions at grid points *that sit directly on the interface* (see the analysis in Subsection 3.3.2). Thus, in an ideal implementation of the procedure, we would temporarily add supplementary grid points as needed, so that the interface always crosses the grid directly at a grid point. For a relatively crude but serviceable alternative to this kind of interpolation, the interface could be temporarily deformed to coincide with the transverse grid at its current location. In this case, the true values of interface parameters such as $\partial f/\partial y$ (i.e., the specified functions of x and y) would still be inserted into the boundary conditions that are used to calculate $\partial^{2n}\chi/\partial y^{2n}$. (These boundary conditions are obtained using the procedure outlined in Appendix G.2 below.) We now have all we need to complete the procedure outlined in Subsection 3.3.2 for calculating $\partial^{2n}\chi/\partial y^{2n}$ and consequently $H\chi$. For a typical quasi-planar surface, the interface is only slightly tilted relative to the horizontal, and so the function χ and its y-derivatives should be nearly continuous near the interface, and the issue of precisely where to place the interface while calculating the $\partial^{n}\chi/\partial y^{n}$ has at best modest importance.

The generalization of the stepping procedure discussed here in Subsection G.1 thus turns out to be the subtlest issue related to adapting the PE formalism developed in this paper (for a 1-dimensional interface embedded in 2-dimensional space) to the problem of a 2-dimensional interface embedded in 3-dimensional space.

G.2 The boundary conditions

This subsection provides an overview of the key issues related to determining the parabolic equation boundary conditions in the full 3-dimensional problem. The discussion builds on the treatment of the 2-dimensional problem provided in Subsection 3.3.3. At the interface, we should make temporary use of a local right-handed orthogonal coordinate system $x - y' - z'$ such that $\hat{z}'$ is the direction locally normal to the cut of the surface in the 2-dimensional $x = \text{constant}$ plane (and of course $\hat{z}'$ is in that plane too). In a notation that is independent of the coordinate system, we denote this 2-dimensional normal by $\hat{n}_{2D}$. If $z = f(x, y)$ in our original coordinate system, then

$$\hat{z}' = \hat{n}_{2D} = \frac{1}{\sqrt{1 + (\partial f/\partial y)^2}}\left(-\frac{\partial f}{\partial y}\hat{y} + \hat{z}\right) = \left(0, -\partial f/\partial y, 1\right)\Big/\sqrt{1 + (\partial f/\partial y)^2}\,.$$

The other axis is given by the unit vector

$$\hat{y}' = \frac{1}{\sqrt{1+\left(\partial f/\partial y\right)^2}}\left(\hat{y}+\frac{\partial f}{\partial y}\hat{z}\right) = \left(0,1,\partial f/\partial y\right)\Big/\sqrt{1+\left(\partial f/\partial y\right)^2}\,.$$

Note that $\hat{y}'$ is in the intersection of the plane locally tangent to the interface and the $x=$ constant plane, and so we will give it the alternate identification $\hat{t}_{2D} \equiv \hat{y}'$.

The boundary conditions are obtained using the $y'-z'$-coordinate system. Then $\partial/\partial y'$ and $\partial/\partial z'$ are expressed in terms of $\partial f/\partial y$, $\partial/\partial y$ and $\partial/\partial z$ so that we can evaluate derivatives using the discrete grid tied to our fixed coordinate system. To be specific,

$$\partial/\partial y' = \hat{t}_{2D}\cdot\underline{\nabla}_T \quad \text{and} \quad \partial/\partial z' = \hat{n}_{2D}\cdot\underline{\nabla}_T \tag{G.1}$$

with

$$\underline{\nabla}_T \equiv \hat{y}\frac{\partial}{\partial y}+\hat{z}\frac{\partial}{\partial z}\,.$$

Note that higher-order derivatives of f with respect to y will be generated as $\partial/\partial y$ operates on $\hat{t}_{2D}$ or $\hat{n}_{2D}$. The downrange slope $\dot{f}$ of the interface is as before.

Now, let us examine some of the specific issues related to obtaining the boundary conditions in our local $y'-z'$-coordinate system. Continuity of χ will guarantee that derivatives of χ with respect to y' (these are tangential derivatives) will also be continuous. To show this, use the follow iterative argument. If some arbitrary function, say χ in our case, is continuous at the interface, then the difference between this function evaluated on two sides of this interface is zero (i.e., $\chi_I - \chi_{II} = 0$). Since the quantity $\chi_I - \chi_{II}$ remains the same everywhere on the interface, its tangential derivatives, which measure the rate of change of the function as one slides along the interface, must be zero as well[www]. This in turn implies that the tangential derivative of the function χ is continuous. Choosing the specific tangential direction $\hat{t}_{2D}$, we have

$$0 = \hat{t}_{2D}\cdot\vec{\nabla}\left(\chi_I-\chi_{II}\right) = \hat{t}_{2D}\cdot\vec{\nabla}\chi_I - \hat{t}_{2D}\cdot\vec{\nabla}\chi_{II} = \hat{y}'\cdot\underline{\nabla}_T\chi_I - \hat{y}'\cdot\underline{\nabla}_T\chi_{II} = \frac{\partial\chi_I}{\partial y'}-\frac{\partial\chi_{II}}{\partial y'} = 0\,.$$

Now, iterate and apply the same reasoning to the function $\hat{t}_{2D}\cdot\vec{\nabla}\chi$ to show:

[www] This is one of several spots where things would get more complicated if for some reason χ were not constant on the interface. In this case, the tangential derivatives would track the χ-boundary condition, whatever it is.

$$\hat{t}_{2D}\cdot\vec{\nabla}\hat{t}_{2D}\cdot\vec{\nabla}\chi_I-\hat{t}_{2D}\cdot\vec{\nabla}\hat{t}_{2D}\cdot\vec{\nabla}\chi_{II}=\hat{y}'\cdot\underline{\nabla}_T\hat{y}'\cdot\underline{\nabla}_T\chi_I-\hat{y}'\cdot\underline{\nabla}_T\hat{y}'\cdot\underline{\nabla}_T\chi_{II}=\frac{\partial^2\chi_I}{(\partial y')^2}-\frac{\partial\chi_{II}}{(\partial y')^2}=0\,,$$

and so on. There is a tricky point here. $\hat{y}'$ is an axis on a coordinate system that is only used at one point, so it is itself a function of position. This is a little clearer when we give it the label $\hat{t}_{2D}\equiv\hat{y}'$. The issue is significant, because once we start taking higher-order derivatives, $\underline{\nabla}_T$ will operate on $\hat{t}_{2D}\equiv\hat{y}'$. In other words, we have to be very careful never to treat $\hat{y}'$ and similarly $\hat{z}'$ as ordinary static unit vectors attached to a fixed coordinate axes. Provided this caveat is kept in mind, it is generally best to proceed using compact notation that treats the y' and z' axes like any other axes, obtain the local boundary conditions, and only then use the identification in equation (G.1) above to incorporate the fact that these unit vectors may in fact vary with position.

Proceeding in this manner, note that $H\chi$ will involve terms of the basic form $\partial^n\chi/\partial y^n$, $\partial^n\chi/\partial z^n$, and $\partial^n\chi/\partial y^{n-m}\partial z^m$. These will be extracted from a system of equations generated by the boundary conditions on $\partial^n\chi/(\partial y')^n$, $\partial^n\chi/(\partial z')^n$ and $\partial^n\chi/(\partial y')^{n-m}(\partial z')^m$. $\partial^n\chi/(\partial y')^n$ are continuous at the interface. Just as with two dimensions, terms of the form $\partial^n\chi/(\partial z')^n$ are evaluated using repeated integrations down the z'-axis of the leading order derivative of χ with respect to z'. (Again, we have an infinitesimal integration possibly preceded by one or more indefinite integrations. Note that terms that only involve $\partial^n\chi/(\partial y')^n$ will fall out during the infinitesimal integrations.) As we use repeated integrations to evaluate $\partial^n\chi/(\partial z)^n$, the only tricky part concerns the integration of cross-terms roughly of the form $\partial^n\chi/(\partial y')^{n-m}(\partial z')^m$. We have to place the $\partial/\partial y'$ and $\partial/\partial z'$ derivatives in the order dictated by $H\chi$. As long as "$\partial/\partial z'$"s are to the left of "$\partial/\partial y'$"s, we can integrate as before. Problems arise when we come across the need to integrate expressions of the basic form

$$\int dz'\frac{\partial}{\partial y'}(\cdots)\,. \tag{G.2}$$

To evaluate something of the form (G.2), we will need to reorder the partial differentiations earlier in the procedure than usual. To pick up subtle cross-terms related to second and higher-order y-derivatives of f when we do so, temporarily fix the $y'-z'$-coordinate system, label the fixed axes by $\tilde{y}'$ and $\tilde{z}'$, and write the interface as $\tilde{z}'=\tilde{f}(x,\tilde{y}')$. For convenience, choose the origin to be the location on the interface currently under consideration. The higher-order derivatives of $\tilde{f}$ reflect the curvature of the surface (and derivatives of the curvature), so they not affected by translation and rotation. Thus, $\partial^q\tilde{f}/(\partial\tilde{y}')^q=\partial^q f/(\partial y)^q$ with $q\geq 2$. Now, convert

$$\frac{\partial}{\partial y'} \to \frac{1}{\sqrt{1+\left(\partial\tilde{f}/\partial\tilde{y}'\right)^2}}\left(\frac{\partial}{\partial\tilde{y}'}+\frac{\partial\tilde{f}}{\partial\tilde{y}'}\frac{\partial}{\partial\tilde{z}'}\right)$$
$$\frac{\partial}{\partial z'} \to \frac{1}{\sqrt{1+\left(\partial\tilde{f}/\partial\tilde{y}'\right)^2}}\left(-\frac{\partial\tilde{f}}{\partial\tilde{y}'}\frac{\partial}{\partial\tilde{y}'}+\frac{\partial}{\partial\tilde{z}'}\right).$$

Note that we are ultimately only interested in the behavior at the origin where the slope $\partial\tilde{f}/\partial\tilde{y}'$ is zero, so the distinction between $(\tilde{y}',\tilde{z}')$ and (y',z') is quite subtle. Since the axes are now fixed, the order of $\partial/\partial\tilde{y}'$ and $\partial/\partial\tilde{z}'$ differentiations no longer matters, so send to the right all the $\partial/\partial\tilde{z}'$ derivatives (i.e., those remaining in the expression denoted by the ellipsis in equation (G.2); assume there are p of these). Next, write $H\chi$ in terms of $(\tilde{y}',\tilde{z}')$, and take a sequence of indefinite integrations with respect to $\tilde{z}'$ to get $\partial^p\chi/(\partial\tilde{z}')^p$ in terms of distributions of the form $\delta^k\left(\tilde{z}'-\tilde{f}(x,\tilde{y}')\right)$ (note that $k \le p-1$) and perhaps also steps of the form $\Theta\left(\tilde{z}'-\tilde{f}(x,\tilde{y}')\right)$, and then take $n-m$ $\tilde{y}'$-derivatives[xxx]. The resultant expression can be integrated with respect to z'; we just have to be careful to convert:

$$\int dz' \to \int \hat{n}_{2D}\cdot(d\tilde{y}',d\tilde{z}').$$

All this effort has finally given us the contribution from a handful of problematic terms to the integrations that generate boundary conditions for the derivatives of the basic form $\partial^i\chi/(\partial z')^i$. (These troublesome terms have the basic form $\partial^n\chi/(\partial z')^{m-p}(\partial y')^{n-m}(\partial z')^p$.) From now on, keep track of these specific contributions. Later, when we use equation (G.1) to convert to the $y-z$ coordinate system, treat $\partial f/\partial y$ as a constant for these terms only, because in these terms we have already effectively taken the higher-order y-derivatives of f.

Recall that we currently are in the process of obtaining the full set of equations for the boundary conditions on $\partial^n\chi/\partial y^n$, $\partial^n\chi/\partial z^n$, and $\partial^n\chi/\partial z^m\partial y^{n-m}$. Furthermore recall that

---

[xxx] The fact that $\left(\partial\tilde{f}/\partial\tilde{y}'\right)\Big|_{(\tilde{y}',\tilde{z}')=0} = 0$ simplifies the result. The main pitfall here involves the need to identify new step functions brought in by fresh derivatives $\partial/\partial\tilde{y}'$. These we can deduce from boundary conditions found at an earlier stage of the process, since we do the large number of integrations first in order to bootstrap ourselves from the boundary conditions on the lower orders on up to the higher orders (as in Appendix Q.1).

these come from the boundary conditions on terms of the form $\partial^n \chi / (\partial y')^n$, $\partial^n \chi / (\partial z')^n$ and $\partial^n \chi / (\partial y')^{n-m} (\partial z')^m$, and that so far we have only have methods for the first two forms. We still need to find a way to *explicitly* evaluate the boundary conditions on cross-terms of the form $\partial^n \chi / (\partial y')^{n-m} (\partial z')^m$. Note that the $\partial / \partial y'$s and $\partial / \partial z'$s have once again been grouped to bring the latter all to the right. Start with the boundary condition on $\partial^m \chi / (\partial z')^m$, and this time write it as a difference that comes out to zero. (Cf., $\chi_I - \chi_{II} = 0$ above; the new expression equal to zero will, of course, also involve various quantities evaluated on the two sides of the interface.) As above, all transverse derivatives $\partial^{n-m} / (\partial y')^{n-m}$ of such a difference will also be zero. This gives us the needed boundary conditions on $\partial^n \chi / (\partial y')^{n-m} (\partial z')^m$ (N.B., the derivatives must be taken in this specific order.) We have to be careful to keep the $\partial / \partial y'$ and $\partial / \partial z'$ operators in their present positions, because the identifications in (G.1) generate cross-terms of the form $\underline{\nabla}_T \hat{t}_{2D}, \underline{\nabla}_T \hat{n}_{2D}$, and these in turn generate subtle modifications to the boundary conditions. (Keep in mind that the now order-sensitive result for

$$\partial^n \chi / (\partial y')^{n-m} (\partial z')^m = \left(\hat{t}_{2D} \cdot \underline{\nabla}_T\right)^{n-m} \left(\hat{n}_{2D} \cdot \underline{\nabla}_T\right)^m \chi$$

goes into a system of equations that give us all the needed boundary conditions on $\partial^n \chi / \partial y^n$, $\partial^n \chi / \partial z^n$, and $\partial^n \chi / \partial y^{n-m} \partial z^m$, and that once we have $\partial^n \chi / \partial y^{n-m} \partial z^m$, we will again be free to switch the order of $\partial / \partial y$ and $\partial / \partial z$ as much as we want.)

This is all we need to evaluate the boundary conditions on a 2-dimensional interface embedded in 3-dimensional space. Once we have the boundary conditions, then we use the basic procedure outlined in Subsection 3.3.2 to evaluate transverse derivatives of the wave function χ and so obtain $H\chi$, which is then used to perform the next downrange step.

H Appendix: Key aspects of the full wave boundary conditions for the 2nd transverse derivative of the field

This appendix addresses the following problem: Given that A solves the Helmholtz equation $\left(\vec{\nabla} \cdot \vec{\nabla} + k^2\right) A = 0$ in 2-dimensional $x - z$ space, and that the sound speed (but not the density) jumps along a quasi-planar interface S given by $z = f(x)$, find the boundary condition in terms of f and its derivatives to 2nd order. The appendix ends with a brief discussion of the results.

For the vector $\hat{n}$ normal to the surface $z = f(x)$, we have

$$\vec{\nabla} = \hat{n}\left(\hat{n}\cdot\vec{\nabla}\right) + \left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla} = \hat{n}\frac{\partial}{\partial \hat{n}} + \left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla} \tag{H.1}$$

and

$$\begin{aligned}\vec{\nabla}\cdot\vec{\nabla} = {} & \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right] + \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\hat{n}\frac{\partial}{\partial \hat{n}} + \left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right]\cdot\hat{n}\frac{\partial}{\partial \hat{n}} \\ & + \left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right]\cdot\left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right].\end{aligned} \tag{H.2}$$

Now on S, $\Delta A = A_I - A_{II} = 0$ and also

$$\frac{\partial A_I}{\partial \hat{n}} - \frac{\partial A_{II}}{\partial \hat{n}} = \frac{\partial(\Delta A)}{\partial \hat{n}} = 0\,.$$

Consider

$$\begin{aligned}\vec{\nabla}\cdot\vec{\nabla} = {} & \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right](\Delta A) + \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\hat{n}\frac{\partial(\Delta A)}{\partial \hat{n}} \\ & + \left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right]\cdot\hat{n}\frac{\partial(\Delta A)}{\partial \hat{n}} + \left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right]\cdot\left[\left(\mathbf{1} - \hat{n}\hat{n}\right)\cdot\vec{\nabla}\right](\Delta A)\end{aligned}\,. \tag{H.3}$$

The two terms on the second line involve tangential derivatives of quantities that are always 0 on the interface, so they fall out, leaving us with

$$\begin{aligned}\vec{\nabla}\cdot\vec{\nabla}(\Delta A) &= \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\vec{\nabla}(\Delta A) - \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\hat{n}\frac{\partial(\Delta A)}{\partial \hat{n}} + \hat{n}\frac{\partial}{\partial \hat{n}}\cdot\hat{n}\frac{\partial(\Delta A)}{\partial \hat{n}} \\ &= \hat{n}\hat{n} : \vec{\nabla}\vec{\nabla}(\Delta A)\end{aligned}$$

for $\Delta A = 0$ (i.e., A continuous) on a surface with normal $\hat{n}$.

Now

$$\hat{n} = \frac{\hat{z} - \dot{f}\cdot\hat{x}}{\sqrt{1+\dot{f}^2}}$$

and so

$$\begin{aligned}\hat{n}\hat{n} : \vec{\nabla}\vec{\nabla} &= \frac{1}{1+\dot{f}^2}\left(\hat{z} - \dot{f}\cdot\hat{x}\right)\left(\hat{z} - \dot{f}\cdot\hat{x}\right) : \vec{\nabla}\vec{\nabla} \\ &= \left[\dot{f}^2\hat{x}\hat{x} + \left(1 - \dot{f}^2\right)\hat{z}\hat{z} - \dot{f}\left(\hat{x}\hat{z} + \hat{z}\hat{x}\right)\right] : \vec{\nabla}\vec{\nabla} + \mathrm{O}\left(\dot{f}^3\right) \\ &= \dot{f}^2\frac{\partial^2}{\partial x^2} + \left(1 - \dot{f}^2\right)\frac{\partial^2}{\partial z^2} - 2\dot{f}\frac{\partial^2}{\partial x \partial z} + \mathrm{O}\left(\dot{f}^3\right).\end{aligned} \tag{H.4}$$

Now, the tangent vector is given by $\hat{t} = \hat{x} + \dot{f} \cdot \hat{z} + \mathrm{O}\left(\dot{f}^2\right)$ and the tangential derivative is

$$\hat{t} \cdot \vec{\nabla} = \frac{\partial}{\partial x} + \dot{f} \frac{\partial}{\partial z} + + \mathrm{O}\left(\dot{f}^2\right)$$

or

$$\hat{t} \cdot \vec{\nabla} - \dot{f} \frac{\partial}{\partial z} + \mathrm{O}\left(\dot{f}^2\right) = \frac{\partial}{\partial x},$$

and substituting into $\partial^2 / \partial x \partial z$ in equation (H.4), we have

$$\begin{aligned} \vec{\nabla} \cdot \vec{\nabla} (\Delta A) &= \hat{n}\hat{n} : \vec{\nabla}\vec{\nabla} (\Delta A) \\ &= \dot{f}^2 \frac{\partial^2 (\Delta A)}{\partial x^2} + \left(1 - \dot{f}^2\right) \frac{\partial^2 (\Delta A)}{\partial z^2} \\ &\quad -2\dot{f}\ \hat{t} \cdot \vec{\nabla} \frac{\partial (\Delta A)}{\partial z} + 2\dot{f}^2 \frac{\partial^2 (\Delta A)}{\partial z^2} + \mathrm{O}\left(\dot{f}^3\right) \end{aligned} \quad . \qquad \text{(H.5)}$$

The second to the last term in equation (H.5) involves a tangential derivative of a quantity that is zero on the interface, so it goes away. Also

$$\frac{\partial^2}{\partial x^2} = \hat{t} \cdot \vec{\nabla} \hat{t} \cdot \vec{\nabla} + \mathrm{O}\left(\dot{f}\right),$$

so that

$$\frac{\partial^2 (\Delta A)}{\partial x^2} = \left[\hat{t} \cdot \vec{\nabla}\right]\left[\hat{t} \cdot \vec{\nabla}\right](\Delta A) + \mathrm{O}\left(\dot{f}\right),$$

which is just the repeated application of tangential derivatives on something that is zero on the interface, and so $\partial^2 (\Delta A) / \partial x^2 = 0$. This leaves us with

$$\vec{\nabla} \cdot \vec{\nabla} (\Delta A) = \left(1 + \dot{f}^2\right) \frac{\partial^2 (\Delta A)}{\partial z^2} + \mathrm{O}\left(\dot{f}^3\right). \qquad \text{(H.6)}$$

Also

$$\begin{aligned} 0 &= \vec{\nabla} \cdot \vec{\nabla} A_I + k_I^2 A_I \\ 0 &= \vec{\nabla} \cdot \vec{\nabla} A_{II} + k_{II}^2 A_{II} \end{aligned},$$

so evaluate each of these just on either side of the interface and subtract (recalling $A_I = A_{II} = A$ on S):

$$0 = \vec{\nabla} \cdot \vec{\nabla} (\Delta A) + \left(k_I^2 - k_{II}^2\right) A. \qquad \text{(H.7)}$$

Now let the sound speed in medium I be the reference value c_0.

Thus, with $n \equiv c_0 / c$, we get $n_{II} \equiv c_I / c_{II}$, and $\mu_{II} \equiv \left(1 - n_{II}^2\right) / 2$. This implies:

$$\left.\begin{aligned} k_I &= k_0 \\ k_{II} &= nk_0 \end{aligned}\right\} \Rightarrow k_I^2 - k_{II}^2 = k_0^2\left(1-n^2\right) = 2k_0\mu_{II}\,.$$

Substituting into equation (H.7), we have

$$0 = \vec{\nabla}\cdot\vec{\nabla}\left(\Delta\, A\right) + 2k_0^2\mu_{II}A\,.$$

From equation (H.6), this leaves us with the boundary condition

$$0 = \left(1+\dot{f}^2\right)\frac{\partial^2\left(\Delta\, A\right)}{\partial z^2} + 2k_0^2\mu_{II}A + \mathrm{O}\left(\dot{f}^3\right), \tag{H.8}$$

or more usefully

$$\frac{\partial^2 A_I}{\partial z^2} - \frac{\partial^2 A_{II}}{\partial z^2} = -2\left(1-\dot{f}^2\right)k_0^2\mu_{II}A + \mathrm{O}\left(\dot{f}^3\right). \tag{H.9}$$

This suggests that the $\mathrm{O}\left(\dot{f}^2\right)$ terms in the parabolic equation boundary conditions contributed by the Foldy-Wouthuysen transformation term $\ddot{\mu}/8k_0$ can be understood as contributing to the boundary condition on $\partial^2 A/\partial z^2$.

The $\mathrm{O}\left(\ddot{f}\right)$ term is a little different. We can get the implicit boundary condition on $\partial^3 A/\partial z^3$ by taking ∇_T of equation (H.3). Now the second to the last term of equation (H.3) is nonzero and can produce a term proportional to $\ddot{f}$, and so we would expect the $\mathrm{O}\left(\ddot{f}\right)$ contribution to be associated with the implicit boundary condition on $\partial^3 A/\partial z^3$. The 3rd order transverse derivative is a pretty obscure quantity in the context of the Helmholtz equation. It shows up neither in the equation of motion nor in a finite difference discretization of the Helmholtz equation. Thus, the $\mathrm{O}\left(\ddot{f}\right)$ contribution to the boundary conditions for this quantity involves a subtle effect that is implicit in full wave theory, but must be made explicit in the PE. To get a crude idea of the physics associated with the $\mathrm{O}\left(\ddot{f}\right)$ term, consider the boundary condition

$$\frac{\partial\chi}{\partial z} = -\frac{\mu_{II}}{4}\ddot{f}\chi$$

in isolation. For $\mu_{II}\ddot{f} > 0$, this allows a solution that decays exponentially away from the surface as $\exp\left(-\left(\mu_{II}\ddot{f}\right)z/4\right)$. This topic is considered briefly in Section 4.2, and again in more detail later in Section 5.3.3, and in Appendices N.2 and O. Here, note that these boundary wave solutions look like polaritons (see, for example the work of Soto-Crespo *et al*.[83], or Tang and Frisk directly in the context of acoustics[84]).

In Section 3.2, attention is concentrated on the $\mathrm{O}\left(\dot{f}^2\right)$ component to the boundary conditions, and in particular to the part related to the boundary condition on $\nabla_T^2\chi$ and by extension on $\nabla_T^2 A$. To do so, Section 4.2 considers the tilted interface with no curvature, and examines this issue in some depth.

I Appendix: Constructing an ansatz and obtaining the state space equation when the density is not uniformly constant

The goal of this appendix is the construction of a state space equation that is a suitable starting point for the Foldy-Wouthuysen transformation. To construct such an equation, we need to fully understand the philosophy behind this transformation.

The state space equation will be the equation of motion for a vector of the basic form

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix} \tag{I.1}$$

(e.g., equations (3.2) and (5.2)). For the acoustic field, θ and χ are scalars, but for vector fields they will be vectors. Φ is a 2-dimensional vector in what may be called a state space, where θ and χ are two possible states (of the field). The state space equation has the basic form

$$i\frac{\partial \Phi}{\partial x} = \mathcal{H}\Phi \tag{I.2}$$

where $\mathcal{H}$ is a 2×2 matrix in state space. Each of the four elements of $\mathcal{H}$ can be operators (for vector fields, they can even become matrices themselves). For a classical field, the Foldy-Wouthuysen transformation assumes that the state space equation has been constructed in such a way that $\mathcal{H}$ is pseudo-Hermitian[yyy]. As discussed in reference [1] (or equivalently appendix C.1.2), an operator α is pseudo-Hermitian when $(\eta\alpha)^\dagger = \eta\alpha$ with η as always defined in (3.3). (Note that η and ξ are both 2×2 matrices in state space. η is a kind of metric on our state space, and so magnitudes

[yyy] More generally, this assertion holds for fields that have integer intrinsic spin (bosons). For fermions (half-integer spin), the full matrix Hamiltonian is Hermitian. However, for a fermion field, the equation is in the form of a state space equation from the beginning, and the derivation in this appendix is not needed. Furthermore, this distinction has very minimal effect on the subsequent portions of the calculation.

squared of vectors in this space Φ are inner products of the vectors with themselves under this metric: $\Phi^\dagger \eta \Phi$.) As discussed in reference [1], (or equivalently appendix C.1.2) pseudo-Hermiticity stabilizes the equation by guaranteeing that the magnitude squared of the vector $\Phi^\dagger \eta \Phi$ is conserved under downrange propagation. In fact, this conservation law and the pseudo-Hermiticity of the (matrix) Hamiltonian are simply two manifestations of the same property.

Under the Foldy-Wouthuysen procedure, one then performs a series of canonical transformations $\Phi_{\text{old}} \to \Phi_{\text{new}}$. By canonical, it is meant that the transformation is constructed in such a way that the basic form of the equation of motion is preserved—in this case:

$$i\frac{\partial \Phi_{\text{new}}}{\partial x} = \mathcal{H}_{\text{new}} \Phi_{\text{new}} .$$

Furthermore, $\mathcal{H}_{\text{new}}$ is still pseudo-Hermitian. This latter attribute is obtained by requiring that the transformations be pseudo-unitary (i.e., if $\Phi_{\text{old}} = U\Phi_{\text{new}}$, then $U^\dagger \eta U = \eta$; again this point is discussed in reference [1]). Note that then ${\Phi_{\text{old}}}^\dagger \eta \Phi_{\text{old}} = \Phi_{\text{new}} \eta \Phi_{\text{new}}$, and so the magnitude of Φ_{new} must be preserved during downrange propagation as well, and $\mathcal{H}_{\text{new}}$ must indeed be pseudo-Hermitian.

Thus, the first step toward applying the Foldy-Wouthuysen transformation is the construction of an ansatz (i.e., a definition for θ and χ) that leads to a proper state space equation. To guarantee that the Hamiltonian of the state space equation $\mathcal{H}$ be pseudo-Hermitian, we choose θ and χ such that there are physical constraints that force $\Phi^\dagger \eta \Phi$ to be conserved during downrange propagation. Specifically, if we construct θ and χ from the original field in such a way that $\Phi^\dagger \eta \Phi = |\theta|^2 - |\chi|^2$ is proportional to the downrange flux S_x, then energy conservation would force the required conservation of $\Phi^\dagger \eta \Phi$. Specifically for an acoustic field with a variable density, this means that a factor of $1/\rho$ (as always ρ is the density as a function of position) will somehow need to be built into θ and χ. This leads to the ansatz given in equation (5.2) and repeated here:

$$\begin{aligned} \theta &= \frac{1}{2}\left(A + \frac{\rho_0}{\rho}\frac{i}{k_0}\dot{A} \right) \\ \chi &= \frac{1}{2}\left(A - \frac{\rho_0}{\rho}\frac{i}{k_0}\dot{A} \right) \end{aligned} \qquad \text{(I.3)}$$

(the dot stands for a downrange derivative $\dot{A} = \partial A/\partial x$). Note the general form of this result. If the downrange flux is the product between the field and another quantity, then the ansatz for θ and χ becomes a sum and difference between this field and that other

quantity times i. (When vector fields are considered in Section 7 and Appendices R and S, θ and χ themselves become vector fields, but the above reasoning remains valid.)

Let us verify that this ansatz indeed works:

$$\begin{aligned}\theta\theta^* &= \frac{1}{4}\left[AA^* + \frac{\rho_0^2}{\rho^2}\frac{\dot{A}\dot{A}^*}{k_0^2} + \frac{i}{k_0}\frac{\rho_0}{\rho}\left(A^*\dot{A} - A\dot{A}^*\right)\right] \\ &= \frac{1}{4}\left[AA^* + \frac{\rho_0^2}{\rho^2}\frac{\dot{A}\dot{A}^*}{k_0^2} - \frac{2}{k_0}\frac{\rho_0}{\rho}\mathrm{Im}\left(\dot{A}A^*\right)\right]\end{aligned}.$$

Substituting $-\dot{A}$ for $\dot{A}$ gives

$$\chi\chi^* = \frac{1}{4}\left[AA^* + \frac{\rho_0^2}{\rho^2}\frac{\dot{A}\dot{A}^*}{k_0^2} + \frac{2}{k_0}\frac{\rho_0}{\rho}\mathrm{Im}\left(\dot{A}A^*\right)\right].$$

Thus

$$\theta\theta^* - \chi\chi^* = -\frac{\rho_0}{k_0}\frac{\mathrm{Im}\left(\dot{A}A^*\right)}{\rho} = -2\rho_0 c_0\left[\frac{\mathrm{Im}\left(\dot{A}A^*\right)}{2\rho\omega}\right] = -2\rho_0 c_0 \vec{S}_{\mathrm{ave}}\cdot\hat{x}\,, \qquad \text{(I.4)}$$

where $\vec{S}_{\mathrm{ave}} = \mathrm{Im}\left(A^*\vec{\nabla}A\right)/2\rho\omega$ is the time-averaged flux (see reference [98], equations 64.6 and 65.4 and use a well-known result for the time-averaged product of the real parts of two complex fields; also compare equation 20b in [1]).

Next, we need to manipulate the definitions for θ and χ and the equation of motion for the pressure field A to construct the state space equation. We will need to make use of one more trick to proceed. To preserve Hermiticity down the line, we should follow reference [98] (pp.245, 288-289) and group the overall factor of the density with k^2 as follows:

$$\vec{\nabla}\cdot\left(\frac{1}{\rho}\vec{\nabla}A\right) + \frac{k^2}{\rho}A = 0\,. \qquad \text{(I.5)}$$

Note that

$$\frac{k^2}{\rho} = \frac{k_0^2}{\rho_0}\left(\frac{n^2\rho_0}{\rho}\right) = \frac{k_0^2}{\rho_0} + \left(\frac{n^2\rho_0}{\rho} - 1\right)\frac{k_0^2}{\rho_0} \quad ; \quad \vec{\nabla}\cdot\left(\frac{1}{\rho}\vec{\nabla}\right) = \frac{\partial}{\partial x}\cdot\left(\frac{1}{\rho}\frac{\partial}{\partial x}\right) + \nabla_T\cdot\left(\frac{1}{\rho}\nabla_T\right). \qquad \text{(I.6)}$$

Recall that when the density was everywhere the same, it was convenient to characterize the index of refraction squared by a quantity $\mu = \left(1-n^2\right)/2$ (see equation (2.5)). The left result of equation (I.6) suggests that we now have to generalize this to

$$\mu = \frac{1}{2}\left(1 - \frac{n^2\rho_0}{\rho}\right). \qquad \text{(I.7)}$$

Noting that $n = c_0/c = \sqrt{(\rho K)/(\rho_0 K_0)}$ (recall that K is a compressibility and $c = \sqrt{1/(\rho K)}$), we see that μ is in fact a measure of the change of compressibility

$$\mu = \frac{1}{2}\left(1 - \frac{K}{K_0}\right) \tag{I.8}$$

rather than simply of the square of the index of refraction. The two turn out to be equivalent only in the special case when the density is everywhere constant. Now let us define an operator

$$\tilde{\lambda} \equiv \frac{\nabla_T \left(\rho_0/\rho\right) \nabla_T}{2k_0} - k_0 \mu \,. \tag{I.9}$$

(In this context, this operator turns out to be an intermediate quantity, but it will occasionally reappear in our subsequent analyses−for example in Appendix L.2.) Multiplying equation (I.5) by ρ_0 and making substitutions (I.6) and (I.9), we end up with the following form of the equation of motion:

$$\frac{\partial}{\partial x} \cdot \left(\frac{\rho_0}{\rho} \dot{A}\right) + 2k_0 \tilde{\lambda} A + k_0^2 A = 0 \,. \tag{I.10}$$

Recalling the ansatz (I.3), we have

$$\begin{aligned} A &= \theta + \chi \\ \frac{\rho_0}{\rho}\dot{A} &= \frac{k_0}{i}(\theta - \chi) \quad \Rightarrow \quad \frac{\partial}{\partial x}\left(\frac{\rho_0}{\rho}\dot{A}\right) = \frac{k_0}{i}\left(\dot{\theta} - \dot{\chi}\right), \end{aligned}$$

leaving us with the following alternate form of the wave equation:

$$-ik_0\left(\dot{\theta} - \dot{\chi}\right) + 2k_0\tilde{\lambda}(\theta + \chi) + k_0^2(\theta + \chi) = 0 \,. \tag{I.11}$$

Next, we obtain a second equation for θ and χ by manipulating their definitions in terms of A and $\dot{A}$ (i.e., the ansatz). Adding and subtracting the two equations in (I.3), we have

$$\begin{aligned} A = \theta + \chi \quad &\Rightarrow \quad \dot{A} = \dot{\theta} + \dot{\chi} \\ ik_0 \frac{\rho_0}{\rho}\dot{A} = \theta - \chi \quad &\Rightarrow \quad \dot{A} = -ik_0 \frac{\rho}{\rho_0}(\theta - \chi) \end{aligned} \,. \tag{I.12}$$

Removing $\dot{A}$ from the right hand pair of equations in (I.12), rewriting equation (I.11), and multiplying through by ik_0 leaves us with the following pair of equations

$$\begin{aligned} ik_0\left(\dot{\theta} + \dot{\chi}\right) &= k_0^2 \frac{\rho}{\rho_0}(\theta - \chi) \\ ik_0\left(\dot{\theta} - \dot{\chi}\right) &= 2k_0\tilde{\lambda}(\theta + \chi) + k_0^2(\theta + \chi) \end{aligned} \,. \tag{I.13}$$

Adding and subtracting these two equations, and dividing by $2k_0$ gives us

$$\begin{aligned} i\dot{\theta} &= \tilde{\lambda}(\theta+\chi)+\frac{k_0}{2}(\theta+\chi)+\frac{k_0}{2}\frac{\rho}{\rho_0}(\theta-\chi) \\ i\dot{\chi} &= -\tilde{\lambda}(\theta+\chi)-\frac{k_0}{2}(\theta+\chi)+\frac{k_0}{2}\frac{\rho}{\rho_0}(\theta-\chi) \end{aligned}.$$

Recall $\gamma \equiv \tfrac{1}{2}(1-\rho/\rho_0)$ so that

$$\frac{k_0}{2}\frac{\rho}{\rho_0} = \frac{k_0}{2} - k_0\gamma,$$

and consequently

$$\begin{aligned} i\dot{\theta} &= \left[\tilde{\lambda}+\frac{k_0}{2}+\left(\frac{k_0}{2}-k_0\gamma\right)\right]\theta+\left[\tilde{\lambda}+\frac{k_0}{2}-\left(\frac{k_0}{2}-k_0\gamma\right)\right]\chi \\ i\dot{\chi} &= \left[-\tilde{\lambda}-\frac{k_0}{2}+\left(\frac{k_0}{2}-k_0\gamma\right)\right]\theta+\left[-\tilde{\lambda}-\frac{k_0}{2}-\left(\frac{k_0}{2}-k_0\gamma\right)\right]\chi \end{aligned}.$$

Applying the definition $\lambda \equiv \tilde{\lambda}+k_0\gamma$, this gives us

$$i\begin{pmatrix}\dot{\theta}\\ \dot{\chi}\end{pmatrix} = \begin{pmatrix}\lambda-2k_0\gamma+k_0 & \lambda \\ -\lambda & -(\lambda-2k_0\gamma)-k_0\end{pmatrix}\begin{pmatrix}\theta\\ \chi\end{pmatrix},$$

and finally using (I.1), we have

$$i\dot{\Phi} = \left[\lambda\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}+(\lambda-2k_0\gamma)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}+k_0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right]\Phi, \qquad \text{(I.14)}$$

which is just the state space equation (5.3).

J Appendix: The 4th order Hamiltonian $\mathcal{H}$ for a variable density

Appendix J.1 provides a derivation of the Hamiltonian $\mathcal{H}$ good for an acoustic field, where the density and sound speed are both allowed to vary. The expression is quite general, and it applies even if the density variation involves a discontinuity. Appendix J.2 derives a simplified Hamiltonian for the special case where the density jumps at an interface, but is otherwise constant.

J.1 The general 4th order Hamiltonian $\mathcal{H}$ for a variable density

This appendix provides the details of the derivation of the matrix Hamiltonian $\mathcal{H}$ for a variable density as it is given by equation (5.7).

The starting point deriving our general $\mathcal{H}$ is the state space equation given by equations (5.3) and (5.4) (or equivalently equation (I.14) above), which are reproduced below:

$$i\frac{\partial \Phi}{\partial x} = \mathcal{H}\Phi \quad \text{with} \quad \mathcal{H} \equiv \mathcal{O} + \mathcal{E} + k_0\eta\,,$$

where

$$\begin{aligned} \mathcal{O} &= \lambda\xi \\ \mathcal{E} &= (\lambda - 2k_0\gamma)\eta \end{aligned}\,, \tag{J.1}$$

with the matrices η and ξ as always, and

$$\begin{aligned} \lambda &= \frac{\underline{\nabla}_T \cdot \left(\frac{\rho_0}{\rho}\right)\underline{\nabla}_T}{2k_0} - k_0\mu + k_0\gamma \\ \mu &\equiv \frac{1}{2}\left(1 - \frac{\mathrm{K}}{\mathrm{K}_0}\right) = -\frac{\Delta \mathrm{K}}{2\mathrm{K}_0} = \frac{1}{2}\left(1 - \frac{\rho_0}{\rho}n^2\right). \\ \gamma &\equiv \frac{1}{2}\left(1 - \frac{\rho}{\rho_0}\right) = -\frac{\Delta\rho}{2\rho_0} \end{aligned} \tag{J.2}$$

These values for $\mathcal{O}$ and $\mathcal{E}$ will be substituted into the general 4th order result given by equations (3.9) and (3.10) (and equivalently (C.28) and (C.29)), and reproduced below for convenience:

$$\tilde{\mathcal{H}}^{IV} = k_0\eta + \mathcal{E}^{II}\,, \tag{J.3}$$

where

$$\begin{aligned} \mathcal{E}^{II} = {} & \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\left[\mathcal{O},[\mathcal{O},\mathcal{E}]\right] - \frac{i}{8k_0^2}\left[\mathcal{O},\dot{\mathcal{O}}\right] \\ & + \frac{\eta}{8k_0^3}\left(-[\mathcal{O},\mathcal{E}]^2 - i\left\{\dot{\mathcal{O}},[\mathcal{O},\mathcal{E}]\right\} + \dot{\mathcal{O}}^2\right) + \text{ 5th order} \end{aligned} \tag{J.4}$$

(as always, the dot denotes the downrange derivative $\partial/\partial x$). Beginning with the substitution $\mathcal{E} = (\lambda - 2k_0\gamma)\eta$, this yields

$$\begin{aligned}\mathcal{E}^{II} &= \eta\frac{\mathcal{O}^2}{2k_0} - \eta\frac{\mathcal{O}^4}{8k_0^3} + \lambda\eta - 2\gamma k_0\eta - \frac{1}{8k_0^2}\Big[\mathcal{O},[\mathcal{O},\lambda\eta]\Big] \\ &+ \frac{1}{8k_0^2}\Big[\mathcal{O},[\mathcal{O},2\gamma k_0\eta]\Big] - \frac{i}{8k_0^2}\Big[\mathcal{O},\dot{\mathcal{O}}\Big] \\ &+ \frac{\eta}{8k_0^3}\Big(-\big([\mathcal{O},\lambda\eta]-[\mathcal{O},2\gamma k_0\eta]\big)^2 - i\Big\{\dot{\mathcal{O}},[\mathcal{O},\lambda\eta]\Big\} + i\Big\{\dot{\mathcal{O}},[\mathcal{O},2\gamma k_0\eta]\Big\} + \dot{\mathcal{O}}^2\Big) \\ &+ 5^{\text{th}}\text{ order.}\end{aligned} \tag{J.5}$$

Now expand

$$\begin{aligned}&\big([\mathcal{O},\lambda\eta]-[\mathcal{O},2\gamma k_0\eta]\big)^2 = \\ &[\mathcal{O},\lambda\eta]^2 + [\mathcal{O},2\gamma k_0\eta]^2 - [\mathcal{O},\lambda\eta][\mathcal{O},2\gamma k_0\eta] - [\mathcal{O},2\gamma k_0\eta][\mathcal{O},\lambda\eta]\end{aligned}$$

and recombine terms to get

$$\tilde{\mathcal{H}}^{IV} = k_0\eta + \mathcal{E}^{II} = (1)+(2)+(3), \tag{J.6}$$

where

$$\begin{aligned}(1) &= k_0\eta + \eta\frac{\mathcal{O}^2}{2k_0} - \eta\frac{\mathcal{O}^4}{8k_0^3} + \lambda\eta - \frac{1}{8k_0^2}\Big[\mathcal{O},[\mathcal{O},\lambda\eta]\Big] - \frac{\eta}{8k_0^3}[\mathcal{O},\lambda\eta]^2 \\ &- \frac{i}{8k_0^2}\Big[\mathcal{O},\dot{\mathcal{O}}\Big] - \frac{i\eta}{8k_0^3}\Big\{\dot{\mathcal{O}},[\mathcal{O},\lambda\eta]\Big\} + \frac{\eta\dot{\mathcal{O}}^2}{8k_0^3} \\ (2) &= -2\gamma k_0\eta + \frac{1}{8k_0^2}\Big[\mathcal{O},[\mathcal{O},2\gamma k_0\eta]\Big] - \frac{\eta}{8k_0^3}[\mathcal{O},2\gamma k_0\eta]^2 \\ &+ \frac{\eta}{8k_0^3}\Big[[\mathcal{O},\lambda\eta][\mathcal{O},2\gamma k_0\eta] + [\mathcal{O},2\gamma k_0\eta][\mathcal{O},\lambda\eta]\Big] \\ (3) &= \frac{i\eta}{8k_0^3}\Big\{\dot{\mathcal{O}},[\mathcal{O},2\gamma k_0\eta]\Big\}\end{aligned} \tag{J.7}$$

Note that (1) identically reproduces the terms that were present in the constant density formula, and note that according to equation (J.1), $\mathcal{O}$ is formally the same as it was in the constant density case (only the definition of λ changes a little, and that is immaterial until we explicitly substitute for λ), and so these terms will reproduce the constant density result given by (C.31):

$$(1) = \eta k_0\left(1 + \frac{\lambda}{k_0} - \frac{\lambda^2}{k_0^2} + \frac{\lambda^3}{2k_0^3} - \frac{5\lambda^4}{8k_0^4} - \frac{\dot{\lambda}^2}{8k_0^4}\right) + \frac{i}{8k_0^2}\Big[\lambda,\dot{\lambda}\Big] - \frac{i}{4k_0^3}\Big[\lambda^2,\dot{\lambda}\Big]. \tag{J.8}$$

Next, let us explore (2), the new terms unique to the variable density problem that do not contain explicit range derivatives. To do so, we exploit the following identities (obtained

using the result $\eta\xi = -\xi\eta$, which follows directly from equations (3.3) and (3.6), the definitions of η and ξ):

$$\begin{aligned}
[\mathcal{O}, \lambda\eta] &= \lambda^2 [\xi, \eta] = \lambda^2 \left(\xi\eta - \underbrace{\eta\xi}_{-\xi\eta} \right) = 2\lambda^2 \xi\eta \\
[\mathcal{O}, 2\gamma k_0 \eta] &= 2k_0 [\lambda\xi, \eta\gamma] = 2k_0 \left(\lambda\gamma\xi\eta - \gamma\lambda \underbrace{\eta\xi}_{-\xi\eta} \right) \\
&= 2k_0 (\lambda\gamma + \gamma\lambda) \xi\eta = 2k_0 \{\lambda, \gamma\} \xi\eta
\end{aligned} \tag{J.9}$$

to obtain (again using equation (3.6), the definition of ξ, to get $\xi^2 = -\mathbf{1}$)

$$\begin{aligned}
[\mathcal{O}, \lambda\eta][\mathcal{O}, 2\gamma k_0 \eta] &= 4\lambda^2 k_0 \{\lambda, \gamma\} \xi \underbrace{\eta\xi}_{-\xi\eta} \eta = -4\lambda^2 k_0 \{\lambda, \gamma\} \underbrace{\xi^2}_{-\mathbf{1}} \underbrace{\eta^2}_{\mathbf{1}} \\
&= 4\lambda^2 k_0 \{\lambda, \gamma\}
\end{aligned}.$$

Similarly, we have

$$\begin{aligned}
[\mathcal{O}, 2\gamma k_0 \eta][\mathcal{O}, \lambda\eta] &= 4k_0 \{\lambda, \gamma\} \lambda^2 \cdot \xi \underbrace{\eta\xi}_{-\xi\eta} \eta = -4k_0 \{\lambda, \gamma\} \lambda^2 \cdot \underbrace{\xi^2}_{-\mathbf{1}} \underbrace{\eta^2}_{\mathbf{1}} \\
&= 4k_0 \{\lambda, \gamma\} \lambda^2
\end{aligned},$$

and so

$$[\mathcal{O}, \lambda\eta][\mathcal{O}, 2\gamma k_0 \eta] + [\mathcal{O}, 2\gamma k_0 \eta][\mathcal{O}, \lambda\eta] = 4k_0 \left\{ \lambda^2, \{\lambda, \gamma\} \right\}. \tag{J.10}$$

Also, from the second equation in (J.9), we have

$$\begin{aligned}
[\mathcal{O}, 2\gamma k_0 \eta]^2 &= 4k_0^2 \{\lambda, \gamma\}^2 \xi \underbrace{\eta\xi}_{-\xi\eta} \eta = -4k_0^2 \{\lambda, \gamma\}^2 \underbrace{\xi^2}_{-\mathbf{1}} \underbrace{\eta^2}_{\mathbf{1}} \\
&= 4k_0^2 \{\lambda, \gamma\}^2
\end{aligned}. \tag{J.11}$$

To finish evaluating (2), we also need

$$\begin{aligned}\frac{1}{8k_0^2}\left[\mathcal{O},\left[\mathcal{O},2\gamma k_0\eta\right]\right] &= \frac{1}{8k_0^2}\left[\lambda\xi,2k_0\{\lambda,\gamma\}\xi\eta\right] \\ &= \frac{1}{8k_0^2}2k_0\left(\lambda\xi\cdot\xi\eta\{\lambda,\gamma\}-\xi\eta\{\lambda,\gamma\}\lambda\xi\right) \\ &= \frac{1}{4k_0}\left(\lambda\{\lambda,\gamma\}\xi^2\eta-\{\lambda,\gamma\}\lambda\xi\underbrace{\eta\xi}_{-\xi\eta}\right) \\ &= \frac{1}{4k_0}\underbrace{\xi^2}_{-1}\eta\left(\lambda\{\lambda,\gamma\}+\{\lambda,\gamma\}\lambda\right) \\ &= -\frac{\eta}{4k_0}\left\{\lambda,\{\lambda,\gamma\}\right\}.\end{aligned} \tag{J.12}$$

Thus,

$$(2) = -2\gamma k_0\eta - \frac{\eta}{4k_0}\left\{\lambda,\{\lambda,\gamma\}\right\} - \underbrace{\frac{\eta}{8k_0^3}}_{2k_0}\cancel{4k_0^2}\{\lambda,\gamma\}^2 + \underbrace{\frac{\eta}{8k_0^3}}_{2k_0^2}\cancel{4k_0}\left\{\lambda^2,\{\lambda,\gamma\}\right\},$$

and pulling out a factor of $k_0\eta$, we have

$$(2) = k_0\eta\left(-2\gamma - \frac{1}{4k_0^2}\left\{\lambda,\{\lambda,\gamma\}\right\} - \frac{\eta}{2k_0^2}\{\lambda,\gamma\}^2 + \frac{\eta}{2k_0^3}\left\{\lambda^2,\{\lambda,\gamma\}\right\}\right). \tag{J.13}$$

Finally, for (3) we have

$$\begin{aligned}(3) &= \frac{i\eta}{8k_0^3}\left\{\dot{\mathcal{O}},\underbrace{\left[\mathcal{O},2\gamma k_0\eta\right]}_{2k_0\{\lambda,\gamma\}\xi\eta}\right\} = \frac{i\eta}{8k_0^3}\left\{\dot{\lambda}\xi,2k_0\{\lambda,\gamma\}\xi\eta\right\} \\ &= \underbrace{\frac{i\eta}{8k_0^3}}_{4k_0^2}\cancel{2k_0}\left(\dot{\lambda}\{\lambda,\gamma\}\xi\cdot\xi\eta+\{\lambda,\gamma\}\dot{\lambda}\xi\underbrace{\eta\xi}_{-\xi\eta}\right) \\ &= \frac{i\eta}{4k_0^2}\underbrace{\xi\cdot\xi}_{-1}\eta\left(\dot{\lambda}\{\lambda,\gamma\}-\{\lambda,\gamma\}\dot{\lambda}\right) = -\frac{i}{4k_0^2}\left[\dot{\lambda},\{\lambda,\gamma\}\right]\end{aligned} \tag{J.14}$$

Combining the three results, we have from equation (J.6)

$$
\begin{aligned}
\tilde{\mathcal{H}}^{IV} &= (1)+(2)+(3) \\
&= \eta k_0 \left(\begin{array}{l} 1-2\gamma+\dfrac{\lambda}{k_0}-\dfrac{\lambda^2}{k_0^2}+\dfrac{\lambda^3}{2k_0^3}-\dfrac{5\lambda^4}{8k_0^4}-\dfrac{\dot{\lambda}^2}{8k_0^4} \\ -\dfrac{1}{4k_0^2}\{\lambda,\{\lambda,\gamma\}\}-\dfrac{\eta}{2k_0^2}\{\lambda,\gamma\}^2+\dfrac{\eta}{2k_0^3}\{\lambda^2,\{\lambda,\gamma\}\} \end{array} \right), \\
&\quad +\frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right]-\frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right]-\frac{i}{4k_0^2}\left[\dot{\lambda},\{\lambda,\gamma\}\right]+\ 5^{\text{th}}\ \text{order}
\end{aligned}
\tag{J.15}
$$

which is equation (5.7) in slightly rearranged form. In equation (5.7), the tilde $\sim$ and superscript IV have been dropped from $\mathcal{H}$.

J.2 The 4th order Hamiltonian $\mathcal{H}$ good at a density jump

In this section, we take the general 4th order Hamiltonian for an acoustic field in an environment where the density varies (equation (5.7) and equivalently (J.15)) and adapt it to the special case where the density ρ (and so $\gamma = \tfrac{1}{2}(1-\rho/\rho_0)$) jumps at an interface, but is otherwise constant. The result is equation (J.24), which is equivalent to equation (5.9). While this discussion invokes single a quasi-planar interface, there is nothing to preclude its application to multiple interfaces, or ones that are not quasi-planar.

To simplify the discussion, it will be assumed that in the half-space the compressibility K (or equivalently $\mu = \tfrac{1}{2}(1-K/K_0)$) does not depend on the range in the half-spaces (although it may, of course, jump along the range-dependent interface). A modest correction to the formalism accounting for range dependence of μ in the half-spaces will be noted and tracked through the calculation. The resulting correction term is given in equation (J.26), which is the same as equation (5.10).

This effort generalizes the calculation that led to the manifestly range-reciprocal form of the parabolic equation for the case where the density was held constant (see Appendix C.2.5) by applying the same basic strategy to the case where the density varies (i.e., now use equation (5.7)/(J.15) as the starting point). The extra terms associated with the parameter γ (which reflects density variation away from a reference value) would significantly complicate the result. However, if we exploit the assumption that the density is constant within a given medium and only changes along interfaces, then the result simplifies to a rather straightforward generalization of result for the constant density problem (i.e., the result expressed in equation (C.35) or equivalently in equation (3.11)). Thus, we will apply extra Foldy-Wouthuysen transformations patterned after those in Appendix C.2.5, use the δ-function procedure outlined in Section 5.2 and Appendix K to evaluate the resultant expressions, and exploit the assumption that the density is constant away from the interface to simplify the result.

The extra Foldy-Wouthuysen transformations that generate the manifestly range-reciprocal form involve the terms in equation (5.7)/(J.15) that are induced by range dependence. (Id est, those terms containing a downrange derivative signified with a dot. These also happen to be the terms associated with "vacuum polarization" effects.) These four terms are

$$\begin{matrix} -\eta k_0\left(\frac{\dot{\lambda}^2}{8k_0^4}\right) & \frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right] \\ -\frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right] & -\frac{i}{4k_0^2}\left[\dot{\lambda},\{\lambda,\gamma\}\right] \end{matrix}.$$

Since only these terms will be involved in the operations considered here, it is convenient to isolate these terms from the rest of the Hamiltonian $\tilde{\mathcal{H}}^{IV}$ by rewriting equation (5.7) /(J.15) as

$$\tilde{\mathcal{H}}^{IV} = \eta H_{\mathrm{RI}} - \eta\frac{\dot{\lambda}^2}{8k_0^3} + \frac{i}{8k_0^2}\left[\lambda,\dot{\lambda}\right] - \frac{i}{4k_0^3}\left[\lambda^2,\dot{\lambda}\right] - \frac{i}{4k_0^2}\left[\dot{\lambda},\{\lambda,\gamma\}\right] + \text{ 5}^{\text{th}}\text{ order} \quad \text{(J.16)}$$

where

$$H_{\mathrm{RI}} \equiv k_0\begin{pmatrix} 1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{k_0^2}+\frac{\lambda^3}{2k_0^3}-\frac{5\lambda^4}{8k_0^4} \\ -\frac{1}{4k_0^2}\{\lambda,\{\lambda,\gamma\}\}-\frac{\eta}{2k_0^2}\{\lambda,\gamma\}^2+\frac{\eta}{2k_0^3}\{\lambda^2,\{\lambda,\gamma\}\} \end{pmatrix}. \quad \text{(J.17)}$$

(The subscript RI stands for range-independent. Note that for the moment we follow equation (J.15) and retain the tilde and superscript IV on $\mathcal{H}$.) Equations (J.16) and (J.17) reduce to the constant density result (C.31) if we set $\gamma = 0$.

Let us begin with the term proportional to $\dot{\lambda}^2$. Note that

$$\dot{\lambda}^2 = \frac{\partial}{\partial x}\left(\lambda\dot{\lambda}\right) - \lambda\ddot{\lambda}. \quad \text{(J.18)}$$

Since $\dot{\lambda}$ and $\ddot{\lambda}$ are proportional to bifurcated $\delta^{(n)}$-functions, λ is evaluated in the half-spaces. Recalling the definition of λ, equation (5.4), we note that the range derivative of ∇_T is zero and given our assumptions so are the range derivatives of μ and γ (evaluated in the half-spaces), and consequently in the half-spaces λ is also independent of the range. Thus (J.18) becomes

$$\dot{\lambda}^2 = \lambda\frac{\partial\dot{\lambda}}{\partial x} - \lambda\ddot{\lambda} = \lambda\ddot{\lambda} - \lambda\ddot{\lambda} = 0$$

and this term drops out.

Now, note what happens when we drop our assumption that μ is range-independent. At the surface, $\dot{\lambda}$ of course still involves a linear combination of bifurcating δ and δ'-functions, and so when we multiply it by another $\dot{\lambda}$, we just pick up that factor evaluated an infinitesimal distance in the half-spaces. In this case, the associative property to be discussed in Appendix K.3 is violated: in other words it matters which $\dot{\lambda}$ we choose to be the first one (and consequently bifurcate), so we symmetrize the choice of which $\dot{\lambda}$ to bifurcate. This gives us

$$\dot{\lambda}^2 \to \frac{1}{2}\left\{\left(\frac{\partial\lambda}{\partial x}\right)^{\pm}, \dot{\lambda}_S\right\}.$$

The subscript S signifies that $\dot{\lambda}_S$ is to be evaluated right on the surface S. The superscript $\pm$ serves to remind us that as $\dot{\lambda}_S$ bifurcates, its coefficients are evaluated in the two half-spaces. Note that since we now are allowing μ and consequently λ to depend on the range away from the interface, the term proportional to $\dot{\lambda}^2$ will also have to be added to the Hamiltonian $\mathcal{H}$ away from the interface. Indicating that the operator $\dot{\lambda}^2$ in its usually understood simple form will be evaluated everywhere except right on top of the interface, we will call it a principal value denoted by PV. This gives us result

$$\dot{\lambda}^2 \to \frac{1}{2}\left\{\left(\frac{\partial\lambda}{\partial x}\right)^{\pm}, \dot{\lambda}_S\right\} + \mathrm{PV}\left[\dot{\lambda}^2\right]. \tag{J.19}$$

For the moment, we will put result (J.19) aside, and proceed assuming $\dot{\lambda} = 0$. It will turn out that there is the only one other place where we use the assumption that μ is range-independent: in equation (J.23). Therefore, we will return to result (J.19) at the end of the calculation, and examine how it would modify the final result for $\tilde{\mathcal{H}}^{IV.2}$.

Now, let us apply the extra Foldy-Wouthuysen transformations used in Appendix C.2.5 to create a manifestly range-reciprocal Hamiltonian. Once again, we have (as in equation (C.32))

$$S^{IV.1} = \frac{\eta\dot{\lambda}}{8k_0^2}$$

and as in equation (C.33)

$$\tilde{\mathcal{H}}^{IV.1} = \tilde{\mathcal{H}}^{IV} + i\left[S^{IV.1}, \eta\left(k_0 + \lambda\underbrace{-2\gamma}_{\substack{\text{This is}\\ \text{new!}}} - \frac{\lambda^2}{2k_0}\right)\right] \underbrace{-\frac{1}{2}\left[S^{IV.1}, \left[S^{IV.1}, \eta k_0\right]\right]}_{\substack{\text{This term is always zero}\\ \text{because } \eta \text{ commutes with itself}}} - \dot{S}^{IV.1} + 5^{\text{th}} \text{ order} \tag{J.20}$$

Note that the term $-\frac{1}{2}\left[S^{IV.1}, \left[S^{IV.1}, \eta k_0\right]\right]$ is always zero because it reduces to

$$-\frac{1}{2}\frac{1}{64k_0^3}\left[\dot{\lambda}\eta,\dot{\lambda}\underbrace{[\eta,\eta]}_{0}\right]=0\,.$$

Note that here we do *not* need to invoke our assumption that μ is range-independent and so that $\dot{\lambda}^2=0$.

This leaves us with

$$\tilde{\mathcal{H}}^{IV.1}=\tilde{\mathcal{H}}^{IV}+i\left[\frac{\eta\dot{\lambda}}{8k_0^2},\eta\left(k_0+\lambda\underbrace{-2k_0\gamma}_{\substack{\text{This is}\\ \text{new!}}}-\frac{\lambda^2}{2k_0}\right)\right]-\frac{\eta\ddot{\lambda}}{8k_0^2}+5^{\text{th}}\text{ order}\,. \tag{J.21}$$

The only change between this result and the equivalent result in Appendix C.2.5 is the additional term

$$-2k_0\left[\frac{\eta\dot{\lambda}}{8k_0^2},\eta\gamma\right].$$

Once again, δ-function bifurcation causes $\dot{\lambda}$ to "lift off" the interface, so γ acts like a constant, and this commutator is zero. The new term disappears. Thus, we fully reproduce equation (C.33) with the range-independent "square-root operator" suitably generalized as in equation (J.17), the $\dot{\lambda}^2$-term gone (for now, but we note that it is passing through as before and would now equal $-\eta k_0\left(\dot{\lambda}^2/8k_0^4\right)$ if we kept it), and we also are carrying along a new term proportional to $-\left[\dot{\lambda},\{\lambda,\gamma\}\right]$. The explicit answer (with H_{RI} given by equation (J.17)) is

$$\tilde{\mathcal{H}}^{IV.1}=\eta H_{\text{RI}}-\frac{\eta\ddot{\lambda}}{8k_0^2}-\frac{3i}{16k_0^3}\left[\lambda^2,\dot{\lambda}\right]-\frac{i}{4k_0^2}\left[\dot{\lambda},\{\lambda,\gamma\}\right]+\ 5^{\text{th}}\text{ order}\,.$$

Now, let us again continue as in Appendix C.2.5, and choose

$$S^{IV.2}=\frac{-3\eta}{16k_0^3}\left\{\lambda,\dot{\lambda}\right\} \tag{J.22}$$

as in equation (C.34). Following equation (C.35), we have

$$\tilde{\mathcal{H}}^{IV.2} = \tilde{\mathcal{H}}^{IV.1} + i\left[S^{IV.2}, \eta\left(k_0 + \lambda \underbrace{-2k_0\gamma}_{\text{This is new}} \right) \right] - \underbrace{\dot{S}^{IV.2}}_{\substack{\text{This term includes contribution} \propto \dot{\lambda}^2 \\ \text{which falls out given our current assumptions}}} + 5^{\text{th}} \text{ order}$$

$$= \eta H_{\text{RI}} + \eta k_0 \left(-\frac{\ddot{\lambda}}{8k_0^3} + \frac{3\{\lambda, \ddot{\lambda}\}}{16k_0^4} \right) - \frac{i}{4k_0^2}\left[\dot{\lambda}, \{\lambda, \gamma\} \right] \tag{J.23}$$

$$+ \underbrace{i\left[\frac{-3\eta}{16k_0^3}\{\lambda, \dot{\lambda}\}, -2k_0\gamma\eta \right]}_{\text{This extra term is zero}} + 5^{\text{th}} \text{ order}$$

Once again, note that bifurcation of $\dot{\lambda}$ lifts everything off the interface, and γ operates like a constant in the half-space and so commutes with $\{\lambda, \dot{\lambda}\}$. Thus the new term falls out. Also note that the term $-\dot{S}^{IV.2}$ includes a portion that is proportional to $\dot{\lambda}^2$. Given our current working assumption that in the half-spaces μ is range-independent and γ is constant, this contribution is zero. Otherwise, this term will provide exactly the same contribution proportional to $\dot{\lambda}^2$ that it had previously in Appendix C.2.5. Recall that rather than explicitly tracking the $\dot{\lambda}^2$-terms, we are simply verifying that they are going through unchanged as we follow the procedure pursued in Appendix C.2.5. At the end, we will simply write down the final result of that previous calculation, and only then make the substitution (J.19). Based on comparison with equation (3.11)/(C.35), the current running value of the term proportional to $\dot{\lambda}^2$ is $\eta k_0 \left(\dot{\lambda}^2 / 4k_0^4 \right)$. This will not change anymore.

Thus, we used the assumption that the density is constant in the half-spaces and that the compressibility is range-independent in the half-spaces to reproduce equation (3.11) /(C.35) with the range-independent "square-root operator" suitably generalized as in equation (J.17), the $\dot{\lambda}^2$-term gone (for now), and with a new term proportional to $-\left[\dot{\lambda}, \{\lambda, \gamma\} \right]$:

$$\tilde{\mathcal{H}}^{IV.2} = \eta H_{\text{RI}} + \eta k_0 \left(-\frac{\ddot{\lambda}}{8k_0^3} + \frac{3\{\lambda, \ddot{\lambda}\}}{16k_0^4} \right) - \frac{i}{4k_0^2}\left[\dot{\lambda}, \{\lambda, \gamma\} \right] + 5^{\text{th}} \text{ order}.$$

Now, let us consider that last term proportional to $-\left[\dot{\lambda}, \{\lambda, \gamma\} \right]$. Now:

$$-\frac{i}{4k_0^2}\left[\dot{\lambda}, \{\lambda, \gamma\} \right] \rightarrow \text{bifurcate } \dot{\lambda} \rightarrow -\frac{i}{4k_0^2}\left[\dot{\lambda}, \{\lambda^{\pm}, \gamma^{\pm}\} \right],$$

and $\gamma^{\pm}$ works like a constant so that

$$-\frac{i}{4k_0^2}\Big[\dot\lambda,\{\lambda,\gamma\}\Big]=-\frac{i}{4k_0^2}\left(2\gamma^+\left[\frac{\dot\lambda^+}{2},\lambda^+\right]+2\gamma^-\left[\frac{\dot\lambda^-}{2},\lambda^-\right]\right)$$
$$=-\frac{i2\gamma}{4k_0^2}\Big[\dot\lambda,\lambda\Big]=4\gamma\left(\frac{i}{8k_0^2}\Big[\lambda,\dot\lambda\Big]\right)$$

Thus, back in equation (J.16), we can drop the term proportional to $-\Big[\dot\lambda,\{\lambda,\gamma\}\Big]$ and replace it with the rescaling

$$\frac{i}{8k_0^2}\Big[\lambda,\dot\lambda\Big]\to(1+4\gamma)\frac{i}{8k_0^2}\Big[\lambda,\dot\lambda\Big].$$

Now, $S^{IV.1}$ gets rescaled by the same factor. The "additional term" is still zero, but there is a new term proportional to $\Big[\gamma\dot\lambda,\lambda^2\Big]$. However, this is 5th order, and so we drop it. Thus, the only change to $\tilde{\mathcal{H}}^{IV.1}$ is the rescaling

$$\eta k_0\left(-\frac{\ddot\lambda}{8k_0^3}\right)\to\eta k_0\left(-(1+4\gamma)\frac{\ddot\lambda}{8k_0^3}\right).$$

Transformation $S^{IV.2}$ is unchanged, and so we have

$$\tilde{\mathcal{H}}^{IV.2}=\eta H_{\rm RI}+\eta k_0\left(-\frac{\ddot\lambda}{8k_0^3}(1+4\gamma)+\frac{3\{\lambda,\ddot\lambda\}}{16k_0^4}\right)+5^{\rm th}\text{ order},\qquad\text{(J.24)}$$

with $H_{\rm RI}$ given by equation (J.17). Dropping the tilde $\sim$ and superscript $IV.2$ on $\mathcal{H}$, this is just equation (5.9).

Now, we add the term proportional to $\dot\lambda^2$. From comparison to equation (3.11)/(C.35), noting that we have been careful to monitor our modifications to make sure that nothing new crept in (i.e., the $\dot\lambda^2$-term should be the same as in that equation), we have the following contribution proportional to $\dot\lambda^2$:

$$\eta k_0\left(\frac{\dot\lambda^2}{4k_0^4}\right).\qquad\text{(J.25)}$$

Now making the substitution (J.19), we have the additional term

$$\eta k_0\left[\frac{1}{4k_0^4}\cdot\frac{1}{2}\left\{\left(\frac{\partial\lambda}{\partial x}\right)^{\pm},\dot\lambda_S\right\}+\text{PV}\left(\frac{\dot\lambda^2}{4k_0^4}\right)\right]\qquad\text{(J.26)}$$

This is equation (5.10).

K Appendix: A heuristic development of the rules for δ-function bifurcation

This appendix provides a plausibility argument for the δ-function bifurcation rules given in Section 5.2. Appendix K.1 considers two cases where the rules apply:

- Subsection K.1.1 examines a flat interface where the sound speed jumps, but not the density,
- Subsection K.1.2 considers the 2-fluid interface (including a density jump) in the full wave (Helmholtz equation) problem.

Then Appendix K.2 discusses the limits of the δ-function bifurcation prescription. Appendix K.2.1 examines two cases, where the prescription only seems to work to 1st order:

- The substitution $\alpha = 1/\rho$ is analyzed in Subsection K.2.1.1 and
- Tappert's change of variable substitution $u = A/\sqrt{\rho}$ is evaluated in Subsection K.2.1.2.

In Appendix Section K.2.2, we examine why some cases only seem to work to first order. Specially, the need for undistorted steps is discussed in this section, and then in Appendix Subsection K.2.3 our observations are verified when the $\alpha = 1/\rho$ case is extended to 2nd order using a Taylor series expansion. Finally, the associative property for our prescription is briefly examined in Appendix K.3. It should be noted that it is implicitly assumed in this section that the parameters jump at an interface, but do not otherwise vary in the vicinity of the interface. If this condition is violated, the associative property in choosing which distributions to bifurcate may not hold, and explicit symmetrization may be necessary.

For convenience, the δ-function bifurcation rules given in Section 5.2 and supported by the arguments in this appendix are repeated here: The basic rule is that the first δ-function obtained splits in half (i.e., bifurcates). The two halves are displaced in opposite directions away from the interface. Any other distributions in the product collapse since they are smooth functions in the half-spaces away from interface. The procedure is associative in the sense that it does not matter which δ-function is chosen to be the first one. On the way to generating that first δ-function, the chain rule for differentiation applies. The ∇_T operating on the δ-function will generate higher-order derivatives of the δ-function. It is permitted to multiply through by a density since it involves an undistorted step, but in general it is not permitted to multiply through by distorted steps produced by taking functions of steps.

K.1 Cases where the δ-function bifurcation rules clearly apply

In this section, we consider two cases where the formalism must somehow work, and show that the δ-bifurcation rules reproduce the known correct answers. Subsection K.1.1 considers the parabolic equation for a flat interface with a sound speed jump only

(no density jump), and Subsection K.1.2 considers the 2-fluid interface (including density jumps) for the full Helmholtz equation.

K.1.1 Flat interface with no density jump ($\delta\rho = 0$)

Consider an interface with a sound speed jump (but a single value of the density everywhere). In Appendix Subsection 0 we derive the implicit boundary conditions for $\nabla_T^2 A$ and $\nabla_T^4 A$ by using standard manipulations on the Helmholtz equation. Later, in Appendix Subsection K.1.1.2, we re-derive these boundary conditions in the context of the parabolic equation for a flat interface. In this context, the boundary conditions for $\nabla_T^2 A$ and $\nabla_T^4 A$ become explicit. They appear in cross-terms where derivatives operate on step functions to produce δ-functions, which in turn are converted to boundary conditions using transverse integration. δ-function bifurcation must be used to obtain some of these boundary conditions. Note that when the interface is flat (i.e., range-independent), there is no backscatter and the ∞-order parabolic equation is exact. Therefore, the precise boundary conditions obtained for the Helmholtz equation in Appendix Subsection K.1.1.1 should apply. Since the orders decouple (see the discussion at the beginning of K.1.1.2; higher orders add new explicit boundary conditions but do not modify existing lower-order boundary conditions), this agreement should hold even for finite-order parabolic equations. Therefore, agreement between the results obtained using δ-function bifurcation (Appendix Subsection K.1.1.2) and those obtained using conventional methods (Appendix Subsection K.1.1.1) establishes a context in which the δ-function bifurcation prescription is indeed valid.

K.1.1.1 Reality check: The implicit boundary conditions on $\nabla_T^2 A$ and $\nabla_T^4 A$ obtained directly from the Helmholtz equation

To serve as a point of comparison with the parabolic equation for a flat interface with a sound speed jump (but a single value of the density everywhere); let us begin by first considering the corresponding Helmholtz equation. This is a 2nd order partial differential equation

$$\left(\nabla^2 + k^2\right) A = 0 \tag{K.1}$$

with boundary conditions $A, \hat{n} \cdot \vec{\nabla} A$ constant (as always, $\hat{n}$ is the normal to the interface). The boundary conditions on higher-order derivatives of A do not need to be explicitly spelled out, because a 2nd order differential equation with 2 boundary conditions fully determines the problem.

Now consider the simplest type of interface: the sound speed discontinuity (the density is the same everywhere) is now assumed to occur along a flat range-*in*dependent interface. The basic geometry is shown in Figure K.1 below.

Figure K.1 - The basic geometry for a flat range-independent interface, where the sound speed jumps, but not the density. When we consider the parabolic equation, we will simplify things yet again, and let the 2-dimensional transverse vector $\underline{R}_T = (y,z)$ become the 1-dimensional variable z (the depth). For the moment, as we consider the full Helmholtz equation, we will keep the 2-dimensional vector $\underline{R}_T = (y,z)$ and its corresponding gradient $\underline{\nabla}_T$, but keep in mind that although results (K.3) and (K.8) below will in principle apply when the interface is a function of the transverse coordinate y, it is the 1-dimensional result that will be of interest once we move on to Subsection K.1.1.2.

Now, the boundary conditions are continuity of A and $\vec{\nabla}A$. The continuity of components of $\vec{\nabla}A$ in the tangential direction comes as a bonus from the continuity of A. Recall the discussion leading to equation (3.51) in Subsection 3.3.2 for a derivation of this result. There, it was stated that the continuity of a given function implies that the difference between the values of the function evaluated on the two sides of the interface is zero, which in turn implies that the tangential derivative of the difference is also zero. Note that we can iterate this argument, beginning with the continuity of the derivative in the tangential direction, to show that a succession of two or more derivatives all in a tangential direction is also continuous. Specifically, with x in a tangential direction and A continuous, we have $\partial^n A/\partial x^n$ continuous at the interface for all n.

Now, let us examine some of the implicit boundary conditions on the higher-order transverse derivatives $\underline{\nabla}_T^m$. As discussed just below Figure 3.8 in Section 3.3.2, the boundary conditions on higher-order derivatives become an issue in the higher-order parabolic equation. Then, the boundary conditions on higher-order transverse derivatives can no longer remain implicit.

The Helmholtz equation gives

$$\begin{aligned} \nabla_T^2 A_I &= \left(-\frac{\partial^2}{\partial x^2} - k_I^2 \right) A_I \qquad \text{just inside Region } I \\ \nabla_T^2 A_{II} &= \left(-\frac{\partial^2}{\partial x^2} - k_{II}^2 \right) A_{II} \qquad \text{just inside Region } II \end{aligned} \quad . \tag{K.2}$$

Taking the difference between the two equations and using continuity of A and $\partial^2 A/\partial x^2$, we have the implicit boundary condition on $\nabla_T^2 A$:

$$\Delta\left(\nabla_T^2 A\right) = -\left(\delta k^2\right) A \tag{K.3}$$

where

$$\begin{aligned}\Delta\left(\nabla_T^2 A\right) &\equiv \nabla_T^2 A_{II} - \nabla_T^2 A_I \\ \delta k^2 &\equiv k_{II}^2 - k_I^2\end{aligned}. \tag{K.4}$$

Next, let us obtain the boundary condition on $\nabla_T^4 A$. Take ∇_T^2 of both parts of equation (K.2):

$$\begin{aligned}\nabla_T^4 A_I &= \left(-k_I^2 - \frac{\partial^2}{\partial x^2}\right)\nabla_T^2 A_I \\ \nabla_T^4 A_{II} &= \left(-k_{II}^2 - \frac{\partial^2}{\partial x^2}\right)\nabla_T^2 A_{II}\end{aligned}, \tag{K.5}$$

and use (K.2) to substitute for $\nabla_T^2 A$:

$$\begin{aligned}\nabla_T^4 A_I &= \left(-k_I^2 - \frac{\partial^2}{\partial x^2}\right)\left(-k_I^2 - \frac{\partial^2}{\partial x^2}\right)A_I = \left(k_I^4 + 2k_I^2\frac{\partial^2}{\partial x^2} + \frac{\partial^4}{\partial x^4}\right)A_I \\ \nabla_T^4 A_{II} &= \left(-k_{II}^2 - \frac{\partial^2}{\partial x^2}\right)\left(-k_{II}^2 - \frac{\partial^2}{\partial x^2}\right)A_{II} = \left(k_{II}^4 + 2k_{II}^2\frac{\partial^2}{\partial x^2} + \frac{\partial^4}{\partial x^4}\right)A_{II}\end{aligned}.$$

Now, subtract these two equations, recalling that $\partial^4 A/\partial x^4$ and $\partial^2 A/\partial x^2$ are continuous. This leaves us with

$$\nabla_T^4 A_{II} - \nabla_T^4 A_I = \left(k_{II}^4 - k_I^4\right)A + 2\left(k_{II}^2 - k_I^2\right)\frac{\partial^2 A}{\partial x^2}.$$

With δk^2 as defined in equation (K.4) above and $\overline{k^2} \equiv \left(k_I^2 + k_{II}^2\right)/2$, this becomes

$$\begin{aligned}\nabla_T^4 A_{II} - \nabla_T^4 A_I &= 2\overline{k^2}\left(\delta k^2\right)A + 2\left(\delta k^2\right)\frac{\partial^2 A}{\partial x^2} \\ &= -2\left(\delta k^2\right)\left[-\overline{k^2}A - \frac{\partial^2 A}{\partial x^2}\right]\end{aligned}. \tag{K.6}$$

Adding the two parts of equation (K.2) and dividing by 2, we get

$$\overline{\nabla_T^2 A} \equiv \frac{\nabla_T^2 A_I + \nabla_T^2 A_{II}}{2} = -\overline{k^2}A - \frac{\partial^2 A}{\partial x^2}, \tag{K.7}$$

and so

$$\Delta\left(\nabla_T^4 A\right) \equiv \nabla_T^4 A_{II} - \nabla_T^4 A_I = -2\left(\delta k^2\right)\overline{\nabla_T^2 A}. \tag{K.8}$$

Thus, equations (K.3) and (K.8) give the implicit boundary conditions on $\nabla_T^2 A$ and $\nabla_T^4 A$ respectively. Note that as we compare results (K.3) and (K.8) to the corresponding parabolic equation result in the next subsection, we will go to the 1-dimensional problem where $\underline{\nabla}_T \to \nabla_T = \partial/\partial z$.

K.1.1.2 The same boundary conditions on $\nabla_T^2 A$ and $\nabla_T^4 A$ obtained from the parabolic equation using δ-function bifurcation

Recall that we are considering the range-independent constant density problem so that, as discussed in Appendix C.2.2 (especially the discussion surrounding equation (C.16)), the parabolic equation can be used to propagate the acoustic field A itself, and not just the auxiliary field χ. Furthermore, the "exact" scalar Hamiltonian H is the infinite order expansion in $2\lambda/k_0$ of $k_0\sqrt{1+2\lambda/k_0}$ (keeping in mind the usual caveats concerning the assumption that the operator λ is in some sense small). It follows immediately that at any finite order, the commutator $[\lambda, H]=0$, and so λ is an observable. Therefore, we can always in principle expand the solution A into eigenvectors and replace λ with eigenvalues. It follows that for any given power n, δ-functions generated internally to λ^n must cancel, and the orders (in n) must decouple. Therefore, higher orders can only add new boundary conditions, but they cannot modify the old ones (when one uses the transverse integration technique outlined in Section 3.3.3 to convert the contact potentials to boundary conditions). Specifically, when we add a new order λ^n, only the first two integrations count, and these will provide the boundary conditions on the two new derivatives that now need specified boundary conditions: $\nabla_T^{2n-1}A$ and $\nabla_T^{2n-2}A$. (The new explicit boundary conditions become required in the context of the new Hamiltonian where lead order is now $\nabla_T^{2n}A$ rather than just $\nabla_T^{2n-2}A$.) For our current purposes, we will only consider the boundary conditions on $\nabla_T^2 A$ and $\nabla_T^4 A$, and use λ^2 theory and λ^3 theory respectively to derive them. We will use δ-function bifurcation on distributions generated by cross-terms in these products of differential operators. The fact that the correct boundary conditions are indeed generated will contribute to our heuristic validation for the δ-function bifurcation technique.

The contact potentials (e.g., potentials proportional to δ or δ') generated by cross-terms in λ^n play a crucial role. For example, in λ^2 theory, a δ'-contact potential is needed if we are to avoid having our transverse integration incorrectly predict that $\nabla_T^2 A$ is continuous (i.e., $\Delta\left(\nabla_T^2 A\right)=0$). Continuing on up to λ^3 theory, if we were to throw out all contact potentials, then we would incorrectly conclude $\Delta\left(\nabla_T^4 A\right)=0$. This, of course, contrasts with the discussion just above in Section 0 concerning the Helmholtz equation. In this equation, no derivatives of higher than 2nd order appear explicitly, and so the additional boundary conditions involving discontinuity of the second and fourth tangential derivatives of the wave function were extracted from the Helmholtz equation only indirectly, and no contact potentials were needed in the Helmholtz equation itself. (However, they *effectively* appeared when we took derivatives of the Helmholtz equation.)

From now until the end of this subsection (Appendix K.1.1.2), we will revert to the 2-dimensional problem, where x is the range and z is the depth. Thus, $z\hat{z}$ replaces $\underline{R}_T = (y,z)$ and ∇_T and $\partial/\partial z$ are the same. As always, the positive z-axis points up from Region II into Region I (e.g., see Figure K.1 with $\underline{R}_T \to z\hat{z}$). We follow the notation first outlined back in Section 2.1, noting especially that equation (2.5) implies that $\mu \equiv \left(1-n^2\right)/2$ and $k_0 n = k$. Then, choosing the reference wave number $k_0 = k_I$, it follows that $\mu = \Theta(-z)\,\mu_{II}$ and

$$2k_0^2\mu = 2k_0^2\mu_{II}\Theta(-z) = k_0^2\left(1-n_{II}^2\right)\Theta(-z) = \left(k_I^2 - k_{II}^2\right)\Theta(-z) = -\left(\delta k^2\right)\Theta(-z).$$

Note that $\delta k^2 = k_{II}^2 - k_I^2$ as in equation (K.4), and Θ is as always the Heaviside step function given by equation (3.22). All this gives us

$$\underbrace{2k_0}_{\substack{\text{Irrelevant}\\ \text{overall}\\ \text{factor!}}}\ \lambda = \nabla_T^2 + \left(\delta k^2\right)\Theta(-z). \tag{K.9}$$

Note the λ theory (i.e., 1st order) instantly gives us continuity of A and $\nabla_T A$ (using infinitesimal transverse integration).

Now let us look at λ^2 theory and deduce the boundary condition on $\nabla_T^2 A$. Start with

$$\begin{aligned}\left(2k_0\lambda\right)^2 A &= \left(\nabla_T^2 + \left(\delta k^2\right)\Theta(-z)\right)\left(\nabla_T^2 + \left(\delta k^2\right)\Theta(-z)\right)A(z)\\ &= \nabla_T^4 A(z) + \underbrace{\nabla_T^2\left(\delta k^2\cdot\Theta(-z)\,A(z)\right)}_{\text{Expand this term}}\\ &\quad + \underbrace{\delta k^2\cdot\Theta(-z)\nabla_T^2 A\big|_z + \left(\delta k^2\right)^2\Theta^2(-z)\,A(z)}_{\substack{\text{These terms play no role in determining}\\ \text{the boundary condition on } \nabla_T^2 A}}\end{aligned}. \tag{K.10}$$

The last two terms in equation (K.10) do not matter in the present context. This is so because $\nabla_T^2 A$ has at worst a step function and A is continuous, and neither has the requisite δ'- (or δ-) function for actually generating a discontinuity boundary condition in $\nabla_T^2 A$ (or $\nabla_T^3 A$) via the infinitesimal-transverse-integral procedure outlined in Section 3.3.3. In fact, if we integrate either of these terms over an infinitesimal transverse integral, we will get zero.

Expanding the interesting term gives

$$\begin{aligned}\nabla_T^2\left(\delta k^2\cdot\Theta(-z)\,A(z)\right) &= \nabla_T\left[-\delta k^2\cdot\delta(z)\,A(z) + \delta k^2\cdot\Theta(-z)\nabla_T A\big|_z\right]\\ &= -\delta k^2\cdot\delta'(z)\,A(z) - \delta k^2\cdot\delta(z)\nabla_T A\big|_z\\ &\quad -\delta k^2\cdot\delta(z)\nabla_T A\big|_z + \underbrace{\delta k^2\cdot\Theta(-z)\nabla_T^2 A\big|_z}_{\substack{\text{Once again there are no } \delta\text{'s}\\ \text{here and this gives 0 after}\\ \text{infinitesimal integration}}}.\end{aligned}$$

Recalling equation (3.54) (for the flat interface $z = f = 0$), we have

$$\delta(z)\chi(z) = \delta(z)\chi(0)$$
$$\delta'(z)\chi(z) = \delta'(z)\chi(0) - \delta(z)\chi'(0),$$

and so

$$\nabla_T^2\left(\delta k^2 \cdot \Theta(-z)\, A(z)\right) = -\delta k^2 \cdot \delta'(z)\, A(0) - \delta k^2 \cdot \delta(z)\nabla_T A\big|_0 + \underbrace{\delta k^2 \cdot \Theta(-z)\nabla_T^2 A\big|_z}_{\text{Stays finite at the origin}}. \quad \text{(K.11)}$$

Substituting into (K.10), this gives us

$$\begin{aligned}\left(2k_0\lambda\right)^2 A &= \left(\nabla_T^2 + \left(\delta k^2\right)\Theta(-z)\right)\left(\nabla_T^2 + \left(\delta k^2\right)\Theta(-z)\right)A(z) \\ &= \nabla_T^4 A(z) - \delta k^2 \cdot \delta'(z)\, A(0) - \delta k^2 \cdot \delta(z)\nabla_T A\big|_0 \\ &\underbrace{+2\delta k^2 \cdot \Theta(-z)\nabla_T^2 A\big|_z + \left(\delta k^2\right)^2 \Theta^2(-z)\, A(z)}_{\substack{\text{Finite stuff which} \\ \text{integrates to zero for} \\ \text{infinitesimal intervals}}}.\end{aligned} \quad \text{(K.12)}$$

Now perform the infinitesimal-transverse-integral procedure outlined in Section 3.3.3, noting the geometry in Figure K.2 below.

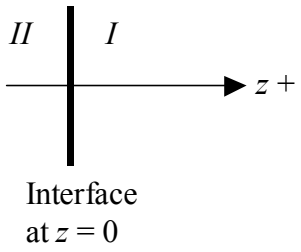

Figure K.2 - For the infinitesimal integration, recall that the interface is along the $z = 0$ line and that the positive z-axis points from Region II into Region I.

Following equation (3.53), we perform the integration $\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz$ (with $\varepsilon \to 0$) on equation (K.12) to obtain

$$\nabla_T^2 A_I - \nabla_T^2 A_{II} - \delta k^2 \cdot A(0) = 0$$

or

$$\nabla_T^2 A_{II} - \nabla_T^2 A_I = \Delta\left(\nabla_T^2 A\right) = -\delta k^2 \cdot A(0), \quad \text{(K.13)}$$

which is exactly equation (K.3). Note that we needed the δ'-function from the cross-terms in λ^2 to get this result. Incidentally, integrating (K.12) once also gives us the similar result

$$\Delta\left(\nabla_T^3 A\right) = -\delta k^2 \cdot \nabla_T A\big|_0 .$$

It is now possible to see where we are heading with this. On the one hand, we need the cross-term between the differential operator ∇_T^2 and step function Θ to generate the proper boundary conditions on $\nabla_T^2 A$. On the other hand, for higher-order λ^n (where $n > 2$) we will rapidly begin to pick up products of distributions: first the product $\Theta\delta$ appears and if we do nothing about that, then the cross-terms will eventually generate products of δ-functions. Note that all this is happening in a trivial range-independent problem where the density is constant, and everything should work out! The bottom line is this: if the first time we create a δ-function, we split it into a pair of half δ-functions:

$$\delta \to \frac{\delta^{II}}{2} + \frac{\delta^{I}}{2} = \frac{\delta^{-}}{2} + \frac{\delta^{+}}{2} \tag{K.14}$$

then we avoid problems associated with the multiplication of distributions. Very significantly, we will also get boundary conditions that are fully consistent with the wave equation.

With this in mind, let us examine the λ^3-term and use the δ-function bifurcation rules to reproduce the boundary condition on $\nabla_T^4 A$ given by equation (K.8). We have

$$\left(2k_0\lambda\right)^3 A = \left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)\underbrace{\left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)\left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)}_{\text{Substitute for this}} A . \tag{K.15}$$

Next, using equation (K.12) evaluate the two right-hand appearances of the operator $\left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)$ first, and then operate on the result with the left-most appearance of the operator $\left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)$[zzz]. This gives us

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[zzz] Since the evaluation of this expression will eventually require use of the new procedure of δ-function bifurcation, it is fair to question whether evaluating this expression by expanding it using the product rule for differentiation first and only then replacing derivatives of the step function with δ-functions is really equivalent to expanding the two right-hand internal operators first, replacing them with δ-functions, and only after that applying the left-most operator. In other words, does the associative property for the multiplication of distributions apply even when δ-function bifurcation is involved? In Section K.3 this issue will be addressed, and it will be argued that the associative property for multiplication applies, even when δ-function bifurcation is involved.

$$
\begin{aligned}
\left(2k_0\lambda\right)^3 A = &\left(\nabla_T^2 + \delta k^2 \cdot \Theta(-z)\right)\cdot \\
&\begin{bmatrix} \nabla_T^4 A\big|_z - \delta k^2 \cdot \delta'(z) A(0) - \delta k^2 \cdot \delta(z) \nabla_T A\big|_0 \\ +2\delta k^2 \cdot \Theta(-z) \nabla_T^2 A\big|_z + \left(\delta k^2\right)^2 \Theta(-z)\Theta(-z) A(z) \end{bmatrix} \\
&= \nabla_T^6 A\big|_z + 2\delta k^2 \cdot \nabla_T^2 \left(\Theta(-z) \nabla_T^2 A\big|_z\right) + \left(\delta k^2\right)^2 \nabla_T^2 \left(\Theta(-z)\Theta(-z) A(z)\right) \\
&-\delta k^2 \cdot \delta'''(z) A(0) - \delta k^2 \cdot \delta''(z) \nabla_T A\big|_0 + \delta k^2 \cdot \Theta(-z) \nabla_T^4 A\big|_z \\
&+2\left(\delta k^2\right)^2 \cdot \Theta(-z)\Theta(-z) \nabla_T^2 A\big|_z + \left(\delta k^2\right)^3 \Theta(-z)\Theta(-z)\Theta(-z) A(z) \\
&-\left(\delta k^2\right)^2 \underbrace{\Theta(-z)\cdot\delta'(z)}_{\delta^-/2} A(0) - \left(\delta k^2\right)^2 \cdot \underbrace{\Theta(-z)\cdot\delta(z)}_{\delta^-/2} \nabla_T A\big|_0 .
\end{aligned}
\tag{K.16}
$$

Since these are the only ones that contribute as we take a double integral to obtain the boundary condition on $\nabla_T^4 A$, we will only consider terms that pick up a δ' function:

$$
\begin{aligned}
\boxed{1} &= 2\delta k^2 \cdot \nabla_T^2 \left(\Theta(-z) \nabla_T^2 A\big|_z\right) \\
\boxed{2} &= \left(\delta k^2\right)^2 \nabla_T^2 \left(\Theta(-z)\Theta(-z) A(z)\right) \\
\boxed{3} &= \delta k^2 \cdot \Theta(-z) \nabla_T^4 A\big|_z \\
\boxed{4} &= -\left(\delta k^2\right)^2 \underbrace{\Theta(-z)\cdot\delta'(z)}_{\delta^-/2} A(0)
\end{aligned}
\quad . \tag{K.17}
$$

Thus,

$$
\left(2k_0\lambda\right)^3 A = \nabla_T^6 A\big|_z + \boxed{1} + \boxed{2} + \boxed{3} + \boxed{4} + \text{non-}\delta' \text{ terms} . \tag{K.18}
$$

Now,

$$
\begin{aligned}
\boxed{1} &= 2\delta k^2 \cdot \nabla_T^2 \left(\Theta(-z) \nabla_T^2 A\big|_z\right) \\
&= 2\delta k^2 \cdot \nabla_T \left[\underbrace{-\delta(z) \nabla_T^2 A\big|_z}_{\substack{\text{use } \delta\text{-function} \\ \text{bifurcation}}} + \Theta(-z) \nabla_T^3 A\big|_z \right] .
\end{aligned}
$$

Follow the δ-function bifurcation prescription: $\delta \to \delta^I/2 + \delta^{II}/2 = \delta^+/2 + \delta^-/2$:

$$
\delta(z) \nabla_T^2 A = \frac{\delta^+}{2} \nabla_T^2 A_I\big|_0 + \frac{\delta^-}{2} \nabla_T^2 A_{II}\big|_0 .
$$

Under the relevant infinitesimal integration $\int_{-\varepsilon}^{\varepsilon} dz$, $\left[\delta^{+}/2\right]\nabla_T^2 A_I\big|_0 + \left[\delta^{-}/2\right]\nabla_T^2 A_{II}\big|_0$ integrates to $\left(\nabla_T^2 A_I\big|_0 + \nabla_T^2 A_{II}\big|_0\right)\big/2 = \overline{\nabla_T^2 A}\big|_0$. Thus, as long as we are clear about how we got there, we can use the shorthand

$$\delta(z)\nabla_T^2 A = \frac{\delta^{+}}{2}\nabla_T^2 A_I\big|_0 + \frac{\delta^{-}}{2}\nabla_T^2 A_{II}\big|_0 \leftrightarrow \delta(z)\overline{\nabla_T^2 A}.$$

Always exercising caution, it will often prove convenient to proceed in this way and recombine are bifurcated δ-functions into an ordinary δ-functions times averages. We will move freely from one form to the other as needed.

Thus,

$$\begin{aligned}\boxed{1} &= 2\delta k^2 \cdot \nabla_T\left[-\delta(z)\overline{\nabla_T^2 A}\big|_0 + \Theta(-z)\nabla_T^3 A\big|_z\right] \\ &= -2\delta k^2 \cdot \delta'(z)\overline{\nabla_T^2 A}\big|_0 + 2\delta k^2 \cdot \delta(z)\nabla_T^3 A\big|_z + 2\delta k^2 \cdot \Theta(-z)\nabla_T^4 A\big|_z .\end{aligned}$$

Again, $\delta(z)$ is really $\sum_{\pm}\left[\delta^{\pm}/2\right] \equiv \left[\delta^{+}/2\right] + \left[\delta^{-}/2\right]$, and so

$$\delta(z)\nabla_T^3 A\big|_z = \left[\delta^{+}/2\right]\nabla_T^3 A_I\big|_0 + \left[\delta^{-}/2\right]\nabla_T^3 A_{II}\big|_0 \leftrightarrow \delta\cdot\overline{\nabla_T^3 A}\big|_0 ,$$

and we have

$$\boxed{1} = -2\delta k^2 \cdot \delta'(z)\overline{\nabla_T^2 A}\big|_0 + \underbrace{2\delta k^2 \cdot \delta(z)\overline{\nabla_T^3 A}\big|_0}_{\substack{\text{This term is not } \propto \delta', \text{ so} \\ \text{it will not survive the double} \\ \text{integral } \int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz}} + 2\delta k^2 \cdot \Theta(-z)\nabla_T^4 A\big|_z . \qquad \text{(K.19)}$$

Now recall the argument at the beginning of this subsection (Subsection K.1.1.2). Range independence implies that the distributions internal to $\lambda^2 A$ must cancel. Equation (K.12) therefore implies that

$$\nabla_T^4 A = \delta k^2 \cdot \delta'(z)\, A(0) + \text{terms that are not } \propto \delta' .$$

In expression $\boxed{1}$, this is multiplied by the step function

$$\Theta(-z) = \begin{cases} 0 & z > 0 \text{ (Region } I\text{)} \\ 1 & z < 0 \text{ (Region } II\text{)} \end{cases}, \qquad \text{(K.20)}$$

so that

$$\Theta(-z)\delta'(z) = \frac{\Theta(0_-)\delta'^{-}(z)}{2} + \frac{\Theta(0_+)\delta'^{+}(z)}{2} = \frac{\delta'^{-}(z)}{2} .$$

Noting that A is continuous even at $z=0$, we have

$$\begin{aligned}\Theta(-z)\nabla_T^4 A\big|_z &= \delta k^2\cdot\Theta(-z)\delta'(z)A(0)+\left\{\begin{array}{c}\text{terms that are}\\ \text{not } \propto \delta'\end{array}\right\}\\ &= \delta k^2\cdot\frac{\delta'^{-}(z)}{2}A(0)+\left\{\begin{array}{c}\text{terms that are}\\ \text{not } \propto \delta'\end{array}\right\}\end{aligned}. \qquad \text{(K.21)}$$

Again, at this point we might as well drop the superscript "$-$" from the δ'-function. Note the δ-function-bifurcation prescription at work here: it has generated a factor of $\frac{1}{2}$ that we would otherwise have missed!

Combining (K.19) and (K.21), we have

$$\begin{aligned}\boxed{1} &= -2\delta k^2\cdot\delta'(z)\overline{\nabla_T^2 A}\big|_0+\left(\delta k^2\right)^2\cdot\delta'(z)A(0)\\ &\quad+\left\{\begin{array}{c}\text{terms that will not contribute}\\ \text{to the double integration}\end{array}\right\}.\end{aligned} \qquad \text{(K.22)}$$

Next, let us evaluate $\boxed{2}$. This will be a great test for the δ-function-bifurcation prescription.

$$\begin{aligned}\boxed{2} &= \left(\delta k^2\right)^2\nabla_T^2\left(\Theta(-z)\Theta(-z)A(z)\right)\\ &= \left(\delta k^2\right)^2\nabla_T\left(\begin{array}{l}\left[\nabla_T\Theta(-z)\right]\Theta(-z)A(z)+\Theta(-z)\left[\nabla_T\Theta(-z)\right]A(z)\\ +\Theta(-z)\Theta(-z)\nabla_T A(z)\end{array}\right)\cdot\end{aligned}$$

Now use the prescription

$$\nabla_T\Theta(-z)=-\frac{\delta^+}{2}-\frac{\delta^-}{2},$$

and equation (K.20) to get

$$\left[\nabla_T\Theta(-z)\right]\Theta(-z)=\Theta(-z)\left[\nabla_T\Theta(-z)\right]=0-\frac{\delta^-}{2}=-\frac{\delta^-}{2}.$$

Again, since A is continuous and we will integrate, we can drop the superscript "$-$" to get

$$
\begin{aligned}
\boxed{2} &= \left(\delta k^2\right)^2 \nabla_T \left(-\frac{\delta}{2} A(0) - \frac{\delta}{2} A(0) \right) \\
&+ \left(\delta k^2\right)^2 \underbrace{\left[\nabla_T \Theta(-z)\right] \Theta(-z)}_{\text{Again } -\delta/2} \nabla_T A(z) + \left(\delta k^2\right)^2 \underbrace{\Theta(-z)\left[\nabla_T \Theta(-z)\right]}_{\text{Again } -\delta/2} \nabla_T A(z) \\
&+ \left(\delta k^2\right)^2 \Theta(-z)\Theta(-z)\nabla_T^2 A(z) \qquad \text{(K.23)} \\
&= -\left(\delta k^2\right)^2 \delta'(z) \cdot A(0) - \underbrace{\left(\delta k^2\right)^2 \delta(z) \nabla_T A(0) + \left(\delta k^2\right)^2 \Theta(-z)\Theta(-z)\nabla_T^2 A(z)}_{\text{These terms go out after double integration}} \\
&= -\left(\delta k^2\right)^2 \delta'(z) \cdot A(0) + \left\{ \begin{array}{c} \text{terms that will not contribute} \\ \text{to the double integration} \end{array} \right\}.
\end{aligned}
$$

Note that $\boxed{2}$ and the 2nd term in $\boxed{1}$ will cancel.

Next we can use equation (K.21) to obtain

$$
\boxed{3} = \delta k^2 \cdot \Theta(-z) \nabla_T^4 A\Big|_z = \left(\delta k^2\right)^2 \cdot \frac{\delta'(z)}{2} A(0) + \left\{ \begin{array}{c} \text{terms that are} \\ \text{not } \propto \delta' \end{array} \right\}. \qquad \text{(K.24)}
$$

Now consider

$$
\boxed{4} = -\left(\delta k^2\right)^2 \underbrace{\Theta(-z) \cdot \delta'(z)}_{\delta'^-/2} A(0).
$$

As already noted above, δ' splits:

$$
\delta'(z) \to \frac{\delta'^+(z)}{2} + \frac{\delta'^-(z)}{2},
$$

and $\Theta(-z)$ is given by equation (K.20) so that

$$
\Theta(-z)\frac{\delta'^-(z)}{2} = \frac{\delta'^-(z)}{2}
$$

$$
\Theta(-z)\frac{\delta'^+(z)}{2} = 0
$$

and

$$
\Theta(-z) \cdot \delta'(z) = \frac{\delta'^-(z)}{2}.
$$

Again dropping labels since A is constant and δk^2 is just a constant parameter, we simply pick up a factor of $\frac{1}{2}$ and end up with

$$\boxed{4} = -\left(\delta k^2\right)^2 \frac{\delta'(z)}{2} A(0). \tag{K.25}$$

Note that $\boxed{3}$ and $\boxed{4}$ cancel.

Combining (K.18), (K.22), (K.23), (K.24) and (K.25), we have

$$\begin{aligned}\left(2k_0\lambda\right)^3 A &= \nabla_T^6 A\big|_z + \boxed{1} + \boxed{2} + \boxed{3} + \boxed{4} + \left\{\begin{array}{c}\text{terms that are}\\ \text{not } \propto \delta'\end{array}\right\} \\ &= \nabla_T^6 A\big|_z - 2\delta k^2 \cdot \delta'(z)\overline{\nabla_T^2 A}\big|_0 + \left\{\begin{array}{c}\text{terms that are}\\ \text{not } \propto \delta'\end{array}\right\}.\end{aligned}$$

Now, substitute into the λ^3-parabolic equation corresponding to the Helmholtz equation (e.g., see equation (C.35) or equation (5.7) or (J.15) with $\gamma = 0$). As noted at the beginning of this subsection, since this particular problem is range-independent, we can replace the auxiliary field χ with the acoustic field A:

$$-i\frac{\partial A}{\partial x} = \left[k_0 + \lambda - \frac{\lambda^2}{2k_0} + \frac{\lambda^3}{2k_0^2}\right] A.$$

This gives us

$$0 = \nabla_T^6 A\big|_z - 2\delta k^2 \cdot \delta'(z)\overline{\nabla_T^2 A}\big|_0 + \left\{\begin{array}{c}\text{non-}\delta'\text{ terms}\\ \textbf{or}\\ \delta'\text{ terms internal to }\lambda^2\text{ that}\\ \text{must cancel each other out}\end{array}\right\}. \tag{K.26}$$

Integrating twice (i.e., $\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz \cdots$), we obtain

$$0 = \nabla_T^4 A_I - \nabla_T^4 A_{II} - 2\delta k^2 \cdot \overline{\nabla_T^2 A}\big|_0$$

or with $\Delta\left(\nabla_T^4 A\right) \equiv \nabla_T^4 A_{II} - \nabla_T^4 A_I$, we get

$$\Delta\left(\nabla_T^4 A\right) = -2\delta k^2 \cdot \overline{\nabla_T^2 A}\big|_0, \tag{K.27}$$

which is exactly equation (K.8), the implicit boundary condition for the full wave equation.

Thus, by requiring that as the PE adds higher-order powers of the transverse Laplacian ∇_T^2, the boundary conditions at a flat horizontal (i.e., range-*in*dependent) interface remain consistent with those set by the wave equation, we find that the physics clearly forces a specific extension to distribution theory: The δ-functions on the interface must

"bifurcate". Next, in Subsection K.1.2 we will show that the same extension to distribution theory is also necessary to recover the 2-fluid boundary conditions at an interface where the density ρ and the sound speed parameter $\mu = \left(1 - c_0^2/c^2\right)/2$ both jump (i.e., ρ and μ are functions of the coordinates that contain step functions at the discontinuity).

K.1.2 2-fluid full wave interface ($\delta\rho \neq 0$)

In this subsection, we demonstrate that the δ-function-bifurcation rules reproduce the boundary conditions on a 2-fluid interface embedded in 2-dimensional $x-z$ space. Once again, let us set up the same (local) coordinate system we typically use in such circumstances (see Figure K.3 below). In particular, note that in the local coordinate system, the interface is at $z=0$ and the z-axis is (locally) normal to the interface.

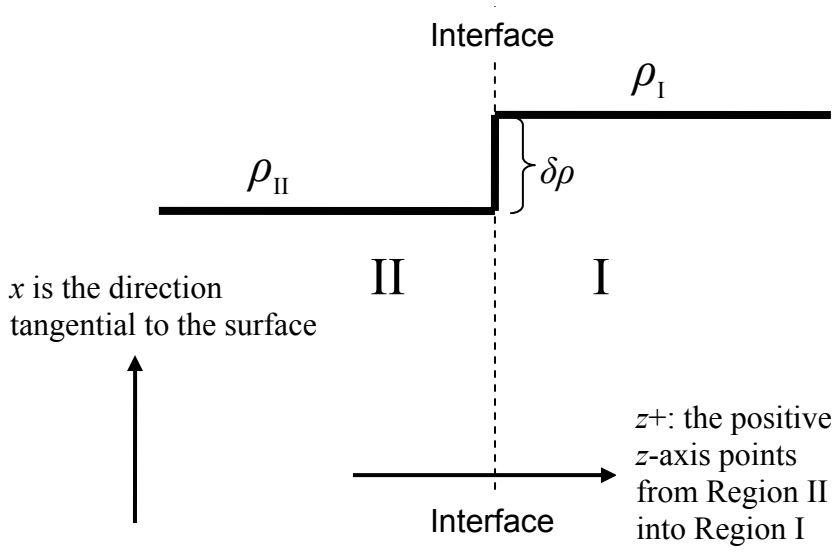

Figure K.3 - The geometry used in this section. The z-axis is locally normal to the interface and the x-axis is locally tangent.

The density jump is given by $\delta\rho \equiv \rho_{II} - \rho_I$ and

$$\rho = \rho_{II} - \delta\rho \cdot \Theta(z) = \begin{cases} \rho_I & z > 0 \\ \rho_{II} & z < 0 \end{cases}.$$

The field A obeys the variable density acoustic equation (equations (2.1) and (5.1))

$$\frac{\partial}{\partial z}\left(\frac{1}{\rho}\frac{\partial}{\partial z}A\right) + \underbrace{\frac{\partial}{\partial x}\left(\frac{1}{\rho}\frac{\partial}{\partial x}A\right)}_{\text{Tangent to the surface; no distributions generated here}} + \frac{k_0^2 n^2}{\rho}A = 0\,. \qquad \text{(K.28)}$$

Note that the x-direction is tangential to the interface, and so ρ, n, A are all locally continuous with respect to this variable. A translation in the x-direction encounters no jumps in the density, and so no distributions are generated by the $\partial/\partial x$ derivative. This term is therefore not a player in determining the boundary conditions via transverse integration.

Now, let us proceed to step one of our prescription: until we generate a δ-function, treat ρ just like any other variable (i.e., use the chain rule for differentiation and multiply, etc.). The usual rules for differentiation give us

$$\frac{\partial}{\partial z}\left(\frac{1}{\rho}\frac{\partial}{\partial z}A\right) = -\frac{1}{\rho^2}\frac{\partial \rho}{\partial z}\frac{\partial A}{\partial z} + \frac{1}{\rho}\frac{\partial^2 A}{\partial z^2}. \tag{K.29}$$

Substituting (K.29) into the wave equation (K.28) and multiplying through by ρ, we get

$$\frac{\partial^2 A}{\partial z^2} - \frac{1}{\rho}\frac{\partial \rho}{\partial z}\frac{\partial A}{\partial z} + \frac{\partial^2 A}{\partial x^2} + k_0^2 n^2 A = 0. \tag{K.30}$$

Now, naively we have

$$\frac{\partial \rho}{\partial z} = -\delta\rho \cdot \delta(z)$$

where $\delta\rho$ is a fixed "density jump" parameter.

Now we are ready to move to step two of our prescription and bifurcate δ:

$$\delta(z) \to \frac{\delta^+(z)}{2} + \frac{\delta^-(z)}{2}$$

or

$$\frac{\partial \rho}{\partial z} = -\frac{\delta\rho}{2}\cdot\delta^+(z) - \frac{\delta\rho}{2}\cdot\delta^-(z).$$

Substituting into the modified Helmholtz equation (K.30), this leads to

$$\frac{\partial^2 A}{\partial z^2} + \frac{1}{\rho_I}\frac{\delta\rho}{2}\frac{\partial A_I}{\partial z}\bigg|_0 \delta^+(z) + \frac{1}{\rho_{II}}\frac{\delta\rho}{2}\frac{\partial A_{II}}{\partial z}\bigg|_0 \delta^-(z) + \frac{\partial^2 A}{\partial x^2} + k_0^2 n^2 A = 0.$$

Integrating once across the interface (over the infinitesimal interval: $\int_{-\varepsilon}^{\varepsilon} dz \cdots$), we have

$$0 = \frac{\partial A_I}{\partial z} - \frac{\partial A_{II}}{\partial z} + \frac{1}{\rho_I}\frac{\delta\rho}{2}\frac{\partial A_I}{\partial z}\bigg|_0 + \frac{1}{\rho_{II}}\frac{\delta\rho}{2}\frac{\partial A_{II}}{\partial z}\bigg|_0$$

$$0 = \frac{\partial A_I}{\partial z} - \frac{\partial A_{II}}{\partial z} + \frac{1}{2}\left(\frac{\rho_{II}}{\rho_I} - 1\right)\frac{\partial A_I}{\partial z}\bigg|_0 + \frac{1}{2}\left(1 - \frac{\rho_I}{\rho_{II}}\right)\frac{\partial A_{II}}{\partial z}\bigg|_0$$

$$0 = \frac{1}{2}\left(\frac{\rho_{II}}{\rho_I} + 1\right)\frac{\partial A_I}{\partial z}\bigg|_0 + \frac{1}{2}\left(-1 - \frac{\rho_I}{\rho_{II}}\right)\frac{\partial A_{II}}{\partial z}\bigg|_0$$

or

$$\begin{aligned}\left(\frac{\rho_{II} + \rho_I}{\rho_I}\right)\frac{\partial A_I}{\partial z}\bigg|_0 &= \left(\frac{\rho_{II} + \rho_I}{\rho_{II}}\right)\frac{\partial A_{II}}{\partial z}\bigg|_0 \\ \frac{1}{\rho_I}\frac{\partial A_I}{\partial z}\bigg|_0 &= \frac{1}{\rho_{II}}\frac{\partial A_{II}}{\partial z}\bigg|_0\end{aligned}. \qquad \text{(K.31)}$$

Similarly, two integrations give us continuity of the field A. Thus, the δ-function-bifurcation prescription correctly reproduces the boundary conditions on the field at an interface where the density jumps: continuity of the field and of the normal derivative divided by the density.

K.2 An important caveat concerning the δ-function bifurcation procedure

As noted in the discussion in Section 5.2, the δ-function bifurcation prescription only applies in certain specified contexts, and it must be applied with care. The prescription works well when the associated step functions are raised to simple powers, and when it is used in conjunction with the ordinary rules of differentiation such as the chain rule and the product rule. However, naively multiplying through by *functions of the step function* will cause problems. For example, in Subsection K.2.1, we will see that multiplications such as $\left[1/(1+\text{constant}\cdot\Theta)\right]\cdot\delta$ or $\left[1/\sqrt{1+\text{constant}\cdot\Theta}\right]\cdot\delta$ will produce incorrect results when combined with the bifurcation prescription (at least if both sides are weighted equally). As discussed in Subsection K.2.2, these functions apparently distort the step and change the relative weighting factor assigned to the two halves of the bifurcated δ-function. On the other hand, as will be demonstrated in Subsections K.2.1 and K.2.3, we can expand these functions into Taylor series expansions, and these consist of sums of terms that are products of the basic form $\Theta^n\cdot\delta$. Now, for these clean undistorted steps we can use the δ-function bifurcation prescription.

K.2.1 Cases where δ-function bifurcation only seems to work to 1st order

Here we examine two cases, where the δ-function-bifurcation prescription only works to to 1st order: the substitution $\alpha = 1/\rho$ and Tappert's change of variable (COV) substitution $u = A/\sqrt{\rho}$.

K.2.1.1 2-fluid full wave interface with the substitution $\alpha = 1/\rho$

As in Appendix Subsection K.1.2, let us consider a 2-fluid interface embedded in a 2-dimensional $x-z$ space. Now, instead of using the variable ρ, let us consider the variable $\alpha = 1/\rho$. As shown in Figure K.4, α jumps at the interface, and so it can be expressed as $\alpha = \alpha_{II} - \delta\alpha \cdot \Theta(z)$ where $\delta\alpha \equiv \alpha_{II} - \alpha_I$. Note that once again we use a local coordinate system so that the interface is at $z = 0$ and the z-axis is (locally) normal to the interface.

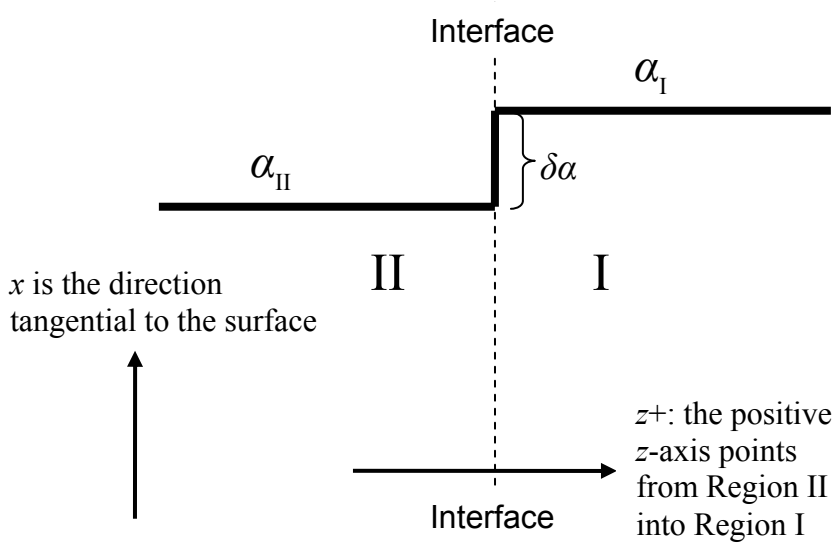

Figure K.4 - The geometry used in this section. The z-axis is locally normal to the interface. We use the new variable $\alpha \equiv 1/\rho$, and $\alpha = \alpha_{II} - \delta\alpha \cdot \Theta(z)$ where $\delta\alpha \equiv \alpha_{II} - \alpha_I$.

The variable density acoustic wave equation (K.28) now takes the form

$$0 = \nabla_T \left([\alpha \nabla_T A] \right) + \cdots$$

where the ellipsis stands for terms that will not a play a role in determining the boundary conditions on the field A. By integrating directly, we see the boundary conditions are

$$A \text{ continuous} \quad ; \quad \alpha \cdot \frac{\partial A}{\partial z} \text{ continuous}. \tag{K.32}$$

Now, let us show that to 1st order in $\delta\alpha$, δ-function bifurcation reproduces the boundary conditions (K.32). The continuity of A is trivial, because there is only a first derivative of α, and so no δ' will be generated. It remains to derive the continuity of $\alpha \cdot \partial A/\partial z$.

The chain rule for differentiation gives us

$$0 = \left(\nabla_T \alpha\right)\left(\nabla_T A\right) + \alpha \nabla_T^2 A + \cdots .$$

Now, δ-function bifurcation gives us

$$\nabla_T \alpha = -\delta\alpha \frac{\delta}{2} \nabla_T A \to -\delta\alpha \sum_{\pm} \frac{\delta^{\pm}}{2} \nabla_T A^{\pm} = -\delta\alpha \left(\frac{\delta^{+}}{2} \nabla_T A^{+} + \frac{\delta^{-}}{2} \nabla_T A^{-} \right)$$

and the wave equation becomes

$$0 = \alpha \nabla_T^2 A - \delta\alpha \left(\frac{\delta^{+}}{2} \nabla_T A^{+} + \frac{\delta^{-}}{2} \nabla_T A^{-} \right) + \cdots . \tag{K.33}$$

Now comes the crucial (and as it turns out partly illegal) step: divide by $\alpha = \alpha_{II} - \delta\alpha \cdot \Theta(z)$. Note that in Subsection K.1.2 above, we *multiplied* by $\rho_{II} - \delta\rho \cdot \Theta(z)$. In other words, earlier we multiplied by the step function, but now we multiply by the step function Θ *embedded in another function;* in this case the other function has the basic form $1/[1 + \text{constant} \cdot \Theta]$.

At any rate, dividing equation (K.33) by α gives us

$$0 = \nabla_T^2 A - \left(\frac{\delta^{+}}{2\alpha_I} \nabla_T A_I + \frac{\delta^{-}}{2\alpha_{II}} \nabla_T A_{II} \right) \delta\alpha + \cdots .$$

Next, we perform the infinitesimal integration $\int_{-\varepsilon}^{\varepsilon} dz$ and recall that $\nabla_T = \partial/\partial z$ for the 2-dimensional problem. This gives us

$$\nabla_T A_I - \nabla_T A_{II} = \frac{\delta\alpha}{2\alpha_I} \nabla_T A_I + \frac{\delta\alpha}{2\alpha_{II}} \nabla_T A_{II}$$

and so

$$\nabla_T A_I \left(1 - \frac{\delta\alpha}{2\alpha_I} \right) = \left(1 + \frac{\delta\alpha}{2\alpha_{II}} \right) \nabla_T A_{II} . \tag{K.34}$$

Result (K.34) would produce a mess if we continued without imposing a trick: let us use a 1st order Taylor series expansion to rewrite (K.34) as

$$\frac{\nabla_T A_I}{1+\frac{\delta\alpha}{2\alpha_I}} = \frac{\nabla_T A_{II}}{1-\frac{\delta\alpha}{2\alpha_{II}}}. \tag{K.35}$$

Now,

$$1+\frac{\delta\alpha}{2\alpha_I} = \frac{2\alpha_I}{2\alpha_I} + \frac{\alpha_{II}-\alpha_I}{2\alpha_I} = \frac{\alpha_I+\alpha_{II}}{2\alpha_I}$$
$$1-\frac{\delta\alpha}{2\alpha_{II}} = \frac{2\alpha_{II}}{2\alpha_{II}} - \frac{\alpha_{II}-\alpha_I}{2\alpha_{II}} = \frac{\alpha_I+\alpha_{II}}{2\alpha_{II}},$$

leading to the correct answer

$$\alpha_I \frac{\partial A_I}{\partial z} = \alpha_{II} \frac{\partial A_{II}}{\partial z}. \tag{K.36}$$

However, note that we had to restrict ourselves to 1st order in $\delta\alpha$. Let us consider another example, Tappert's change of variable substitution, and show that the same sort of thing happens.

K.2.1.2 The change of variable substitution $A \to u/\sqrt{\rho}$

In this subsection, we will apply the change of variable substitution suggested by Tappert (see pp. 262-264 of reference [15]), and show that to 1st order, δ-function bifurcation will be needed to correctly reproduce the continuity condition on the field $A = u/\sqrt{\rho}$. Once again as in Subsections K.1.2 and K.2.1.1, let us consider a 2-fluid interface embedded in 2-dimensional $x-z$ space. We use a local coordinate system so that the interface is at $z=0$ and the z-axis is (locally) normal to the interface. Thus, the geometry outlined in Figure K.3 holds here as well.

Under the change of variable substitution, the wave equation becomes

$$0 = \rho\vec{\nabla}\cdot\left[\frac{1}{\rho}\vec{\nabla}\left(\sqrt{\rho}\cdot u\right)\right] + k^2\cdot\sqrt{\rho}\cdot u. \tag{K.37}$$

The boundary condition on u itself (as opposed to its normal derivative) will come from terms involving the second transverse derivative on a step function (which in this case comes from the density ρ) and terms involving the second transverse derivative of u [aaaa]. Thus, equation (K.37) becomes

[aaaa] The first transverse derivatives of the step function and of u will be involved in a calculation of the boundary condition on $\nabla_T u$ much like that presented in Subsection K.1.2 for the calculation of $\nabla_T A$.

$$0 = \sqrt{\rho}\nabla_T^2 u + \left[\nabla_T^2\sqrt{\rho}\right]u + \cdots \tag{K.38}$$

where the ellipsis once again stands for terms that will not be involved in determining the boundary condition on u. Now, we divide by $\sqrt{\rho}$ (or equivalently multiply by $1/\sqrt{\rho}$). Once again, as in the calculation following equation (K.33), this is the crucial and, as it turns out, partly illegal step. Once again in contrast to Subsection K.1.2, where we *multiplied* by $\rho_{II} - \delta\rho\cdot\Theta(z)$, here we multiply by the step function Θ *embedded* in another function of the basic form $1/\sqrt{1+\text{constant}\cdot\Theta}$.

At any rate, dividing equation (K.38) by $\sqrt{\rho}$ gives us the equation

$$0 = \nabla_T^2 u + \frac{1}{\sqrt{\rho}}\left[\nabla_T^2\sqrt{\rho}\right]u + \cdots . \tag{K.39}$$

Note that z is in the normal direction, and so $\nabla_T^2 = \partial^2/\partial z^2$ stands for two derivatives in the normal direction. Thus, it is undone by the infinitesimal double integration in the normal direction $\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz \cdots$, and so $\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz\cdot\nabla_T^2 u = u_I - u_{II}$.

We will also need to use δ-function bifurcation to evaluate

$$\frac{1}{\sqrt{\rho}}\left[\nabla_T^2\sqrt{\rho}\right]u .$$

Since $\rho = \rho_{II} - \delta\rho\cdot\Theta(z)$, we have

$$\begin{aligned}\nabla_T^2\sqrt{\rho} &= \frac{\partial}{\partial z}\left[\frac{\partial}{\partial z}\sqrt{\rho}\right] = \frac{\partial}{\partial z}\left[\frac{1}{2\sqrt{\rho}}(-\delta\rho)\left(\frac{\delta^+}{2}+\frac{\delta^-}{2}\right)\right] \\ &= -\frac{\delta\rho}{4}\frac{\partial}{\partial z}\left(\frac{\delta^+}{\sqrt{\rho_I}}+\frac{\delta^-}{\sqrt{\rho_{II}}}\right) = -\frac{\delta\rho}{4}\left(\frac{\delta'^+}{\sqrt{\rho_I}}+\frac{\delta'^-}{\sqrt{\rho_{II}}}\right),\end{aligned}$$

and multiplying by $u/\sqrt{\rho}$ gives us

$$\frac{1}{\sqrt{\rho}}\left[\nabla_T^2\sqrt{\rho}\right]u = -\frac{\delta\rho}{4\rho}u\left(\delta'^+ + \delta'^-\right) = -\frac{\delta\rho}{4}\left(\frac{u_I}{\rho_I}\delta'^+ + \frac{u_{II}}{\rho_{II}}\delta'^-\right).$$

Proceeding in much the same way as in the discussion in Subsection K.1.1.2 (a little below equation (K.18)), we note that under the relevant infinitesimal integration

$\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz \cdots$,

$$\left[\delta'^{+}/2\right](u_I/\rho_I)+\left[\delta'^{-}/2\right](u_{II}/\rho_{II})$$

integrates to $(u_I/\rho_I)+(u_{II}/\rho_{II})$, which is the same as

$$\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz\left[(u_I/\rho_I)+(u_{II}/\rho_{II})\right]\cdot\delta'(z).$$

and so we now are free to pull out the bifurcated δ'-function and replace it with an ordinary δ'-function[bbbb]:

$$\frac{1}{\sqrt{\rho}}\left[\nabla_T^2\sqrt{\rho}\right]u=-\frac{\delta\rho}{4}\left(\frac{u_I}{\rho_I}\delta'^{+}+\frac{u_{II}}{\rho_{II}}\delta'^{-}\right)=-\frac{\delta\rho}{4}\left(\frac{u_I}{\rho_I}+\frac{u_{II}}{\rho_{II}}\right)\delta'. \qquad \text{(K.40)}$$

Substituting (K.40) into (K.39) leaves us with

$$0=\nabla_T^2 u-\frac{\delta\rho}{4}\left(\frac{u_I}{\rho_I}+\frac{u_{II}}{\rho_{II}}\right)\delta'+\cdots$$

and integrating twice $\int_{-\varepsilon}^{\varepsilon} dz' \int_{-\infty}^{z'} dz\cdots$ gives us

$$\begin{aligned} u_I-u_{II}&=\frac{\delta\rho}{4}\left(\frac{u_I}{\rho_I}+\frac{u_{II}}{\rho_{II}}\right)\\ u_I\left[1-\frac{\delta\rho}{4\rho_I}\right]&=u_{II}\left[1+\frac{\delta\rho}{4\rho_{II}}\right] \end{aligned}. \qquad \text{(K.41)}$$

Once again we need to restrict ourselves to 1st order ($\mathrm{O}(\delta\rho/\rho)$). Now equation (K.41) becomes:

$$u_I\left[1+\frac{\delta\rho}{2\rho_I}\right]^{-1/2}=u_{II}\left[1-\frac{\delta\rho}{2\rho_{II}}\right]^{-1/2}. \qquad \text{(K.42)}$$

Noting that

$$\begin{aligned} 1+\frac{\delta\rho}{2\rho_I}&=\frac{2\rho_I+\rho_{II}-\rho_I}{2\rho_I}=\frac{\bar{\rho}}{\rho_I}\\ 1-\frac{\delta\rho}{2\rho_{II}}&=\frac{2\rho_{II}-\rho_{II}+\rho_I}{2\rho_{II}}=\frac{\bar{\rho}}{\rho_{II}}\ , \end{aligned}$$

[bbbb] The details have been repeated here in order to help us familiarize ourselves with this useful aspect of the δ-function bifurcation formalism.

equation (K.42) implies

$$u_I\sqrt{\rho_I} = u_{II}\sqrt{\rho_{II}}\ .$$

Furthermore,

$$u_I = \frac{A_I}{\sqrt{\rho_I}} \quad ; \quad u_{II} = \frac{A_{II}}{\sqrt{\rho_{II}}}$$

and we have recovered the continuity condition

$$A_I = A_{II}\ . \tag{K.43}$$

Thus, we have again shown that δ-function bifurcation works to $\mathrm{O}\left(\delta\rho/\rho\right)$.

The reason that we needed to restrict ourselves to 1st order ($\mathrm{O}\left(\delta\rho/\rho\right)$) in the example just given here in K.2.1.2, as well as in the example given earlier in Subsection K.2.1.1, will be examined in Subsection K.2.2 below.

Finally, note that in addition to casting light on the applicability of δ-function bifurcation, the change of variable procedure raises a number of other interesting issues, and so we also further examine this substitution in Sections 2.2 and 6.2.1.

K.2.2 The need for clean (undistorted) steps

When applied "naively," the δ-function bifurcation procedure appears to work only to 1st order in some cases and exactly in others. It turns out that the problem does not lie with the δ-function bifurcation prescription per se. It is perfectly sensible that a δ-function will pick up the average between the values of a discontinuous variable, provided that once we introduce a step into a given parameter (and subsequently take derivatives of it to produce a δ-function), we do not expect the exact same (undistorted) step to also govern the behavior of the jump associated with another parameter that depends on the original parameter in some non-trivial manner. The reason is this: According to generalized function (i.e., distribution) theory, the Heaviside step function $\Theta\left(z\right)$ is really a sequence of functions symmetric about the origin ($z = 0$) that converge to the step. Once we operate on the functions in this sequence (e.g., take the reciprocal, the square root, etc.), this distorts the symmetry, and the functions will be weighted differently when they multiply the corresponding δ-function. In other words, the δ-function no longer bifurcates evenly $\delta \to \delta^+/2 + \delta^-/2$, but now we have the more general condition:

$$\delta \to a\delta^+ + \left(1-a\right)\delta^- \quad 0 < a < 1\ . \tag{K.44}$$

To further examine these issues, we begin by once again considering the operator that appears in the variable density acoustic equation (K.28): $\nabla_T \left(1/\rho\right) \nabla_T$. Recall that our prescription requires that the chain rule (for differentiation) be applied first, and the step is only subsequently put directly into the density ($\rho = \rho_{II} - \delta\rho \cdot \Theta(z)$). It is important to note that our concerns about distorting the step function do <u>not</u> extend to the $-1/\rho^2$ that is generated when we have used the product and chain rules to expand the operator:

$$\nabla_T \left(1/\rho\right) \nabla_T = -\frac{\nabla_T \rho}{\rho^2} \nabla_T + \frac{1}{\rho} \nabla_T^2 . \tag{K.45}$$

One the other hand, as an alternative we could have proceeded roughly as in Subsection K.2.1.1, and first put the step directly into $1/\rho$. To clarify certain issues relevant to the current discussion, let us recast the equation $\alpha = \alpha_{II} + \delta\alpha \cdot \Theta(z)$ to

$$\frac{1}{\rho} = \frac{1}{\rho_{II}} - \Theta(z) \left[\frac{1}{\rho_{II}} - \frac{1}{\rho_I} \right]. \tag{K.46}$$

Substituting equation (K.46) directly into equation $\nabla_T \left(1/\rho\right) \nabla_T$, we generate a δ-function by operating on the step function $\Theta(z)$ with ∇_T. Now it will be the step in $1/\rho$ that is symmetric about $z = 0$ and rather than the step in ρ. By itself, this is fine. However, in the other term in the expansion of $\nabla_T \left(1/\rho\right) \nabla_T$, $\left(1/\rho\right) \nabla_T^2$, we are left with a factor of $1/\rho$ in front of the leading operator ∇_T^2. To integrate with respect to z (in our usual 1-dimensional example) and obtain the boundary conditions, we will need to get rid of that $1/\rho$ in front of ∇_T^2 by multiplying through by a ρ. But now we are multiplying a δ-function by an asymmetric step, and we would have to adjust the weighting factor accordingly. It is not obvious how to do that. Now we can understand why we are better off putting our step directly into ρ (as originally suggested in the previous paragraph). Somehow, the chain rule automatically provides extra coefficients for the two halves of the bifurcated δ-function generated by $\nabla_T \left(1/\rho\right)$ so that it properly corresponds to an undistorted step for ρ itself (that the chain rule is really capable of doing so is not self-evident—see, for example footnote zz and the related discussion in Section 5.2—but it does seem to do the job!). Thus, we are free to multiply through by a ρ and apply simple δ-function bifurcation (i.e., $a = 1 - a = ½$ in (K.44)). It is the coefficients generated by the chain rule that provide the asymmetrical weighting.

Let us now summarize these insights in way that ties them to the parts of Appendix K that have come previous to this point. We see that the trouble actually begins after the δ-bifurcation procedure has been completed, and we are left with a discontinuous function in front of the leading order derivative (i.e., the one that will be integrated one, two and in general three, four, or more times). For the constant density parabolic equation ($\delta\rho = 0$), there is no such function, and the issue never comes up. On the other

hand, as noted in the previous paragraph, for the $\nabla_T (1/\rho)\nabla_T$ operator, we get $(1/\rho)\nabla_T^2$: i.e., $1/\rho$ times the leading order derivative. Now we multiply by ρ (i.e., a simple step function) so that the $1/\rho$ in front of ∇_T^2 cancels. Elsewhere, this leads us to multiply our δ-functions by a simple step. The step is effectively averaged, and our prescription remains fine. However, in the two examples that fail at 2nd order (see section K.2.1), the leading order derivative ∇_T^2 was multiplied by α, a function with a step, or $\sqrt{\rho}$, the square root of a function with a step. If we now multiply through by the reciprocal (formally $1/\alpha$ and $1/\sqrt{\rho}$ in our examples), we run into trouble. Since we have distorted the associated series of functions that (in the generalized sense) approach the step function, we cannot expect the relative weights in the δ-function bifurcation to provide a simple averaging, and indeed they do not (i.e., $a \neq ½$). We obtain the wrong answer if we assume that to be the case. On the other hand, if we content ourselves with a 1st order result, then multiplication by the reciprocal is converted into multiplication by a clean step, and we do indeed obtain the correct answer to 1st order in both our examples.

Note that this reasoning apparently implies that we can in general use Taylor series expansions to guarantee that we are always multiplying by powers of undistorted steps, and so place any problem into a form where the δ-function-bifurcation prescription applies. In Section K.2.3 just below, we will provide an example of this principle at work.

Before proceeding to this example, let us consider one more issue: what happens if we mix two *in*dependent parameters, say the density ρ and the compressibility K. Everything should work fine without further consideration provided the parameters are truly independent. However, what if we use the density ρ, but now replace the compressibility K with the sound speed $c = 1/\sqrt{\rho K}$? This raises the question: does a step in ρ go with a step in K or a step in c? The answer depends on the context. Either K or c may in principle be considered independent of ρ. The context, however, will determine which variable we choose to consider independent of ρ, and that is the one with which we associate a clean (undistorted) step. In the full wave equation, the only δ-functions involve ρ, and these δ-functions never multiply a sound speed or a compressibility, so the point is mute. However, the issue arises in the parabolic equation. In this case, the chain rule will keep things consistent, but one choice will be more convenient. If we choose the compressibility K as the variable that is independent of the density ρ, then the key PE parameter μ depends (linearly) on K alone, and we can step K (or absolutely equivalently μ) and ρ in tandem, and make no further adjustments. On the other hand, if we choose ρ and c as our independent variables, now μ picks up a ρ-dependence (as well as a $1/c^2$-dependence), and we will need to use the chain rule

in evaluating μ when it is operated on by a derivative[cccc]. Since things are much simpler when we use the compressibility K (or completely equivalently μ), we will take this to be the physical parameter that is independent of the density ρ.

K.2.3 Example: Extending the treatment of $\alpha = 1/\rho$ to 2nd order using Taylor series expansion

To further verify the hypothesis that the δ-function-bifurcation procedure applies as long as the δ-function is multiplied by clean undistorted steps, let us return to the example in Subsection K.2.1.1, and expand to 1st order in $\delta\alpha$ the factor of $1/\alpha$ multiplying the bifurcating δ-function. Previously, we used 0th order, so this will overall generate an extra order in $\delta\alpha$ beyond that previously used. Having expanded in a Taylor series, we are now simply multiplying through by a legitimate (undistorted) step function. Since the step function multiplies a δ-function that is already 1st order in $\delta\alpha$, this maneuver will gain us one more order of accuracy overall than the order of the expansion of $1/\alpha$—an overall accuracy to $\mathrm{O}\left(\delta\alpha^2\right)$ in this case.

Note that the geometry is again given by Figure K.4. We consider 2-dimensional $x-z$ space and we have $\alpha = \alpha_{II} - \delta\alpha \cdot \Theta(z)$, where $\delta\alpha \equiv \alpha_{II} - \alpha_I$. We are evaluating the equation

$$0 = \nabla_T \left([\alpha \nabla_T A] \right) + \cdots$$

(where the ellipsis stands for terms that will not a play a role in determining the boundary conditions on the field A). Applying the chain rule in this context gives us

$$\begin{aligned} 0 &= \nabla_T \left([\alpha \nabla_T A] \right) + \cdots = \alpha \nabla_T^2 A + (\nabla_T \alpha) \nabla_T A + \cdots \\ &= \alpha \nabla_T^2 A - \delta\alpha \left(\frac{\delta^+}{2} \nabla_T A^+ + \frac{\delta^-}{2} \nabla_T A^- \right) + \cdots . \end{aligned} \tag{K.47}$$

[cccc] Even cross-terms between $\nabla_T (1/\rho) \nabla_T$ and $1/\rho$ should pose no problems provided we use the chain rule for differentiation to generate our first δ-function. In fact, the same is also true for all the cross-terms associated with higher orders of the operator $\nabla_T (1/\rho) \nabla_T$. To see that this must be true for the broad class of cases mentioned here, just let everything to the right of the leftmost $\nabla_T (1/\rho) \nabla_T$ operator take the place of A in the calculation of Section K.1.2.

Now we multiply through by a $1/\alpha$. The α in the first term cancels. Now, as advertised, let us take the factor of $1/\alpha$ multiplying the bifurcating δ-function and expand it to first order:

$$\frac{1}{\alpha}=\frac{1}{\alpha_{II}\left(1-\dfrac{\delta\alpha}{\alpha_{II}}\Theta(z)\right)}=\frac{1}{\alpha_{II}}\left(1+\frac{\delta\alpha}{\alpha_{II}}\Theta(z)\right)+\mathrm{O}\left(\delta\alpha^2\right). \tag{K.48}$$

Substituting (K.48) into (K.47) multiplied by $1/\alpha$, we obtain

$$0=\nabla_T^2 A-\delta\alpha\left(\frac{\delta^+}{2}\frac{1}{\alpha_{II}}\left(1+\frac{\delta\alpha}{\alpha_{II}}\right)\nabla_T A_I+\frac{\delta^-}{2}\frac{1}{\alpha_{II}}\nabla_T A_{II}\right)+\cdots+\mathrm{O}\left(\delta\alpha^3\right). \tag{K.49}$$

Recall that for our 2-dimensional example, $\nabla_T=\partial/\partial z$ and integrate $\int_{-\varepsilon}^{\varepsilon} dz$ to get

$$0=\nabla_T A_I-\nabla_T A_{II}-\frac{\delta\alpha}{2\alpha_{II}}\left(1+\frac{\delta\alpha}{\alpha_{II}}\right)\nabla_T A_I-\frac{\delta\alpha}{2\alpha_{II}}\nabla_T A_{II}+\mathrm{O}\left(\delta\alpha^3\right),$$

and consequently

$$\nabla_T A_I\left(1-\frac{\delta\alpha}{2\alpha_{II}}-\frac{(\delta\alpha)^2}{2\alpha_{II}^2}\right)=\nabla_T A_{II}\left(1+\frac{\delta\alpha}{2\alpha_{II}}\right)+\mathrm{O}\left(\delta\alpha^3\right)$$

$$\nabla_T A_I\left(1-\frac{\delta\alpha}{2\alpha_{II}}-\frac{(\delta\alpha)^2}{4\alpha_{II}^2}\right)-\frac{(\delta\alpha)^2}{4\alpha_{II}^2}\nabla_T A_I=\nabla_T A_{II}\left(1+\frac{\delta\alpha}{2\alpha_{II}}\right)+\mathrm{O}\left(\delta\alpha^3\right).$$

Now, $\nabla_T A_I=\nabla_T A_{II}+\mathrm{O}(\delta\alpha)$ and so to $\mathrm{O}\left(\delta\alpha^3\right)$ we can replace $\nabla_T A_I$ with $\nabla_T A_{II}$ in the term just to the left of the = sign and move it to the right side of the equation:

$$\nabla_T A_I\left(1-\underbrace{\frac{\delta\alpha}{2\alpha_{II}}-\frac{(\delta\alpha)^2}{4\alpha_{II}^2}}_{\substack{\text{Substitute } \alpha_I \\ \text{for } \alpha_{II} \text{ here}}}\right)=\nabla_T A_{II}\left(1+\frac{\delta\alpha}{2\alpha_{II}}+\frac{(\delta\alpha)^2}{4\alpha_{II}^2}\right)+\mathrm{O}\left(\delta\alpha^3\right). \tag{K.50}$$

Now, note that

$$\frac{1}{\alpha_{II}}=\frac{1}{\alpha_I+\delta\alpha}=\frac{1}{\alpha_I\left(1+\delta\alpha/\alpha_I\right)}=\frac{1}{\alpha_I}\left(1-\frac{\delta\alpha}{\alpha_I}\right)+\mathrm{O}\left(\delta\alpha^2\right)$$

and

$$\frac{1}{\alpha_{II}^2}=\frac{1}{\alpha_I^2}+\mathrm{O}(\delta\alpha).$$

Thus to $\mathrm{O}\left(\delta\alpha^3\right)$ we can substitute α_I for α_{II} on the left side of equation (K.50):

$$\nabla_T A_I\left(1-\frac{\delta\alpha}{2\alpha_I}\left(1-\frac{\delta\alpha}{\alpha_I}\right)-\frac{\left(\delta\alpha\right)^2}{4\alpha_I^2}\right)=\nabla_T A_I\left(1-\frac{\delta\alpha}{2\alpha_I}+\frac{\left(\delta\alpha\right)^2}{2\alpha_I^2}-\frac{\left(\delta\alpha\right)^2}{4\alpha_I^2}\right)=$$

$$\nabla_T A_I\left(1-\frac{\delta\alpha}{2\alpha_I}+\frac{\left(\delta\alpha\right)^2}{4\alpha_I^2}\right)=\nabla_T A_{II}\left(1+\frac{\delta\alpha}{2\alpha_{II}}+\frac{\left(\delta\alpha\right)^2}{4\alpha_{II}^2}\right)+\mathrm{O}\left(\delta\alpha^3\right)$$

Now use

$$\frac{1}{1-x}=1+x+x^2+\cdots \quad \text{with} \quad x=\frac{\delta\alpha}{2\alpha_{II}}$$

$$\frac{1}{1+x}=1-x+x^2+\cdots \quad \text{with} \quad x=\frac{\delta\alpha}{2\alpha_I}$$

to obtain

$$\frac{\nabla_T A_I}{1+\dfrac{\delta\alpha}{2\alpha_I}}=\frac{\nabla_T A_{II}}{1-\dfrac{\delta\alpha}{2\alpha_{II}}}+\mathrm{O}\left(\delta\alpha^3\right). \tag{K.51}$$

This is exactly equation (K.35) in Subsection K.2.1.1. As noted there, this quickly leads to

$$\frac{\nabla_T A_I}{\left[\dfrac{2\alpha_I+\alpha_{II}-\alpha_I}{2\alpha_I}\right]}=\frac{\nabla_T A_{II}}{\left[\dfrac{2\alpha_{II}-\alpha_{II}+\alpha_I}{2\alpha_{II}}\right]}+\mathrm{O}\left(\delta\alpha^3\right)$$

$$\Downarrow \tag{K.52}$$

$$\alpha_I\nabla_T A_I=\alpha_{II}\nabla_T A_{II}+\mathrm{O}\left(\delta\alpha^3\right)$$

as desired.

By expanding the coefficient of the bifurcating δ-function in a Taylor series, we have converted from multiplication by *distorted* steps to multiplication by *undistorted* steps, and so we have been able to increase the order to which the final result is valid. Since the bifurcating δ-function already carries one order, the order of validity turns out to be one greater than the order of the Taylor series employed.

K.3 Verification of the associative property for δ-function bifurcation

The associative property is built into basic distribution theory. This is the main reason behind those expansions connecting $\delta^{(n)}\left(z-f\right)\chi\left(z\right)$ with $\delta^{(n)}\left(z-f\right)\chi\left(f\right)$ (see

footnote ll concerning equation (3.54)). δ-function bifurcation is a linear operation, and it does not affect these equalities.

However, the δ-function bifurcation prescription begs the following question: does the order in which we take nested derivatives and consequently "kick up" δ-functions matter? Interestingly, the answer seems to be that the order does not matter. Let us consider several examples.

In the first example to be considered here in Section K.3, note that we evaluated equation (K.15) by going from right to left, taking derivatives and converting to bifurcated δ-functions as they are generated. This is sensible, but if the associative property for multiplication were to hold, we should also be able to apply the chain rule going from left to right, and get the same answer. This is indeed the case.

To see why things will always work out, first consider

$$\frac{\partial}{\partial z}\left[\Theta(z)\frac{\partial\Theta}{\partial z}\right].$$

We could either begin with

$$\frac{\partial\Theta}{\partial z}=\delta(z)\rightarrow\frac{\delta^{+}(z)}{2}+\frac{\delta^{-}(z)}{2}$$

and so (recalling $\Theta^{+}=\Theta(z>0)=1$ and $\Theta^{-}=\Theta(z<0)=0$)

$$\Theta(z)\frac{\partial\Theta}{\partial z}=\frac{\delta^{+}(z)}{2}$$

and thus

$$\frac{\partial}{\partial z}\left[\Theta(z)\frac{\partial\Theta}{\partial z}\right]=\frac{\delta'^{+}(z)}{2}. \tag{K.53}$$

Alternately, we could proceed as follows:

$$\begin{aligned}\frac{\partial}{\partial z}\left[\Theta(z)\frac{\partial\Theta}{\partial z}\right]&=\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z}+\Theta(z)\frac{\partial^{2}\Theta}{\partial z^{2}}\\&=\frac{\delta'^{+}(z)}{2}\frac{\partial[1]}{\partial z}-\frac{\delta'^{-}(z)}{2}\frac{\partial[0]}{\partial z}+\frac{\delta'^{+}(z)}{2}=\frac{\delta'^{+}(z)}{2}\ .\end{aligned} \tag{K.54}$$

The "extra" terms go away, and we see that we can evaluate derivatives (and replace them with bifurcating δ-functions) at any time during the calculation.

Similarly, note that

$$\frac{\partial^2}{\partial z^2}\left[\Theta(z)\Theta(z)\right] = \frac{\partial}{\partial z}\left[\frac{\partial\Theta}{\partial z}\Theta(z) + \Theta(z)\frac{\partial\Theta}{\partial z}\right] = \frac{\partial}{\partial z}\left[\frac{\delta^+(z)}{2} + \frac{\delta^+(z)}{2}\right]$$
$$= \delta'^+(z) \ ,$$

or alternately

$$\frac{\partial^2}{\partial z^2}\left[\Theta(z)\Theta(z)\right] = \frac{\partial^2\Theta(z)}{\partial z^2}\Theta(z) + \Theta(z)\frac{\partial^2\Theta(z)}{\partial z^2} + 2\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z}$$
$$= \frac{\delta'^+(z)}{2}\cdot 1 + \frac{\delta'^-(z)}{2}\cdot 0 + 1\cdot\frac{\delta'^+(z)}{2} + 0\cdot\frac{\delta'^-(z)}{2}$$
$$+2\delta^+(z)\frac{\partial[1]}{\partial z} + 2\delta^-(z)\frac{\partial[0]}{\partial z}$$
$$= \frac{\delta'^+(z)}{2} + \frac{\delta'^+(z)}{2} = \delta'^+(z)$$

Again, the "extra" terms disappear and we can proceed in either order.

Now, consider λ^4 ($\delta\rho = 0$) theory. Here, we would get a term roughly like

$$\frac{\partial^2}{\partial z^2}\left[\Theta(z)\Theta(z)\Theta(z)\right]$$
$$= \frac{\partial}{\partial z}\left[\delta(z)\Theta(z)\Theta(z) + \Theta(z)\delta(z)\Theta(z) + \Theta(z)\Theta(z)\delta(z)\right].$$
$$= \frac{\partial}{\partial z}\left[\frac{\delta^+}{2} + \frac{\delta^+}{2} + \frac{\delta^+}{2}\right] = \frac{3}{2}\delta'^+$$

Alternately, we could proceed with

$$\frac{\partial^2}{\partial z^2}\left[\Theta(z)\Theta(z)\Theta(z)\right] = \frac{\partial^2\Theta}{\partial z^2}\Theta\Theta + \frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z}\Theta + \frac{\partial\Theta}{\partial z}\Theta\frac{\partial\Theta}{\partial z}$$
$$+\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z}\Theta + \Theta\frac{\partial^2\Theta}{\partial z^2}\Theta + \Theta\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z}$$
$$+\frac{\partial\Theta}{\partial z}\Theta\frac{\partial\Theta}{\partial z} + \Theta\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z} + \Theta\Theta\frac{\partial^2\Theta}{\partial z^2}$$
$$= \frac{3}{2}\delta'^+$$

Again, all the "extra" terms contain a product of the form

$$\frac{\partial\Theta}{\partial z}\frac{\partial\Theta}{\partial z} = \frac{\delta^+}{2}\frac{\partial[1]}{\partial z} = 0 \ ,$$

and so they go away. The same goes for a term like $\nabla_T^2 \Theta \nabla_T^2 \Theta$ (which is similar to one associated with a term like $\nabla_T^2 \left[\mu \nabla_T^2 (\mu\chi) \right]$).

We can start to see why things are working out. Cross-terms of the basic form

$$\frac{\partial \Theta}{\partial z} \frac{\partial \Theta}{\partial z}$$

always go away. Thus, every time we have a product of step functions, and start taking derivatives, the chain rule for multiplication will lead to a sum of terms each with one step function differentiated and the others untouched. Henceforth, all further derivatives in a given product of step functions will focus only on one step function. In other words, the first δ-function caused the rest of them to collapse. We can either apply δ-function bifurcation right away and so avoid generating the superfluous terms; or we can wait and drop the superfluous terms later. We will get the same answer either way.

Note that these arguments also apply to the theory for variable density ($\delta\rho \neq 0$). For example, consider the "sandwich term" in λ^2-theory:

$$\nabla_T \left(\frac{1}{\rho} \nabla_T (\mu\chi) \right).$$

Whether we apply to the chain rule to the "inner" ∇_T operator first and bifurcate immediately as δ-functions are generated, or apply the chain rule for multiplication from left to right and again bifurcate as δ-functions are generated, or apply the chain rule for multiplication from left to right and bifurcate at the end, we will get the same answer in all cases.

Now, note also that as we introduce downrange derivatives $\partial/\partial x$, the associative property continues to apply. For example, let us consider the important example

$$\left[\dot{\lambda}, \gamma \right] = -\left[\nabla_T \frac{\dot{\rho}}{\rho} \nabla_T, \gamma \right]. \tag{K.55}$$

(This expression shows up as we derive the manifestly reciprocal form for the Hamiltonian where there is a density jump, equation (5.9); see also Appendix J.2 for the details.) Of course, if we take $\partial\lambda/\partial x$ first, bifurcation puts us in one medium or the other, and γ is a constant in the half-spaces and commutes with everything, and so the commutator in equation (K.55) is obviously zero. Now, let us evaluate the expression another way:

$$-\left[\dot{\lambda}, \gamma \right] = \nabla_T \left[\frac{\dot{\rho}}{\rho} \nabla_T (\gamma\chi) \right] - \gamma \nabla_T \left[\frac{\dot{\rho}}{\rho} \nabla_T \chi \right].$$

Expanding ∇_T, we have

$$-\left[\dot{\lambda},\gamma\right]=\frac{\dot{\rho}}{\rho}\nabla_T^2(\gamma\chi)+\left(\nabla_T\left[\frac{\dot{\rho}}{\rho}\right]\right)\nabla_T(\gamma\chi)-\gamma\left(\nabla_T\left[\frac{\dot{\rho}}{\rho}\right]\right)\nabla_T\chi-\gamma\frac{\dot{\rho}}{\rho}\left(\nabla_T^2\chi\right).$$

Now,

$$\nabla_T(\gamma\chi)=(\nabla_T\gamma)\chi+\gamma(\nabla_T\chi)$$

and

$$\begin{aligned}\nabla_T^2(\gamma\chi)&=\nabla_T\left[(\nabla_T\gamma)\chi+\gamma(\nabla_T\chi)\right]\\&=\left(\nabla_T^2\gamma\right)\chi+2(\nabla_T\gamma)(\nabla_T\chi)+\gamma\left(\nabla_T^2\chi\right).\end{aligned}$$

Thus, we have

$$\begin{aligned}-\left[\dot{\lambda},\gamma\right]=&\frac{\dot{\rho}}{\rho}\left(\left(\nabla_T^2\gamma\right)\chi+2(\nabla_T\gamma)(\nabla_T\chi)+\cancel{\gamma\left(\nabla_T^2\chi\right)}\right)+\left(\nabla_T\left[\frac{\dot{\rho}}{\rho}\right]\right)(\nabla_T\gamma)\chi\\&+\cancel{\left(\nabla_T\left[\frac{\dot{\rho}}{\rho}\right]\right)\gamma(\nabla_T\chi)}-\cancel{\gamma\left(\nabla_T\left[\frac{\dot{\rho}}{\rho}\right]\right)\nabla_T\chi}-\cancel{\gamma\frac{\dot{\rho}}{\rho}\left(\nabla_T^2\chi\right)}.\end{aligned}$$

Thus, we only have products of derivatives of steps left. Bifurcating $\nabla_T\gamma$ first, ρ is constant in the half-space and $\dot{\rho}=0$; bifurcating $\dot{\rho}$ first, $\nabla_T\gamma=0$. Either way, $\left[\dot{\lambda},\gamma\right]=0$.

For clarity, we will always take $\partial/\partial x$ first and generate our bifurcating δ-functions right away, but we could in principle proceed in any order.

Thus, here in Appendix K.3, we have seen that at least for the kind of simple scenarios that arise in the context of the parabolic equation when the parameters jump (but do not vary otherwise), the δ-function bifurcating formalism obeys an associative property. To be specific, even with our modifications to distribution theory, it does not matter which order we take nested derivatives and in the process "kick up" bifurcating δ-functions.

Finally, note that in Appendix J.2 (specifically, the argument leading to equation (J.19)), we came across an example where the associative property did *not* hold. This is connected to the fact that there, we not only had an interface where the parameters jump, but we also allowed for further variation of the parameter μ in the vicinity of the interface. Thus, it should be emphasized that it is implicitly assumed in the δ-function-bifurcation rules that the parameters jump at an interface, but do not otherwise vary in the vicinity of the interface. If this condition is violated, the associative property in choosing which distributions to bifurcate may not hold, and explicit symmetrization may be necessary.

L Appendix: The Hamiltonian in the half-space where the density is locally constant, but differs from the reference density

In this appendix, we derive the Hamiltonian in the half-space where the density is locally constant. We obtain two closed-form square-root operators that generate the same infinite-order Hamiltonian. The square-root operator derived in Appendix L.1 and presented at the end of equation (L.8) follows from an intuitive derivation and provides an easily remembered closed form operator that generates the acoustic Foldy-Wouthuysen expansion in the half-space where the density is *locally* constant (but different from the reference density). However, this closed form suggests a grouping of terms that provides overly pessimistic convergence criteria for the expansion. Appendix L.2 explores the correct grouping of terms in the expansion, and demonstrates that broad convergence criteria apply. In particular, the approach in Appendix L.2 does not mix orders in the correct expansion parameters, while the expansion in Appendix L.1 does. However, the closed form obtained using the approach of Appendix L.2 (equation (L.14)) is comparatively difficult to work with, so it is preferable in practice to generate the finite-order half-space Hamiltonian using result (L.8).

L.1 Derivation of the form useful as a mnemonic

Recall from equation (5.3) that

$$\begin{aligned} \mathcal{H} &= \mathcal{O} + \mathcal{E} + k_0\eta \\ \mathcal{E} &= \left(\lambda - \boxed{2k_0\gamma}\right)\eta, \\ \mathcal{O} &= \lambda\xi \end{aligned} \tag{L.1}$$

where λ and γ are again given by equation (5.4), while the box again in this appendix indicates a term specific to the case when the reference density ρ_0 differs from the local density ρ. η and ξ are once again given by equations (3.3) and (3.6) respectively. For present purposes, the properties

$$\eta\xi = -\xi\eta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad ; \quad \eta^2 = -\xi^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ; \quad [\eta,\xi]^2 = 4\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{L.2}$$

will turn out to be useful.

From equations (3.9) and (3.10) with the (local) range dependence set to zero, we have to 4th order

$$\tilde{\mathcal{H}} = \eta\left(\frac{\mathcal{O}^2}{2k_0} - \frac{\mathcal{O}^4}{8k_0^3}\right) + \mathcal{E} - \frac{1}{8k_0^2}\big[\mathcal{O},[\mathcal{O},\mathcal{E}]\big] + \frac{\eta}{8k_0^3}\Big(-[\mathcal{O},\mathcal{E}]^2\Big). \tag{L.3}$$

Substituting for $\mathcal{O}$ and $\mathcal{E}$ gives

$$\begin{aligned}\tilde{\mathcal{H}} &= k_0\eta+\eta\left(-\frac{\lambda^2}{2k_0}-\frac{\lambda^4}{8k_0^3}\right)+\eta\left(\lambda-\boxed{2k_0\gamma}\right)-\frac{1}{8k_0^2}\left[\lambda\xi,[\lambda\xi,\lambda\eta]\right] \\ &\quad \boxed{+\frac{2k_0}{8k_0^2}\left[\lambda\xi,[\lambda\xi,\gamma\eta]\right]}+\frac{\eta}{8k_0^3}\left(-\left[\lambda\xi,\left(\lambda-\boxed{2k_0\gamma}\right)\eta\right]^2\right).\end{aligned} \tag{L.4}$$

Expanding the last term:

$$\begin{aligned}\left[\lambda\xi,\left(\lambda-\boxed{2k_0\gamma}\right)\eta\right]^2 &= \left([\lambda\xi,\lambda\eta]\boxed{-[\lambda\xi,2k_0\gamma\eta]}\right)^2 \\ &= [\lambda\xi,\lambda\eta]^2\boxed{-[\lambda\xi,\lambda\eta][\lambda\xi,2k_0\gamma\eta]} \\ &\quad \boxed{-[\lambda\xi,2k_0\gamma\eta][\lambda\xi,\lambda\eta]+[\lambda\xi,2k_0\gamma\eta]^2}\end{aligned}$$

using identities (L.2) and $\left[\xi,[\xi,\eta]\right]=-4\eta$ leads to

$$\begin{aligned}\tilde{\mathcal{H}} &= \eta k_0\left(1+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}+\frac{\lambda^3}{2k_0^3}-\frac{5\lambda^4}{8k_0^4}\right) \\ &\quad \boxed{-2k_0\gamma\eta+\frac{2k_0}{8k_0^2}\left[\lambda\xi,[\lambda\xi,\gamma\eta]\right]} \\ &\quad \boxed{\frac{-\eta}{8k_0^3}\left(-[\lambda\xi,\lambda\eta][\lambda\xi,2k_0\gamma\eta]-[\lambda\xi,2k_0\gamma\eta][\lambda\xi,\lambda\eta]+[\lambda\xi,2k_0\gamma\eta]^2\right)}.\end{aligned} \tag{L.5}$$

Next, again use $\left[\xi,[\xi,\eta]\right]=-4\eta$ and the fact that γ is locally constant in the half-space to show

$$\frac{2k_0}{8k_0^2}\left[\lambda\xi,[\lambda\xi,\gamma\eta]\right]=\frac{2k_0\gamma\lambda^2}{8k_0^2}\left[\xi,[\xi,\eta]\right]=\eta\frac{-\lambda^2}{2k_0^2}(2k_0\gamma). \tag{L.6}$$

Now, we consider the terms in the third line of equation (L.5). Holding γ locally constant, we have

$$[\lambda\xi,\lambda\eta][\lambda\xi,2k_0\gamma\eta]=[\lambda\xi,2k_0\gamma\eta][\lambda\xi,\lambda\eta]=2k_0\gamma\lambda^3[\xi,\eta]^2=4(2k_0\gamma)\lambda^3\cdot 1$$

and

$$[\lambda\xi,2k_0\gamma\eta]^2=4k_0^2\gamma^2\lambda^2[\xi,\eta]^2=4(2k_0\gamma)^2\lambda^2\cdot 1,$$

so that

$$\frac{-\eta}{8k_0^3}\Big(-[\lambda\xi,\lambda\eta][\lambda\xi,2k_0\gamma\eta]-[\lambda\xi,2k_0\gamma\eta][\lambda\xi,\lambda\eta]+[\lambda\xi,2k_0\gamma\eta]^2\Big)=$$
$$\frac{\eta}{8k_0^3}\Big(8(2k_0\gamma)\lambda^3-4(2k_0\gamma)^2\lambda^2\Big)=k_0\eta\frac{-\lambda^2}{2k_0^2}(2\gamma)^2+k_0\eta\frac{\lambda^3}{2k_0^3}2\cdot(2\gamma). \tag{L.7}$$

Thus, we have to 4th order (recalling $\alpha\equiv\rho_0/\rho$)

$$\begin{aligned}
\tilde{\mathcal{H}} &= \eta k_0\left(1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}-\frac{\lambda^2}{2k_0^2}(2\gamma)-\frac{\lambda^2}{2k_0^2}(2\gamma)^2+\frac{\lambda^3}{2k_0^3}+\frac{\lambda^3}{2k_0^3}2\cdot(2\gamma)-\frac{5\lambda^4}{8k_0^4}\right)\\
&= \eta k_0\left(1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}\Big(1+2\gamma+(2\gamma)^2\Big)+\frac{\lambda^3}{2k_0^3}\Big(1-2\cdot(-2\gamma)\Big)-\frac{5\lambda^4}{8k_0^4}\right)\\
&= \eta k_0\left(1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}\frac{1}{1-2\gamma}+\frac{\lambda^3}{2k_0^3}\frac{1}{(1-2\gamma)^2}-\frac{5\lambda^4}{8k_0^4}\right)+\text{5th order}\\
&= \eta k_0\left(\frac{1}{\alpha}+\frac{\lambda}{k_0}-\frac{\alpha\lambda^2}{2k_0^2}+\frac{\alpha^2\lambda^3}{2k_0^3}-\frac{5\alpha^3\lambda^4}{8k_0^4}\right)+\text{5th order}\\
&= \frac{\eta k_0}{\alpha}\left(1+\frac{\alpha\lambda}{k_0}-\frac{(\alpha\lambda)^2}{2k_0^2}+\frac{(\alpha\lambda)^3}{2k_0^3}-\frac{5(\alpha\lambda)^4}{8k_0^4}\right)+\text{5th order}\\
&= \frac{\eta k_0}{\alpha}\sqrt{1+\frac{2\alpha\lambda}{k_0}}.
\end{aligned} \tag{L.8}$$

This is the result we are looking for.

Finally we show that the final form of $\tilde{\mathcal{H}}$ obtained in equation (L.8) is indeed equivalent to the known "correct" (i.e., ∞-order) answer for the Hamiltonian in a half-space where the density is locally constant. We begin with

$$\tilde{\mathcal{H}}=\eta\sqrt{\frac{k_0^2}{\alpha^2}+\frac{2k_0\lambda}{\alpha}}$$

and use equation (5.4) with the density locally constant to obtain

$$\frac{2k_0}{\alpha}\lambda=\frac{2k_0}{\alpha}\left(\frac{\alpha}{2k_0}\nabla_T^2-k_0\mu+k_0\gamma\right)=\nabla_T^2-\frac{2k_0^2}{\alpha}\mu+\frac{2k_0^2}{\alpha}\gamma.$$

Now,

$$\frac{2k_0^2}{\alpha}\mu=\frac{2k_0^2}{\alpha}\frac{(1-n^2\alpha)}{2}=k_0^2\left(\frac{1}{\alpha}-n^2\right)\quad;\quad\frac{2k_0^2}{\alpha}\gamma=\frac{2k_0^2}{\alpha}\frac{\left(1-1/\alpha\right)}{2}=k_0^2\left(\frac{1}{\alpha}-\frac{1}{\alpha^2}\right),$$

and so

$$\frac{2k_0}{\alpha}\lambda = \nabla_T^2 - \frac{k_0^2}{\alpha} + k_0^2 n^2 + \frac{k_0^2}{\alpha} - \frac{k_0^2}{\alpha^2} = \nabla_T^2 + k_0^2 n^2 - \frac{k_0^2}{\alpha^2}.$$

Note the cancellation leaving us with

$$\tilde{\mathcal{H}} = \eta\sqrt{\frac{k_0^2}{\alpha^2} + \frac{2k_0\lambda}{\alpha}} = \eta\sqrt{\nabla_T^2 + k_0^2 n^2} = \eta\sqrt{\nabla_T^2 + k^2}\ . \tag{L.9}$$

This is indeed the standard ∞-order PE Hamiltonian given, for example in equation (9.52) of reference [57]. It is completely equivalent to equation (3.11) above with the (local) range dependence set to zero (the square-root operator there also reduces to $\eta\sqrt{\nabla_T^2 + k^2}$). When there is no (local) range dependence, we can also use the PE Hamiltonian to propagate the pressure field A, and equation (L.9) then also recovers equation (2.4) above. We have therefore shown that in the half-space where the density is locally constant, the Foldy-Wouthuysen procedure generates a PE expansion of the PE square root operator, where the expansion parameters now measure the departure of the local values of *both* the sound speed and density from their reference values.

L.2 Heuristic derivation of a form that accurately reflects the convergence properties of the expansion

Appendix L.2 considers the convergence properties of the series for the Hamiltonian in the half-space. In Subsection L.2.1, we demonstrate that the convergence criteria obtained by naively expanding the closed form of the scalar Hamiltonian obtained in Appendix L.1 are quite strict. In Subsection L.2.2 we use general arguments to obtain an alternate closed form for the Hamiltonian in the half-space that suggests that these convergence criteria are too strict. Subsection L.2.3, we demonstrate that the looser convergence conditions given in Section L.2.2 are indeed the correct ones. We begin by grouping terms in such a way that we preserve the intra-order cancellations that are present in the Foldy-Wouthuysen expansion and are needed to generate its true convergence properties. The resultant closed form manifestly incorporates these cancellations and thus reflects the true convergence properties of the expansion.

L.2.1 Why there is an issue here?

The result for the scalar Hamiltonian H:

$$H = \frac{k_0}{\alpha}\sqrt{1 + \frac{2\alpha\lambda}{k_0}} \tag{L.10}$$

derived in Appendix L.1 must be interpreted as an expansion in the dimensionless operator $2\lambda/k_0$ and the dimensionless scalar function 2γ (which comes from $\alpha = 1/(1-2\gamma)$). Used properly, this expansion is taken order by order with these

expansion parameters (and more generally also the downrange derivative $\partial/\partial x$ acting on λ) contributing equally to the order. In this sense equation (L.10) is a mnemonic that encapsulates this expansion. We have to be careful about taking this mnemonic too literally. Specifically, we cannot treat the operator $2\alpha\lambda/k_0$ as an expansion parameter. To see why, note that if the density ρ and the compressibility K are range independent, then we can decompose the solution into eigenvectors. For each eigenvector, we can replace the operator H with its eigenvalue k_x (the downrange wave number of the eigenvector solution) so that

$$\frac{k_0}{\alpha}\sqrt{1+\frac{2\alpha\lambda}{k_0}} = k_x ,$$

and so noting that $k_0^2 = \omega\rho_0 K_0$, $k^2 = \omega\rho K$ and as always $\alpha = \rho_0/\rho$, we have

$$1+\frac{2\alpha\lambda}{k_0} = \frac{k_x^2}{k_0^2}\alpha^2 = \frac{k_x^2}{k^2}\frac{\rho_0}{\rho}\frac{K}{K_0} .$$

Since k_x is the x-component of the wavevector for the waveguide eigenvector solution, and it is real since the finite-order Hamiltonian is Hermitian, we can write $k_x/k = \cos\theta$, where θ is the grazing angle corresponding to that particular solution. This leads to

$$\frac{2\alpha\lambda}{k_0} = \cos^2\theta\cdot\frac{\rho_0}{\rho}\cdot\frac{K}{K_0} - 1 \qquad \text{(L.11)}$$

To maximize convergence, we typically choose the reference compressibility and density K_0 and ρ_0 to be the maximum values of these parameters found in the problem. A typical problem would involve an interface between water (labeled by the Roman numeral I) and a muddy ocean bottom (labeled by II). Under this scenario, the higher compressibility is the value in water (so $K_0 = K_I$), and the higher density is found in the muddy bottom (so $\rho_0 = \rho_{II}$). Thus for eigenvalue solutions, we have

$$\begin{aligned} \frac{2\alpha\lambda}{k_0} &= \cos^2\theta\cdot\frac{\rho_{II}}{\rho_I} - 1 \quad \text{in medium I} \\ \frac{2\alpha\lambda}{k_0} &= \cos^2\theta\cdot\frac{K_{II}}{K_I} - 1 \quad \text{in medium II} \end{aligned} \qquad \text{(L.12)}$$

Now, we have an interesting problem: for the relatively common scenario $\rho_{II} > 2\rho_I$ and shallow grazing angle (θ small; $\cos(\theta)\approx 1$), our apparent expansion parameter $2\alpha\lambda/k_0$ becomes greater than one. One is tempted to conclude that the validity of our PE is limited to the region $\rho_{II} \le 2\rho_I$. However, as discussed in Section 2.3, the physics of the problem imposes no such limit. We are forced to conclude that the apparent divergence of the expansion is an artifact of the way the terms have been lumped together into the nominal expansion parameter $2\alpha\lambda/k_0$. In the Subsections L.2.2 and L.2.3 we provide

confirmation of this insight by explicitly constructing an alternate grouping of terms that is specifically designed to accurately reflect the true convergence behavior of the underlying PE expansion. We will find that convergence to the correct result $H = \sqrt{\nabla_T^2 + k^2}$ is manifest for all $\Delta\rho/\rho_0 < 1$.

L.2.2 The basic strategy

In the upcoming Subsection L.2.3 that immediately follows the current subsection, a new grouping of terms will be constructed. This grouping, by design, will reflect the true convergence properties of the PE expansion generated by the Foldy-Wouthuysen transformation. The procedure will begin with the observation that the actual order-by-order (in $2\lambda/k_0, 2\gamma$) expansion generated by the Foldy-Wouthuysen transformation contains cancellations that are associated with cross-terms that come from taking powers of $\lambda - \gamma$. (On the other hand, if we let the derivation in Appendix L.1 influence us to consider $2\alpha\lambda/k_0$ as an expansion parameter, then we would be combining terms across orders in the original expansion (i.e., in the expansion in the parameters $2\lambda/k_0$ and 2γ) in a way that does not take advantage of these intra-order cancellations. Crucial cancellations would occur between different orders in the $2\alpha\lambda/k_0$ -expansion rather than within a given order.) The intra-order cancellations will be used to guide us in the construction of an alternate "mnemonic" (i.e., a compact expression that can be used to generate the expansion). Since the cancellations are built in, this alternate form should accurately reflect the true convergence properties of the expansion.

As it turns out, we could almost have guessed the result. It reflects the fact that (locally at least) we are free to make use of the familiar PE operator $\tilde{\lambda}$ and reference wave number $\tilde{k}_0$, where the reference density is temporarily chosen to be the local density (i.e., $\tilde{\rho}_0 = \rho_{\text{Local}} = \rho$ where $\tilde{\rho}_0$ is the reference density used briefly during the argument employed to construct equation (L.14) below), and the difference between the reference and local compressibilities generates the familiar deviation of the index of refraction squared (i.e., $\tilde{K}_0 = K_0$). Thus:

$$\begin{aligned}
&\tilde{k}_0 = \omega\sqrt{K_0\rho} = \frac{\omega}{\tilde{c}_0} \\
&\tilde{\mu} = \mu = \frac{1}{2}\left(1 - \frac{K}{K_0}\right) = \frac{1}{2}\left(1 - \frac{K}{K_0}\frac{\rho}{\rho}\right) = \frac{1}{2}\left(1 - \frac{\tilde{c}_0^2}{c^2}\right) = \frac{1}{2}\left(1 - \tilde{n}^2\right). \qquad \text{(L.13)} \\
&\tilde{\lambda} = \frac{\nabla_T^2}{2\tilde{k}_0} - \tilde{k}_0\tilde{\mu}
\end{aligned}$$

Within the half-space (where the density is constant), $\tilde{\lambda}$ and $\tilde{k}_0$ can be used to express the locally exact PE operator:

$$H = \tilde{k}_0 \sqrt{1 + \frac{2\tilde{\lambda}}{\tilde{k}_0}} = \sqrt{\nabla_T^2 + k^2} \ . \qquad \text{(L.14)}$$

As noted earlier, the latter is equivalent to the mnemonic given in equation (L.10). Using the relations

$$\begin{aligned} \frac{\tilde{\lambda}}{\tilde{k}_0} &= \frac{\nabla_T^2}{2\tilde{k}_0^2} - \tilde{\mu} = \frac{\nabla_T^2}{2\omega^2 K_0 \rho} - \tilde{\mu} = \frac{\nabla_T^2}{2\omega^2 K_0 \rho_0} \frac{\rho_0}{\rho} - \mu = \left(\frac{\rho_0}{\rho} \right) \frac{\nabla_T^2}{2k_0^2} - \mu = \frac{\lambda}{k_0} - \gamma \\ \tilde{k}_0 &= \omega \sqrt{K_0 \rho} = \omega \sqrt{K_0 \rho_0} \sqrt{\frac{\rho}{\rho_0}} = k_0 \sqrt{1 - 2\gamma} \end{aligned} \ , \qquad \text{(L.15)}$$

the new compact expression in equation (L.14) can be expressed and then expanded in the quantities $2\lambda/k_0$ and 2γ. Since for sufficiently small $2\lambda/k_0$ and 2γ, even the expansion derived using equation (L.10) clearly converges, the expansions of (L.10) and of (L.14) must be identical at any given order in $2\lambda/k_0$ and 2γ. Thus, we have a compact expression for the expansion generated by the Foldy-Wouthuysen transformation that implies good convergence properties as long as $2\lambda/k_0$ and 2γ are both less than 1 (i.e., for all densities provided we choose $\rho_0 = \rho_{\max}$). The heuristic development in Subsection L.2.3 roughly proceeds in the reverse direction of the argument in this paragraph. It is useful to consider it in detail because this derivation clearly illustrates why expression (L.14) more accurately reflects the true expansion properties of full PE expansion.

L.2.3 Detailed heuristic analysis

Here we consider the PE expansion for the case when the reference density differs from the local density, and cast it in a form where the natural pairing of λ and γ into the combination $\lambda - \gamma$ is manifestly apparent. We begin by grouping the 1st order of the expansion in the following suggestive manner:

$$k_0 - 2k_0\gamma + \lambda \to k_0 + (\lambda - k_0\gamma) - k_0\gamma + \cdots .$$

This suggests that we try an ansatz with $\lambda_{\text{effective}} = \lambda - k_0\gamma$. In other words, we anticipate a result of the form

$$H = k_0 \sqrt{1 + \frac{2(\lambda - k_0\gamma)}{k_0}} - \gamma k_0 \sqrt{1 + \frac{2(\lambda - k_0\gamma)}{k_0}} + \cdots . \qquad \text{(L.16)}$$

Let us see if the ansatz works to 2nd order. The 2nd order expansion of equation (L.16) is

$$k_0\left(1+\frac{(\lambda-k_0\gamma)}{k_0}-\frac{(\lambda-k_0\gamma)^2}{2k_0^2}\right)-k_0\gamma\left(1+\frac{(\lambda-k_0\gamma)}{k_0}\right)-\frac{k_0\gamma^2}{2}(1+\cdots)$$

$$k_0+\lambda-k_0\gamma-\frac{\lambda^2}{2k_0}+\gamma\lambda-\frac{k_0\gamma^2}{2}-k_0\gamma-\gamma\lambda+k_0\gamma^2-\frac{k_0\gamma^2}{2}+\cdots \quad .$$

$$k_0-2k_0\gamma+\lambda-\frac{\lambda^2}{2k_0}+\cdots$$

Thus we have indeed reproduce the 2nd order result. Especially telling is the fact that the last term on the first line had to be tacked on in order to properly reproduce the expansion generated by the Foldy-Wouthuysen transformation. This is pretty suggestive. We are clearly beginning to obtain a series that looks like

$$\left(k_0-k_0\gamma-\frac{k_0\gamma^2}{2}+\cdots\right)\sqrt{1+\frac{2(\lambda-k_0\gamma)}{k_0}}\,.$$

Thus, noting that $\sqrt{1-2\gamma}=1-\gamma-\gamma^2/2+\cdots$, we have

$$k_0\sqrt{1-2\gamma}\cdot\sqrt{1+\frac{2(\lambda-k_0\gamma)}{k_0}}\,.$$

Now, from equation (L.15) we have

$$\tilde{k}_0=k_0\sqrt{1-2\gamma} \quad ; \quad \frac{\tilde{\lambda}}{\tilde{k}_0}=\frac{\lambda-k_0\gamma}{k_0}\,, \tag{L.17}$$

and so we have reproduced result (L.14).

We have shown that the PE expansion when the reference density differs from the local density is generated by:

- taking the generator of the PE that is commonly used when the density is tacitly assumed to be everywhere the same (for the moment using the local density as the reference density),
- using equation (L.17) to express the associated reference wave number $\tilde{k}_0$ ($=\omega\sqrt{\rho_{\text{Local}}K_0}$) and the related operator $\tilde{\lambda}$ in terms of our usual reference wave number k_0 ($=\omega\sqrt{\rho_0K_0}$) as well as in the expansion parameters associated with the variable density PE (i.e., λ,γ),
- and then expanding in terms of these new expansion parameters.

This result applies in the half-space (or more generally, any finite-size area) where the density is (at least locally) constant, and only the reference compressibility changes to vary the sound speed. Also note that equation (L.14) ($H=\tilde{k}_0\sqrt{1+2\tilde{\lambda}/\tilde{k}_0}$) leads to an expansion in the nominal expansion parameter $2\tilde{\lambda}/\tilde{k}_0$, which has decent convergence

properties provided that the reference compressibility K_0 is greater than the local compressibility K, and the grazing angle is reasonably shallow. The nominal expansion parameter $2\tilde{\lambda}/\tilde{k}_0$ has embedded within it the key cancellation generated by taking the difference $\lambda - k_0\gamma$. The convergence properties related to this nominal expansion parameter are therefore much more indicative of the true convergence properties for PE expansion (generated by the FW transformation for the variable density problem) than are the convergence properties that apply when the nominal expansion parameter is $2\alpha\lambda/k_0$, (the expansion parameter that emerges most naturally from expression (L.10)).

This leaves us with the obvious question: why should we bother with the generator from equation (L.8)

$$H = \frac{k_0}{\alpha}\sqrt{1+\frac{2\alpha\lambda}{k_0}}$$

at all? This result is useful because:

- Its derivation is the most transparent and direct.
- The result is nicely compact and easy to work with.
  - It is useful as a mnemonic
  - When calculating the endpoint correction, this form very naturally generates the compact result

$$\chi = \sqrt{\frac{\alpha}{k_0}}\sqrt{H}\cdot A = \left(1+\frac{2\alpha\lambda}{k_0}\right)^{1/4}\cdot A\,.$$

For these reasons we will henceforth primarily use this form, being careful to use it correctly: i.e., to use it to generate an expansion in 2γ and λ. Both these parameters contribute equally to the power counting, and we must be careful not to "bust up" orders of $\lambda;\gamma$.

M Appendix: The boundary conditions for quasi-1st order deterministic variable density theory

In this appendix, we derive equation (5.16), the boundary conditions for deterministic quasi-1st order acoustic theory, where the density and compressibility jump at an interface. This calculation nicely illustrates many of the ideas developed in Section 5, and so it will be presented in great detail. We operate in standard 2-dimensional $x-z$ space. There are two regions labeled I and II separated by the rough surface $z = f(x)$. The density ρ and compressibility K are constant in the two regions, but both quantities

jump along the interface separating the two regions. The positive z-axis points from Region II into Region I. The starting point is the standard scalar parabolic equation

$$-i\frac{\partial \chi}{\partial x} = H\chi \tag{M.1}$$

where H is given by equation (5.15)

$$H = k_0 + \lambda - 2k_0\gamma - \frac{\ddot{\lambda}}{8k_0^2}. \tag{M.2}$$

From equation (5.4), we have the definitions

$$\begin{aligned}
\lambda &= \frac{\nabla_T\left(\frac{\rho_0}{\rho}\right)\nabla_T}{2k_0} - k_0\mu + k_0\gamma \\
\mu &\equiv \frac{1}{2}\left(1 - \frac{\mathrm{K}}{\mathrm{K}_0}\right) \\
\gamma &\equiv \frac{1}{2}\left(1 - \frac{\rho}{\rho_0}\right)
\end{aligned} \quad . \tag{M.3}$$

(In the 2-dimensional problem, $\nabla_T = \partial/\partial z$.) We also have

$$\begin{aligned}
\rho &= \rho_{II} - \delta\rho\cdot\Theta(z-f) & \delta\rho &= \rho_{II} - \rho_I \\
\gamma &= \gamma_{II} - \delta\gamma\cdot\Theta(z-f) \quad \text{where} & \delta\gamma &= \gamma_{II} - \gamma_I \\
\mu &= \mu_{II} - \delta\mu\cdot\Theta(z-f) & \delta\mu &= \mu_{II} - \mu_I
\end{aligned} .$$

(Note that these definitions are a little more general than the ones that are usually employed. The usual special case will be considered at the end of the calculation.)

We will evaluate equation (M.2), and the δ-function-bifurcation rules outlined in Section 5.2 will be used as needed to properly interpret the results. Then, the result will be substituted into the basic parabolic equation (M.1). To obtain the boundary conditions, a pair of infinitesimal transverse integrations of the type described in Subsection 3.3.3 will be applied to this equation.

Thus, begin by differentiating λ (as always, a dot means the downrange derivative $\partial/\partial x$):

$$\dot{\lambda} = \frac{-\rho_0\nabla_T\left(\frac{1}{\rho^2}\dot{\rho}\right)\nabla_T}{2k_0} - k_0\dot{\mu} + k_0\dot{\gamma}. \tag{M.4}$$

Now,

$$\dot{\rho} = -\delta\rho\left(-\dot{f}\right)\underbrace{\delta\left(z-f\right)}_{\frac{\delta^+}{2}+\frac{\delta^-}{2}} = \dot{f}\cdot\delta\rho\cdot\delta\left(z-f\right)$$

and similarly

$$\dot{\gamma} = \dot{f}\cdot\delta\gamma\cdot\delta\left(z-f\right) \quad ; \quad \dot{\mu} = \dot{f}\cdot\delta\mu\cdot\delta\left(z-f\right).$$

$\delta\left(z-f\right)$ of course bifurcates, but $\delta\rho$, $\delta\gamma$ and $\delta\mu$ are just old-fashioned constants, and in this context $\dot{f}$ might as well be. Bifurcation only becomes an issue when we multiply by another distribution, and so at this point the issue only affects the term in (M.4) that is proportional to $\delta\rho$. In this term, we have

$$\frac{\dot{\rho}}{\rho^2} = \dot{f}\delta\rho\left[\frac{\delta^+}{2\rho_I^2}+\frac{\delta^-}{2\rho_{II}^2}\right]$$

and so

$$\begin{aligned}\dot{\lambda} = \frac{-\rho_0\dot{f}\cdot\delta\rho}{2k_0\cdot 2}\nabla_T\left\{\left(\frac{\delta^+\left(z-f\right)}{\rho_I^2}+\frac{\delta^-\left(z-f\right)}{\rho_{II}^2}\right)\nabla_T\right\} \\ -k_0\cdot\delta\mu\cdot\dot{f}\underbrace{\delta\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}}+k_0\cdot\delta\gamma\cdot\dot{f}\underbrace{\delta\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}}\end{aligned}. \tag{M.5}$$

Taking one more downrange derivative:

$$\begin{aligned}\ddot{\lambda} &= \frac{-\rho_0\ddot{f}\cdot\delta\rho}{2k_0}\nabla_T\left\{\left(\frac{\delta^+\left(z-f\right)}{2\rho_I^2}+\frac{\delta^-\left(z-f\right)}{2\rho_{II}^2}\right)\nabla_T\right\} \\ &-\frac{\rho_0\dot{f}\cdot\delta\rho}{2k_0}\nabla_T\left\{\left(\frac{\left(-\dot{f}\right)\delta'^+\left(z-f\right)}{2\rho_I^2}+\frac{\left(-\dot{f}\right)\delta'^-\left(z-f\right)}{2\rho_{II}^2}\right)\nabla_T\right\} \\ &+\left(-k_0\cdot\delta\mu+k_0\cdot\delta\gamma\right)\dot{f}\left(-\dot{f}\right)\underbrace{\delta'\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}}+\left(-k_0\cdot\delta\mu+k_0\cdot\delta\gamma\right)\ddot{f}\underbrace{\delta\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}} \\ &= \frac{-\rho_0\ddot{f}\cdot\delta\rho}{2k_0}\nabla_T\left\{\left(\frac{\delta^+\left(z-f\right)}{2\rho_I^2}+\frac{\delta^-\left(z-f\right)}{2\rho_{II}^2}\right)\nabla_T\right\} \\ &+\frac{\rho_0\dot{f}^2\cdot\delta\rho}{2k_0}\nabla_T\left\{\left(\frac{\delta'^+\left(z-f\right)}{2\rho_I^2}+\frac{\delta'^-\left(z-f\right)}{2\rho_{II}^2}\right)\nabla_T\right\} \\ &+\left(k_0\cdot\delta\mu-k_0\cdot\delta\gamma\right)\dot{f}^2\underbrace{\delta'\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}}-\left(k_0\cdot\delta\mu-k_0\cdot\delta\gamma\right)\ddot{f}\underbrace{\delta\left(z-f\right)}_{\substack{\text{Will bifurcate}\\ \text{later}}}.\end{aligned} \tag{M.6}$$

Now consider $\ddot{\imath}\chi$. First note that bifurcation gives $\delta^{(n)\pm}\chi = \delta^{(n)\pm}\chi^{\pm}$. Then convert distributions times functions of the transverse coordinate z to distributions times "constants" with respect to z that depend only on $f(x)$ using equation (3.54) for $k=0$ or $k=1$ (the related footnote ll explicitly evaluates these two expressions):

$$\left(\frac{\delta^{+}}{2\rho_I^2}+\frac{\delta^{-}}{2\rho_{II}^2}\right)\nabla_T\chi(z)=\frac{\delta^{+}}{2\rho_I^2}\nabla_T\chi_I(z)+\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(z)$$

$$=\frac{\delta^{+}}{2\rho_I^2}\nabla_T\chi_I(f)+\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(f)$$

$$\frac{\delta'^{+}}{2\rho_I^2}\nabla_T\chi(z)=\frac{\delta'^{+}}{2\rho_I^2}\nabla_T\chi_I(z)=\frac{\delta'^{+}}{2\rho_I^2}\nabla_T\chi_I(f)-\frac{\delta^{+}}{2\rho_I^2}\nabla_T^2\chi_I(f)$$

$$\frac{\delta'^{-}}{2\rho_{II}^2}\nabla_T\chi(z)=\frac{\delta'^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(z)=\frac{\delta'^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(f)-\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T^2\chi_{II}(f).$$

Adding the last two equalities gives us

$$\left(\frac{\delta'^{+}}{2\rho_I^2}+\frac{\delta'^{-}}{2\rho_{II}^2}\right)\nabla_T\chi(z)=\frac{\delta'^{+}}{2\rho_I^2}\nabla_T\chi_I(f)+\frac{\delta'^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(f)$$

$$-\left(\frac{\delta^{+}}{2\rho_I^2}\nabla_T^2\chi_I(f)+\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T^2\chi_{II}(f)\right).$$

Similarly, we have

$$\left(\frac{\delta'^{+}}{2}+\frac{\delta'^{+}}{2}\right)\chi(z)=\frac{\delta'^{+}}{2}\chi_I(f)+\frac{\delta'^{-}}{2}\chi_{II}(f)$$

$$-\left(\frac{\delta^{+}}{2}\nabla_T\chi_I(f)+\frac{\delta^{-}}{2}\nabla_T\chi_{II}(f)\right).$$

Now, let us adopt the following shorthand notation:

$$\frac{\delta^{+}}{2\rho_I^2}\nabla_T\chi_I(f)+\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(f)=\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)$$

$$\frac{\delta'^{+}}{2\rho_I^2}\nabla_T\chi_I(f)+\frac{\delta'^{-}}{2\rho_{II}^2}\nabla_T\chi_{II}(f)=\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)$$

$$\frac{\delta^{+}}{2\rho_I^2}\nabla_T^2\chi_I(f)+\frac{\delta^{-}}{2\rho_{II}^2}\nabla_T^2\chi_{II}(f)=\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T^2\chi_{\pm}(f)$$

etc.

Using these results to evaluate equation (M.6), we have

$$
\begin{aligned}
\ddot{\lambda}\chi = &-\frac{\rho_0 \ddot{f}\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] \\
&+\frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] \\
&-\frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T^2\chi_{\pm}(f)\right] \\
&+(k_0\cdot\delta\mu - k_0\cdot\delta\gamma)\dot{f}^2\left[\frac{1}{2}\sum_{\pm}\delta'^{\pm}\chi_{\pm}(f)\right] \\
&-(k_0\cdot\delta\mu - k_0\cdot\delta\gamma)\dot{f}^2\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\nabla_T\chi_{\pm}(f)\right] \\
&-(k_0\cdot\delta\mu - k_0\cdot\delta\gamma)\ddot{f}\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\chi_{\pm}(f)\right].
\end{aligned}
\tag{M.7}
$$

In the first three terms to the right of the equals-sign (=), the only functions of the transverse coordinate z are the δ and δ'-functions, and so we can operate on these by the transverse derivative $\nabla_T = \partial/\partial z$. This gives us

$$
\begin{aligned}
-\frac{\rho_0 \ddot{f}\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] &\to -\frac{\rho_0 \ddot{f}\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] \\
\frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] &\to \frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\sum_{\pm}\frac{\delta''^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right] \\
-\frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\nabla_T\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}^2}\nabla_T^2\chi_{\pm}(f)\right] &\to -\frac{\rho_0 \dot{f}^2\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T^2\chi_{\pm}(f)\right]
\end{aligned}
\quad . \tag{M.8}
$$

Result (M.7) as modified by (M.8) will be substituted into the quasi-1st order parabolic equation for the right-hand traveling (i.e., downrange) field χ. This parabolic equation comes by combining (M.1) and (M.2) to form

$$
-i\frac{\partial\chi}{\partial x} = k_0\chi + \lambda\chi - 2k_0\gamma\chi - \frac{\ddot{\lambda}}{8k_0^2}\chi\,. \tag{M.9}
$$

As discussed in Section 3.3.4, we ignore the δ-function-like singularity associated with $\partial\chi/\partial x$ primarily because it is of higher order than concerns us here (it involves three downrange derivatives of λ, and so it is effectively a 4th-order term). Furthermore, this term is an artifact of our rather artificial quasi-1st order theory.

Since the lead order transverse derivative in λ is divided by $2k_0$, we multiply the wave equation (M.9) through by $2k_0$, leaving us with

$$0 = 2k_0\lambda\chi - \frac{\ddot{\lambda}}{4k_0}\chi + \left[\begin{array}{l}\text{terms that play no role in}\\ \text{the boundary value problem}\end{array}\right]. \tag{M.10}$$

From definition (M.3), we have

$$2k_0\lambda\chi = \nabla_T\cdot\left(\frac{\rho_0}{\rho}\right)\nabla_T\chi \underbrace{-2k_0^2\mu\chi + 2k_0^2\gamma\chi}_{\substack{\text{These terms are not}\\ \text{players in the boundary}\\ \text{value problem}}}. \tag{M.11}$$

Next, multiply (M.7) as modified by (M.8) by $-1/(4k_0)$, and substitute the result as well as (M.11) into (M.10):

$$\begin{aligned}0 = {} & \nabla_T\left[\left(\frac{\rho_0}{\rho}\right)\nabla_T\chi\right] + \frac{\rho_0\ddot{f}\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right]\\ & - \frac{\rho_0\dot{f}^2\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta''^{\pm}}{\rho_{\pm}^2}\nabla_T\chi_{\pm}(f)\right]\\ & + \frac{\rho_0\dot{f}^2\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\nabla_T^2\chi_{\pm}(f)\right]\\ & - \frac{1}{4\cancel{k_0}}\left(\cancel{k_0}\cdot\delta\mu - \cancel{k_0}\cdot\delta\gamma\right)\dot{f}^2\left[\frac{1}{2}\sum_{\pm}\delta'^{\pm}\chi_{\pm}(f)\right]\\ & + \frac{1}{4\cancel{k_0}}\left(\cancel{k_0}\cdot\delta\mu - \cancel{k_0}\cdot\delta\gamma\right)\dot{f}^2\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\nabla_T\chi_{\pm}(f)\right]\\ & + \frac{1}{4\cancel{k_0}}\left(\cancel{k_0}\cdot\delta\mu - \cancel{k_0}\cdot\delta\gamma\right)\ddot{f}\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\chi_{\pm}(f)\right]\\ & + \left[\begin{array}{l}\text{terms that play no role in}\\ \text{the boundary value problem}\end{array}\right].\end{aligned} \tag{M.12}$$

Now follow the transverse-integration procedure described in general terms throughout Section 3.3.3. For the case directly analogous to the present situation use both single integration as described in equation (3.56) and double integration described in the equation immediately preceding it. The single infinitesimal integration $\int_{f-\varepsilon}^{f+\varepsilon} dz\cdots$ of equation (M.12) gives us

$$0=\frac{\rho_0}{\rho_I}\nabla_T\chi_I-\frac{\rho_0}{\rho_{II}}\nabla_T\chi_{II}+\frac{1}{4}(\delta\mu-\delta\gamma)\dot{f}^2\underbrace{\left(\frac{\nabla_T\chi_I(f)+\nabla_T\chi_{II}(f)}{2}\right)}_{\overline{\nabla_T\chi}|_f}$$
$$+\frac{1}{4}(\delta\mu-\delta\gamma)\ddot{f}\underbrace{\left(\frac{\chi_I(f)+\chi_{II}(f)}{2}\right)}_{\overline{\chi}|_f}. \qquad \text{(M.13)}$$

Now, let us perform the double integral $\int_{f-\varepsilon}^{f+\varepsilon}dz'\int_{-\infty}^{z'}dz\cdots$. We do so in slightly different form: as a sequence of an indefinite integration followed by a second definite integration $\int_{f-\varepsilon}^{f+\varepsilon}dz\cdots$. First, perform the indefinite integration and then multiply by ρ/ρ_0:

$$\begin{aligned}0=&\nabla_T\chi+\frac{\rho_0\ddot{f}\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}}\nabla_T\chi_{\pm}(f)\right]\\&-\frac{\rho_0\dot{f}^2\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}}\nabla_T\chi_{\pm}(f)\right]\\&+\frac{\rho_0\dot{f}^2\cdot\delta\rho}{8k_0^2}\left[\frac{1}{2}\sum_{\pm}\frac{\delta^{\pm}}{\rho_{\pm}}\nabla_T^2\chi_{\pm}(f)\right]\\&-\frac{1}{4}(\delta\mu-\delta\gamma)\dot{f}^2\left[\frac{1}{2\rho_0}\sum_{\pm}\delta^{\pm}\rho_{\pm}\chi_{\pm}(f)\right]\\&+\frac{1}{4}(\delta\mu-\delta\gamma)\dot{f}^2\left[\frac{1}{2\rho_0}\sum_{\pm}\Theta^{\pm}\rho_{\pm}\nabla_T\chi_{\pm}(f)\right]\\&+\frac{1}{4}(\delta\mu-\delta\gamma)\ddot{f}\left[\frac{1}{2\rho_0}\sum_{\pm}\Theta^{\pm}\rho_{\pm}\chi_{\pm}(f)\right].\end{aligned}$$

and now the infinitesimal integral $\int_{f-\varepsilon}^{f+\varepsilon}dz\cdots$ gives us[dddd]:

[dddd] Note the term in $\ddot{\lambda}$ that was proportional to δ'' did not contribute to the boundary conditions for quasi-1st order theory. This is because this $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$ theory is a bit of a hybrid. Once we introduce an $\mathrm{O}\left(\lambda^2\right)$ term (let alone going to true 3rd order theory with the λ^3-term), then the term proportional to δ'' will contribute. Historically, contemplating this term was the catalyst that made the author consider the

$$0 = \chi_I - \chi_{II} + \frac{\delta\rho}{8k_0^2}\left(\ddot{f}\overline{\left(\frac{\nabla_T\chi}{\rho}\right)}\Big|_f + \dot{f}^2\overline{\left(\frac{\nabla_T^2\chi}{\rho}\right)}\Big|_f \right) - \frac{1}{4}(\delta\mu - \delta\gamma)\,\dot{f}^2\frac{\overline{(\rho\chi)}\big|_f}{\rho_0} \quad \text{(M.14)}$$

Equations (M.13) and (M.14) gives us the boundary conditions on χ:

$$\begin{aligned} \chi_{II} &= \chi_I + \frac{\delta\rho}{8k_0^2}\left(\ddot{f}\overline{\left(\frac{\nabla_T\chi}{\rho}\right)}\Big|_f + \dot{f}^2\overline{\left(\frac{\nabla_T^2\chi}{\rho}\right)}\Big|_f \right) - \frac{\dot{f}^2}{4\rho_0}(\delta\mu - \delta\gamma)\overline{(\rho\chi)}\Big|_f \\ \frac{1}{\rho_{II}}\nabla_T\chi_{II} &= \frac{1}{\rho_I}\nabla_T\chi_I + \frac{1}{4\rho_0}(\delta\mu - \delta\gamma)\left[\dot{f}^2\overline{\nabla_T\chi}\Big|_f + \ddot{f}\,\overline{\chi}\Big|_f \right] \end{aligned} \quad \text{(M.15)}$$

Now let us make the standard choices for the reference values of the density and compressibility. This follows Figure 5.1 and the related discussion in Subsection 5.3.2. Specifically, in order to guarantee that the parabolic equation expansion parameters μ and γ be less than 1, we choose for the maximum values for the reference compressibility and density. In our prototypical example where Region I is the ocean water column and Region II is the sediment in the ocean bottom, the compressibility in Region I is the largest and the density in Region II is the bigger value. Thus, the reference compressibility is $K_0 = K_I$ and the reference density is $\rho_0 = \rho_{II}$. This gives us

$$\begin{aligned} \mu_I &= \frac{1}{2}\left(1 - \frac{K_I}{K_I}\right) = 0 & k_0 &= \frac{\omega}{c_0} = \omega\sqrt{\rho_0 K_0} = \omega\sqrt{\rho_{II}K_I} \\ \mu_{II} &= \frac{1}{2}\left(1 - \frac{K_{II}}{K_I}\right) = -\frac{1}{2}\frac{\delta K}{K_I} & \delta\mu &= \mu_{II} - \mu_I = -\frac{1}{2}\frac{\delta K}{K_I} \\ \gamma_I &= \frac{1}{2}\left(1 - \frac{\rho_I}{\rho_{II}}\right) = \frac{1}{2}\frac{\delta\rho}{\rho_{II}} & \delta\gamma &= \gamma_{II} - \gamma_I = -\frac{1}{2}\frac{\delta\rho}{\rho_{II}} \\ \gamma_{II} &= \frac{1}{2}\left(1 - \frac{\rho_{II}}{\rho_{II}}\right) = 0 & \delta\mu - \delta\gamma &= -\frac{1}{2}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right) \end{aligned}$$

and so the boundary conditions (M.15) become

$$\begin{aligned} \chi_{II} &= \chi_I + \frac{\dot{f}^2}{8\rho_{II}}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right)\overline{(\rho\chi)}\Big|_f + \frac{\delta\rho}{8k_0^2}\left(\ddot{f}\overline{\left(\frac{\nabla_T\chi}{\rho}\right)}\Big|_f + \dot{f}^2\overline{\left(\frac{\nabla_T^2\chi}{\rho}\right)}\Big|_f \right) \\ \frac{1}{\rho_{II}}\nabla_T\chi_{II} &= \frac{1}{\rho_I}\nabla_T\chi_I - \frac{1}{8\rho_{II}}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right)\left[\dot{f}^2\overline{\nabla_T\chi}\Big|_f + \ddot{f}\,\overline{\chi}\Big|_f \right] \end{aligned} \quad \text{(M.16)}$$

---

issues of migrating boundary conditions (Section 4.2.2) and thus shortly thereafter, the key result of the whole effort: Bragg-scale vorticity (Section 6).

This is just equation (5.16), the boundary conditions for deterministic quasi-1st order acoustic theory, where the density and compressibility jump at an interface.

N Appendix: A closer look at the higher-order range-dependent terms in the PE

As frequently discussed above, the Foldy-Wouthuysen procedure generates a Hamiltonian that includes a unique series of terms explicitly associated with the range dependence. It was noted in Section 4.4 that the members of this series of terms that are proportional to $\ddot{\lambda}$ correspond to the phenomenon of "vacuum polarization" known from quantum mechanics (because this type of term involves virtual particle pairs). The lowest-order member of this class of terms is the 3rd-order term $-\ddot{\lambda}/\left(8k_0^2\right)$. It was just evaluated in Appendix M (and the results were summarized in Subsection 5.3.2). Examining equation (J.24) (or equivalently (5.9)), we see that there are also two nominally 4th-order terms that contain $\ddot{\lambda}$:

$$\frac{3\left\{\lambda,\ddot{\lambda}\right\}}{16k_0^4} \quad \text{and} \quad -4\gamma\frac{\ddot{\lambda}}{8k_0^3}.$$

In Section N.1, we estimate the magnitude of these terms for typical values of the environmental parameters, and verify that they are indeed getting smaller. The form of the boundary conditions that arise from the $-(4\gamma)\ddot{\lambda}/\left(8k_0^3\right)$ term suggests an infinite series encountered previously. In Section N.2 this infinite series is evaluated in closed form, and the appropriate limit is taken to examine the Dirichlet ($\chi = 0$) and Neumann ($\partial\chi/\partial n = 0$ for the full wave problem, but this changes a little bit for the parabolic equation) boundary conditions. The Neumann boundary conditions for the parabolic equation imply the existence of curvature-induced boundary waves.

N.1 An estimate of the magnitude of the 4th-order terms in the "vacuum polarization" series

To help us develop a feel for the nature of the convergence of the series of terms newly predicted by the Foldy-Wouthuysen procedure, this section examines the magnitude of the 4th order terms relative to that of the 3rd order term. For the sake of this comparison, we take out a common factor in the relevant terms (taken from equation (J.24) (or equivalently (5.9)):

$$-\frac{1}{8k_0^3}\left(\ddot{\lambda}-\frac{3}{2k_0}\left\{\lambda,\ddot{\lambda}\right\}+4\gamma\cdot\ddot{\lambda}\right). \tag{N.1}$$

Now, only the terms in the parenthesis need to be compared. To within a constant, these terms appear in a Hamiltonian, and so it is of course always understood that they are operating on the wave function χ.

N.1.1 An estimate of the magnitude of the $\{\lambda,\ddot{\lambda}\}$-term

Recall that $\{\lambda,\ddot{\lambda}\}/k_0 = (\lambda/k_0)\cdot\ddot{\lambda} + \ddot{\lambda}\cdot(\lambda/k_0)$. Let us evaluate $(\lambda/k_0)\cdot\ddot{\lambda}\chi$ first. We have $\ddot{\lambda}$ from equation (M.7). All terms contain bifurcated $\delta^{(n)}$-functions ($n \geq 0$). Thus, λ/k_0 will be evaluated in the half-spaces. From the definition (5.4) and equivalently (M.3), λ/k_0 in the half-spaces is the sum of the operator

$$\frac{1}{2k_0^2}\frac{\rho_0}{\rho}\nabla_T^2 = \frac{1}{2\omega\cancel{\rho_0}K_0}\frac{\cancel{\rho_0}}{\rho}\nabla_T^2 = \frac{1}{2\omega\rho K}\frac{K}{K_0}\nabla_T^2 = \frac{K}{2K_0}\frac{\nabla_T^2}{k^2} \tag{N.2}$$

and the operator $-\mu+\gamma$. From equation (M.7), the former operating on $\ddot{\lambda}\chi$ generates $\delta^{(n)}$ functions where now $n \geq 2$. Now, $\delta^{(2)} = \delta''$ integrates to zero for quasi-1st order theory (since λ also generates the leading order derivative ∇_T^2), so in this context we can forget about all these terms. This leaves us with $-\mu+\gamma$ multiplying $\ddot{\lambda}\chi$:

$$(\lambda/k_0)\cdot\ddot{\lambda}\chi \to (-\mu+\gamma)\ddot{\lambda}\chi .$$

Since $\ddot{\lambda}$ contains only bifurcating $\delta^{(n)}$-functions, the factor $(-\mu+\gamma)$ operators just like a constant, so we can commute $\ddot{\lambda}$ and $(-\mu+\gamma)$ to obtain:

$$\frac{\lambda}{k_0}\ddot{\lambda}\chi \to \ddot{\lambda}(-\mu+\gamma)\chi . \tag{N.3}$$

Now, let us flip things around and consider $\ddot{\lambda}(\lambda/k_0)\cdot\chi$. Again we pick up two kinds of terms:

$$\begin{aligned}\ddot{\lambda}\frac{\lambda}{k_0}\cdot\chi &= \ddot{\lambda}\left[\frac{K}{2K_0}\frac{\nabla_T^2}{k^2} - \mu + \gamma\right]\chi \\ &= \ddot{\lambda}\left(\frac{K}{2K_0}\frac{\nabla_T^2}{k^2}\chi\right) + \ddot{\lambda}(-\mu+\gamma)\chi\end{aligned} . \tag{N.4}$$

Combining results (N.3) and (N.4), we have

$$\frac{1}{k_0}\{\lambda,\ddot{\lambda}\} = \ddot{\lambda}\left[\left(\frac{K}{2K_0}\frac{\nabla_T^2}{k^2}\chi\right) + 2(-\mu+\gamma)\chi\right]. \tag{N.5}$$

Note that the factor of 2 in front of $(-\mu+\gamma)\chi$ occurs because both halves of the commutator contribute to this term. Equation (N.5) simply gives us all the terms in equation (M.7) (as modified by equation (M.8)) with

$$\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^2}{k_\pm^2}\chi_\pm\right)-2(\mu_\pm-\gamma_\pm)\chi_\pm$$

replacing $\chi_\pm$[eeee]:

$$\begin{aligned}\frac{1}{k_0}\{\lambda,\ddot{\lambda}\}=&-\frac{\rho_0\ddot{f}\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\sum_\pm\frac{\delta'^\pm}{\rho_\pm^2}\left[\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^3\chi_\pm\big|_f}{k_\pm^2}\right)-2(\mu_\pm-\gamma_\pm)\nabla_T\chi_\pm\big|_f\right]\right]\\&-\frac{\rho_0\dot{f}^2\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\sum_\pm\frac{\delta'^\pm}{\rho_\pm^2}\left[\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^4\chi_\pm\big|_f}{k_\pm^2}\right)-2(\mu_\pm-\gamma_\pm)\nabla_T^2\chi_\pm\big|_f\right]\right]\\&+k_0(\delta\mu-\delta\gamma)\dot{f}^2\left[\frac{1}{2}\sum_\pm\delta'^\pm\left[\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^2\chi_\pm\big|_f}{k_\pm^2}\right)-2(\mu_\pm-\gamma_\pm)\chi_\pm\big|_f\right]\right]\\&-k_0(\delta\mu-\delta\gamma)\dot{f}^2\left[\frac{1}{2}\sum_\pm\delta^\pm\left[\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^3\chi_\pm\big|_f}{k_\pm^2}\right)-2(\mu_\pm-\gamma_\pm)\nabla_T\chi_\pm\big|_f\right]\right]\\&-k_0(\delta\mu-\delta\gamma)\ddot{f}\left[\frac{1}{2}\sum_\pm\delta^\pm\left[\left(\frac{K_\pm}{2K_0}\frac{\nabla_T^2\chi_\pm\big|_f}{k_\pm^2}\right)-2(\mu_\pm-\gamma_\pm)\chi_\pm\big|_f\right]\right]\\&+\left[\begin{array}{l}\text{Terms proportional to } \delta^{(n)}\,(n\ge 2)\text{ which}\\ \text{do not contribute to quasi-1st theory}\end{array}\right].\end{aligned}\qquad\text{(N.6)}$$

Note that in quasi-1st order theory, we throw out the terms proportional to δ''.

Equation (N.1) tells us that to compare the 4th-order $\frac{1}{k_0}\{\lambda,\ddot{\lambda}\}$-contribution with that from the 3rd-order term $\ddot{\lambda}$, we will need to multiply equation (N.6) by $-\frac{1}{2}$. Now we find that equation (N.6) contains new 4th-order terms that relate to corresponding ones in the 3rd-order contribution in one of two basic ways:

[eeee] Note that when differential operators are to the right of δ-functions, we must of course first take the derivatives to obtain, for example, $\nabla_T^n\chi(z)$, and only then convert from a function of z to a constant that is nominally evaluated at $z=f$.

- the operator $\left([-3K_{\pm}]/[4K_0]\right)\left(\nabla_T^2/k_{\pm}^2\right)$ has been inserted to operate on the wave function $\chi_{\pm}$, or
- there is an extra factor $3\left(\mu_{\pm}-\gamma_{\pm}\right)$ (this factor simply multiplies the wave function $\chi_{\pm}$ or its transverse derivative $\nabla_T^n\chi_{\pm}$ where $n=1,2$).

Now, let us pick credible parameters for the ocean bottom. We will use values for sand, or sandy mud. Then

$$\begin{aligned} K_{\text{water}} &= K_I = K_0 = 3K_{II} = 3K_{\text{sand}} \\ 2\rho_{\text{water}} &= 2\rho_I = \rho_0 = \rho_{II} = \rho_{\text{sand}} \end{aligned} \tag{N.7}$$

If we set $c_{\text{water}} = 1500\,\text{m/s}$, then the ratios (N.7) correspond to $c_{\text{sand}} \approx 1840\,\text{m/s}$. The ratios (N.7) also give us

$$\begin{aligned} &\frac{-3K_{\pm}}{4K_0} = \begin{cases} -\tfrac{3}{4} & \text{in Region } I \\ -\tfrac{1}{4} & \text{in Region } II \end{cases} \\ &\mu_- = \mu_{II} = \frac{1}{2}\left(1-\frac{K_{II}}{K_0}\right) = \frac{1}{2}\left(1-\frac{K_{II}}{K_I}\right) = \frac{1}{2}\left(1-\frac{K_{II}}{3K_{II}}\right) = \frac{1}{6}. \\ &\gamma_+ = \gamma_I = \frac{1}{2}\left(1-\frac{\rho_I}{\rho_0}\right) = \frac{1}{2}\left(1-\frac{\rho_I}{\rho_{II}}\right) = \frac{1}{2}\left(1-\frac{\rho_I}{2\rho_I}\right) = \frac{1}{4} \\ &\mu_+ = \mu_I = 0 \quad ; \quad \gamma_- = \gamma_{II} = 0 \end{aligned} \tag{N.8}$$

Now, consider the first type of term listed above. In typical problem where the parabolic equation is used, there is long-range propagation down a duct. If we decompose the wave $\chi_{\pm}$ traveling down the duct into modes, we find that the shallow grazing angle modes dominate downrange propagation, and the assumptions behind the low-order parabolic equation are easily satisfied. Modes with a grazing angle on the order of $10\,\text{deg}$ is typical, and for such modes, $\nabla_T^2/k_{\pm}^2$ brings down the sine of the grazing angle squared: $\sin^2\theta_{\text{grazing}} \approx \sin^2(10\,\text{deg}) \approx 0.03$. Multiplying by the factor given by the first line of equation (N.8), we find that in both half-spaces, terms of the first sort will provide a correction on the order of 1%-2%. This is negligible, and we are very safe in ignoring these terms.

Next, consider terms of the second type listed above. We have

$$\begin{aligned} &\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_{\pm}^2}\left[3\left(\mu_{\pm}-\gamma_{\pm}\right)\nabla_T^n\chi_{\pm}\Big|_f\right] = \frac{3}{2}\left(\frac{\delta'^{+}}{\rho_+^2}\left[-\gamma_+\nabla_T^n\chi_+\Big|_f\right]+\frac{\delta'^{-}}{\rho_-^2}\left[\mu_-\nabla_T^n\chi_-\Big|_f\right]\right) \\ &\frac{1}{2}\sum_{\pm}\delta^{(m)\pm}\left[3\left(\mu_{\pm}-\gamma_{\pm}\right)\nabla_T^n\chi_{\pm}\Big|_f\right] = \frac{3}{2}\left(\delta^{(m)+}\left[-\gamma_+\nabla_T^n\chi_+\Big|_f\right]+\delta^{(m)-}\left[\mu_-\nabla_T^n\chi_-\Big|_f\right]\right) \end{aligned} \tag{N.9}$$

(Equality (N.6) contains a subset of all possible permutations on $n=0,1,2; m=0,1$.) We will throw out terms that have an overall power of γ^3,μ^3 (i.e., a power of γ^2,μ^2 relative

to the corresponding term in 3rd-order ($\ddot{\lambda}$) theory). This is completely acceptable, because these terms also contain two downrange derivatives and so they are 5th order by our power counting. Recall that we have already thrown out all terms of this order. Now, note that if $\gamma,\mu \to 0$, then χ, $\nabla_T\chi$ and $\nabla_T^2\chi$ are all continuous. Thus,

$$\begin{aligned}\chi_I &= \chi_{II} + \mathrm{O}(\gamma,\mu)\\ \nabla_T\chi_I &= \nabla_T\chi_{II} + \mathrm{O}(\gamma,\mu)\\ \nabla_T^2\chi_I &= \nabla_T^2\chi_{II} + \mathrm{O}(\gamma,\mu)\end{aligned}. \qquad \text{(N.10)}$$

We also have, $\rho_I = \rho_{II} + \mathrm{O}(\gamma)$. This allows us to make the substitution

$$\begin{aligned}\frac{\nabla_T^n\chi_\pm\big|_f}{\rho_\pm^2} &= \overline{\left[\frac{\nabla_T^n\chi\big|_f}{\rho^2}\right]} + \mathrm{O}(\gamma,\mu)\\ \nabla_T^n\chi_\pm\big|_f &= \overline{\nabla_T^n\chi\big|_f} + \mathrm{O}(\gamma,\mu)\end{aligned},$$

and pull these factors out of (N.9). Also note that $\delta^-\mu_- - \delta^+\gamma_+$ integrates just like $(\mu_- - \gamma_+)\delta$, and so we can make this replacement as well (cf. the discussions a little below equation (K.18) and surrounding (K.21)). Thus, we can collapse the bifurcation and pull out the common factors to get

$$\begin{aligned}\frac{3}{2}\left(\frac{\delta'^+}{\rho_+^2}\left[-\gamma_+\nabla_T^n\chi_+\big|_f\right] + \frac{\delta'^-}{\rho_-^2}\left[\mu_-\nabla_T^n\chi_-\big|_f\right]\right) &\to \frac{3}{2}\delta'\overline{\left[\frac{\nabla_T^n\chi\big|_f}{\rho^2}\right]}(\mu_- - \gamma_+)\\ \frac{3}{2}\left(\delta^{(m)+}\left[-\gamma_+\nabla_T^n\chi_+\big|_f\right] + \delta^{(m)-}\left[\mu_-\nabla_T^n\chi_-\big|_f\right]\right) &\to \frac{3}{2}\delta^{(m)}\overline{\left[\nabla_T^n\chi\big|_f\right]}(\mu_- - \gamma_+)\end{aligned}.$$

Where before we had $\overline{\left[\nabla_T^n\chi\big|_f/\rho^2\right]}$ or $\overline{\nabla_T^n\chi\big|_f}$, we now have

$$\begin{aligned}\frac{3}{2}(\mu_- - \gamma_+)\overline{\left[\frac{\nabla_T^n\chi\big|_f}{\rho^2}\right]}\\ \frac{3}{2}(\mu_- - \gamma_+)\overline{\left[\nabla_T^n\chi\big|_f\right]}\end{aligned}.$$

In other words, the 4th order contribution is picking up an extra factor $\frac{3}{2}(\mu_- - \gamma_+)$ relative to the comparable 3rd-order term. Now, from equation (N.8), we have

$$\frac{3}{2}(\mu_- - \gamma_+) = -\frac{1}{8}$$

or a 12.5% correction. This is not too bad.

Now, let us perform a similar analysis on the term proportional to $4\gamma\cdot\ddot{\lambda}$.

N.1.2 An estimate of the magnitude of the $\gamma\cdot\ddot{\lambda}$-term

Next, let us estimate the magnitude of the term proportional to $4\gamma\cdot\ddot{\lambda}$. Again using equation equation (M.7) (as modified by equation (M.8)) to substitute for $\ddot{\lambda}$, we have (with $\gamma^{-}=\gamma_{II}=0$)

$$\begin{aligned}
4\gamma\ddot{\lambda}\chi = &-\frac{\rho_0\ddot{f}\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\frac{\delta'^{+}}{\rho_+^2}(4\gamma_+)\nabla_T\chi_+(f)\right]\\
&\cancel{+\frac{\rho_0\dot{f}^2\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\frac{\delta''^{+}}{\rho_+^2}(4\gamma_+)\nabla_T\chi_+(f)\right]}\\
&-\frac{\rho_0\dot{f}^2\cdot\delta\rho}{2k_0}\left[\frac{1}{2}\frac{\delta'^{+}}{\rho_+^2}(4\gamma_+)\nabla_T^2\chi_+(f)\right]\\
&+(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\dot{f}^2\left[\frac{1}{2}\delta'^{+}(4\gamma_+)\chi_+(f)\right]\\
&-(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\dot{f}^2\left[\frac{1}{2}\delta^{+}(4\gamma_+)\nabla_T\chi_+(f)\right]\\
&-(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\ddot{f}\left[\frac{1}{2}\delta^{+}(4\gamma_+)\chi_+(f)\right].
\end{aligned}\tag{N.11}$$

Note that the term proportional to δ'' will not contribute to quasi-1st order theory, and so we again throw it out. Also once again throwing out terms that have an overall power of γ^3,μ^3 (and are hence 5th order by our power counting since these terms also contain two downrange derivatives), we can use equation (N.10) (and $\rho_I=\rho_{II}+\mathrm{O}(\gamma)$) to get

$$\begin{aligned}
4\gamma\ddot{\lambda}\chi = &-\frac{\rho_0\ddot{f}\cdot\delta\rho}{2k_0}(2\gamma_+)\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_\pm^2}\nabla_T\chi_\pm(f)\right]+\cancel{\{\delta''\text{ term}\}}\\
&-\frac{\rho_0\dot{f}^2\cdot\delta\rho}{2k_0}(2\gamma_+)\left[\frac{1}{2}\sum_{\pm}\frac{\delta'^{\pm}}{\rho_\pm^2}\nabla_T^2\chi_\pm(f)\right]\\
&+(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\dot{f}^2(2\gamma_+)\left[\frac{1}{2}\sum_{\pm}\delta'^{\pm}\chi_\pm(f)\right]\\
&-(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\dot{f}^2(2\gamma_+)\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\nabla_T\chi_\pm(f)\right]\\
&-(k_0\cdot\delta\mu-k_0\cdot\delta\gamma)\ddot{f}(2\gamma_+)\left[\frac{1}{2}\sum_{\pm}\delta^{\pm}\chi_\pm(f)\right].\\
=&\,2\gamma_+\ddot{\lambda}
\end{aligned}$$

With $\gamma_+ = 1/4$ (from equation (N.8)), this is a 50% correction. The terms are getting smaller, but this is a pretty substantial correction. In many practical instances, it may prove necessary to use higher-order theory to correctly evaluate this term, so in Section N.2 we will attempt to extrapolate the result to infinite orders, and examine its implications.

N.2 Extension to infinite orders and the implications for the Dirichlet and Neumann Boundary Conditions

This section provides a preliminary survey of one of the possibilities of the new formalism, and so we will allow ourselves to use mathematical reasoning that is a little bit looser than that generally employed elsewhere in this study.

As in Section N.1.2, we have

$$\gamma \to \begin{cases} \gamma_I = \dfrac{1}{2}\dfrac{\rho_{II} - \rho_I}{\rho_{II}} \\ \gamma_{II} = 0 \end{cases} \quad . \qquad \text{(N.12)}$$
$$\mu \to \begin{cases} \mu_I = 0 \\ \mu_{II} = \dfrac{1}{2}\dfrac{K_I - K_{II}}{K_I} \end{cases}$$

Under these circumstances, we have the sequence of terms:

$$\left(1 + 2\gamma_+\right)\frac{-\ddot{\lambda}}{8k_0^3}, \qquad \text{(N.13)}$$

which contains the very suggestive factor $\left(1 + 2\gamma_+\right)$. This looks like the beginning of the familiar series (e.g., see equation (5.13))

$$1 + (2\gamma) + (2\gamma)^2 + (2\gamma)^3 + (2\gamma)^4 \cdots = \frac{1}{1 - 2\gamma} = \frac{1}{1 - 1 + \rho_0/\rho} = \frac{\rho_0}{\rho}.$$

With $\gamma = \gamma_+$, we have $\rho_0 = \rho_{II}$ and $\rho = \rho_I$. All this suggests that at infinite order, the series beginning with (N.13) will converge to

$$-\frac{\ddot{\lambda}}{8k_0^3}\frac{\rho_{II}}{\rho_I}. \qquad \text{(N.14)}$$

In quasi-1st order theory, the lead derivative is generated by λ/k_0. From equation (N.2), we can write the term responsible for the lead derivative as

$$\frac{\nabla_T \frac{\rho_0}{\rho} \nabla_T}{2 \underbrace{k_0^2}_{\omega K_0 \rho_0}} = \frac{\nabla_T \frac{1}{\rho} \nabla_T}{2\omega K_0}$$

which is independent of ρ_0, and so it is the same as the corresponding ∞-order in γ operator. Thus, it is consistent to generate boundary conditions by pairing this differential operator with the (also ∞-order in γ) boundary-condition-generating term (N.14). Doing so effectively leads us to take the boundary conditions in equation (M.16), identify the terms that are associated with $\ddot{\lambda}$ by noting that they are the ones proportional to $\ddot{f}$ and $\dot{f}^2$, and multiplying these terms by ρ_{II}/ρ_I. This gives us

$$\begin{aligned} \chi_{II} &= \chi_I + \frac{\dot{f}^2}{8\rho_I}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right)\overline{(\rho\chi)}\Big|_f + \frac{\delta\rho}{8k_I^2}\left(\ddot{f}\overline{\left(\frac{\nabla_T\chi}{\rho}\right)}\Big|_f + \dot{f}^2\overline{\left(\frac{\nabla_T^2\chi}{\rho}\right)}\Big|_f\right), \\ \frac{1}{\rho_{II}}\nabla_T\chi_{II} &= \frac{1}{\rho_I}\nabla_T\chi_I - \frac{1}{8\rho_I}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right)\left[\dot{f}^2\,\overline{\nabla_T\chi}\Big|_f + \ddot{f}\,\overline{\chi}\Big|_f\right] \end{aligned} \qquad \text{(N.15)}$$

where we have used $k_0^2 \cdot {}^{\rho_I}\!/_{\rho_{II}} = \omega K_I \rho_{II} \cdot {}^{\rho_I}\!/_{\rho_{II}} = \omega K_I \rho_I = k_I^2$. To get the Neumann and Dirichlet boundary conditions, we will let both $\rho_{II} \gg \rho_I$ and $K_{II} \ll K_I$, and look at this problem from the point of view of the two different half-spaces.

To get the Neumann boundary conditions, use the second boundary condition in equation (N.15) as viewed from the point of view of the field in Region I. Thus, set $\rho_{II} \to \infty$ and $K_{II} \to 0$. Taking these limits in equation (N.12) gives us

$$\frac{\delta K}{K_I} = \frac{K_{II} - K_I}{K_I} \cong -1 \quad ; \quad \frac{\delta\rho}{\rho_{II}} = \frac{\rho_{II} - \rho_I}{\rho_{II}} \simeq 1 .$$

Now the lower boundary condition in (N.15) becomes

$$\frac{1}{\rho_{II}}\nabla_T\chi_{II} = \frac{1}{\rho_I}\nabla_T\chi_I + \frac{1}{4\rho_I}\left[\dot{f}^2\,\overline{\nabla_T\chi}\Big|_f + \ddot{f}\,\overline{\chi}\Big|_f\right]. \qquad \text{(N.16)}$$

Since c_{II} is finite ($\rho_{II} \to \infty$ and $K_{II} \to 0$ roughly cancel), k_{II} is finite, and so

$$\frac{\nabla_T\chi_{II}}{\rho_{II}} \sim \frac{k_{II} \cdot \text{field amplitude}}{\rho_{II}} \to 0 .$$

Since ρ_I is not large, $\nabla_T\chi_I$ must be zero to $\mathrm{O}\left(\ddot{f}, \dot{f}^2\right)$. Also, from the first boundary condition, $\overline{\chi} = \chi_I + \mathrm{O}\left(\ddot{f}, \dot{f}^2\right)$. Multiplying through by ρ_I, this leaves us with

$$0 = \nabla_T\chi_I + \frac{1}{4}\left[\dot{f}^2\nabla_T\chi_{II} + \ddot{f}\chi_I\right]. \qquad \text{(N.17)}$$

If we make one more rather sensible approximation, we can further simplify equation (N.17). Taking the air-water interface as a prototype (Region I is now air and Region II is the water), we note that $c_{\text{air}} \approx 300\,\text{m/s}$ and as usual $c_{\text{water}} = 1500\,\text{m/s}$. Conversely, we could go from water (this time Region I) to a medium where sound speed is much greater than water's – for example, rock (Region II). Generalizing, we note that c_{II} is typically pretty large in the denser medium (though not as much so as ρ itself). Furthermore, since the wave number is given by $k = \omega/c$, $c_I < c_{II}$ also implies that $k_I > k_{II}$. Now, let us use this insight to examine the term in (N.17) proportional to $\nabla_T \chi_{II}$. By Fourier decomposing χ_{II}, we see that ∇_T roughly brings down a

$$ik_{IIz} \sim i\sqrt{k_{II}^2 - k_I^2 \cos^2\left(\theta_{I;\,\text{grazing}}\right)} \approx -k_I .$$

We can typically only take the branch that decays, so $\nabla_T \chi_{II}$ is not at a phase minimum as is $\nabla_T \chi_I$, and thus $\dot{f}^2 \nabla_T \chi_{II} \approx \dot{f}^2 k_I \chi_{II} = \dot{f}^2 k_I \chi_I$. Also note that $\ddot{f} \sim 1/R$, where R is the radius of curvature of the interface. Let us now compare the two terms in (N.17): $\dot{f}^2 \nabla_T \chi_{II}$ and $\ddot{f}\chi_I$. This amounts to comparing $\dot{f}^2 k_I$ and $1/R$, or equivalently $\dot{f}^2$ and $1/(k_I R)$ [ffff]. Now, keeping the first order in the radius of curvature $\mathrm{O}\left(1/(k_I R)\right)$ and dropping the 2nd order in the slope ($\mathrm{O}\left(\dot{f}^2\right)$) is exactly the kind of approximation that we make when we choose to model the scattering amplitude using the small slope approximation rather than the composite model (Reference [73], Section II). This is often a reasonable thing to do, and we do it here. Thus, the $\mathrm{O}\left(\dot{f}^2\right)$ term in equation (N.17) may be considered small, and we throw it out.

Making this last substitution, we have for the Neumann boundary condition

$$\nabla_T \chi_I = -\frac{\ddot{f}}{4}\chi_I . \qquad \text{(N.18)}$$

Equation (N.18), the result for the Neumann boundary condition, leads to curvature-induced boundary waves along concave surfaces. Note that since the boundary waves are confined to concave surfaces, they cannot lead to an energy flux that propagates down a

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[ffff] Note that the rescaling suggested by equation (N.14): $\ddot{\lambda}/8k_0^2 \Rightarrow -\left(\ddot{\lambda}/8k_0^2\right)\left(\rho_{II}/\rho_I\right) = -\left(\ddot{\lambda}/8k_I^2\right)$ takes the reference wave number k_0 and replaces it with the wave number in Region I, k_I. Recalling the virtual-fluctuation interpretation of Appendix C.2.6, this suggests the virtual fluctuations are actually of magnitude $\delta x \sim i/2k_I$. This in turn suggests that the size cutoff for determining $\ddot{f} = 1/[\text{radius of curvature}]$ should be taken as the wave number in Region I, k_I.

rough surface. Thus, the effect associated with the Neumann boundary conditions is small compared to the analogous effect along a 2-fluid interface. In the latter case, there is always a concave surface available, and so boundary waves can always be present and can even propagate downrange. (As discussed in the text (Section 5.3.3), something similar can occur even for the Neumann boundary conditions along a bossed surface, where it is possible for the surface to be everywhere concave. However, the bossed surface lies outside the purview of the parabolic equation.)

Next, let us consider the Dirichlet boundary conditions. Now, we must view the first boundary condition in equation (N.15) from the point of view of the field in Region II and let $K_I \to \infty$ while $\rho_I \to 0$. The first boundary condition in (N.15) now becomes

$$\chi_{II} = \chi_I - \frac{\dot{f}^2}{4}\left(\chi_I + \frac{\rho_{II}}{\rho_I}\chi_{II}\right) + \frac{1}{8k_I^2}\left(\ddot{f}\nabla_T\chi_{II} + \dot{f}^2\left(\frac{\rho_{II}}{\rho_I}\nabla_T^2\chi_I + \nabla_T^2\chi_{II}\right)\right)$$

Now, at least in the higher-order terms, $\chi_I, \nabla_T^2\chi_I \to 0$. (To convince yourself of this statement for the latter quantity, Fourier decompose and look at the plane wave solutions on a flat interface.) This leaves us with two terms that are proportional to $\dot{f}^2$. They contain the quantities $\left(\rho_{II}/\rho_I\right)\chi_{II}$ and $\left(\rho_{II}/\rho_I\right)\nabla_T^2\chi_I$. These are both finite since χ_{II} and $\nabla_T^2\chi_I$ both go to zero as ρ_I/ρ_{II}. Therefore, (as with the Neuman boundary conditions), we can once again drop the slope-squared terms to get

$$\chi_{II} = \chi_I + \frac{\ddot{f}}{8k_I^2}\nabla_T\chi_{II}\,.$$

Set the field on the far side to zero (assert that the wave is incoming on side II and that nothing bleeds through to the far side — i.e., side I). This gives us

$$\chi_{II} = \frac{\ddot{f}}{8k_I^2}\nabla_T\chi_{II}\,. \qquad \text{(N.19)}$$

This time, the $\mathrm{O}\left(\ddot{f}\right)$-term is insignificant for two reasons. In the first place, a boundary condition of the form (N.19) represents a small displacement of the surface, and this will not affect the scattered wave very much. Even more importantly, as discussed above, we expect the wave number in Region I, k_I to be large on the scales that matter for the field in Region II, and so $1/k_I^2$ is small. Thus, we drop the $\mathrm{O}\left(\ddot{f}\right)$-term, and assert that the Dirichlet boundary conditions are not significantly influenced by the curvature-induced terms introduced by the Foldy-Wouthuysen transformation. The Dirichlet boundary condition is thus unchanged: $\chi_{II} = 0$. This is no surprise, since the new terms introduced by the Foldy-Wouthuysen transformation are connected to phenomena that require renormalization (e.g., vacuum polarization is associated with renormalized Quantum Electro-Dynamics), and Orris and Dashen have shown that the Dirichlet boundary conditions only require renormalization at very high orders[119,120,121]. (As discussed, in

Section 4.4 and in Appendix O, renormalization for the parabolic equation reduces to the simple introduction of the cutoff k_0, or as we have just discovered perhaps k_1.)

The results of this appendix indicate that the parabolic equation may be a good way to study the explicit effects of slope and curvature on scattered fields. This is related to the fact that a good parabolic equation conserves energy, and energy conservation helps to pacify some of the pathologies that perturbative field theories encounter with multiscale rough surfaces. Specifically, the failure of perturbation theories to properly incorporate curvature-induced boundary waves is a cause behind the failure of these theories to conserve energy. This will be discussed further in Appendix O.

O Appendix: Curvature-induced boundary waves in the context of the development of modern rough-surface scattering theory

This Appendix reprises developments in acoustic rough-surface scattering theory since the late 1980's, and points to remaining issues that may be addressed using the "vacuum polarization" series of terms introduced into the parabolic equation by the Foldy-Wouthuysen transformation.

O.1 The status quo in the late 1980s

In the late 1980's, there were a number of competing approaches for calculating acoustic scattering from rough surface.

For some very idealized problems, exact solutions were available. Sometimes, "brute force" numerical calculations were used. These generally made use of either finite difference or finite element approaches. These approaches are practical for 1-dimensional and occasionally even 2-dimensional surfaces with mild roughness (e.g., calm sea surface), and occasionally for 1-dimensional "agitated" surfaces (e.g., heavy seas). For agitated surfaces, the size of the scattering surface had to be limited. Furthermore, to get stochastic answers, many realizations had to be considered. The calculations were quite demanding since many scales are simultaneously involved in such scattering problems. As a consequence, for truly rough surfaces, these brute force approaches were at best research tools, but they were not particularly useful as general algorithms.

There were also perturbative approaches. These typically concerned the scattering amplitude[gggg], which is in principle related to the scattered field everywhere via a 2-dimensional Fourier transform. In practice, the scattering amplitude was typically used to calculate the far field, which is simply proportional to it, or the far field scattering cross-section, which is proportional to the magnitude squared of the scattering amplitude. For quasi-planar rough surfaces, the quantity of interest was the stochastic scattering cross-section per unit area, which measured in decibels, becomes the scattering strength that is generally substituted into the sonar equation. Once the quasi-planar rough surface is introduced, one generally drops the specular δ-function, and only examines the incoherent wave. (The coherent component has a different spreading center than does the incoherent wave, and so extreme care is needed if the specular component is retained in the far-field formalism.)

As of the early 1980's, there were two widely used approximations to calculate the scattering amplitude. The Kirchhoff approximation dates from the 19th century, and it was used in the high frequency limit to calculate the scattering from gently undulating (i.e., slowly varying on the scale of a wavelength) surfaces. For wavelength scale scattering (also known as Bragg scattering), perturbation theory developed by Rayleigh[122], Rice[123] and Waterman[124] was used. Both approaches remained the subject of much tinkering and controversy. In fact, it was not until the mid 1980's that the relationship between the Kirchhoff and perturbation approximations was established independently by Berman and Perkins[125], and by Holliday[126].

A pair of useful new approximations applicable to acoustic scattering from the ocean surface (i.e., Dirichlet boundary conditions) was developed between the early 1960's and the mid 1980's. Various groups in Russia[127,128] and S. McDaniel (with collaborators) in the United States[129,130] developed the composite model (also known as the 2-scale model), which glued physical and geometrical acoustics together, forcing the spectrum of the latter regime to terminate at some fixed, empirically chosen maximum wave number (typically about $\frac{1}{3}$ the Bragg wave number). The mid 1980's also saw the emergence of a new approximation that remains extremely useful to this day: the small slope approximation by Voronovich[131,132]. Its properties have since been firmly established by Thorsos and Broschat[133,134], and it has been extended to a wide variety of fields and boundary conditions[32,135,136,137,138]. The small slope approximation unifies the Kirchhoff approximation and perturbation theory by reducing to each in the proper limit. The Kirchhoff approximation and the composite model have largely been replaced by the small-slope approximation, and this approximation has become the new standard method for calculating the scattering amplitude and cross-section for a quasi-planar rough surface. (Perturbation theory remains in widespread use as well, because it does not contain an integration and is consequently simpler to evaluate than the small slope result.)

[gggg] An exception would be the perturbative normal mode approach of Kuperman and Schmidt mentioned in several places in this report, including for example in Table 6.1.

O.2 Towards a new scattering theory

The various techniques available by the late-1980's all had some qualitative or formal validity criteria, but there was nothing to provide an overall context for the various approaches. This void helped generate a widespread distrust of the results of rough surface scattering theory. When in the mid-1980's it became clear that theory and experiment were not in agreement (sometimes they differed by a factor of 100), it was claimed by many that the rough-surface scattering theories were inadequate, and that this mechanism could still not be ruled out. Since perturbation theory works well in predicting HH electromagnetic scattering[hhhh] when the same air-sea interface is impacted from the other side[139], it should have been clear all along that scattering theory was not the problem, and indeed it was eventually established that the true cause of the anomaly was scattering from near-surface bubble clouds[140]. Nevertheless the controversy of the late-1980's sparked new developments in scattering theory.

For example, this state of affairs prompted R. Dashen, *et. al.* to begin a wide-ranging examination of the problem of scattering from the rough air-sea interface[73]. Even before this effort began, it had already become clear to Dashen that there was a strong need to relate the existing approaches to one another and to a clear physical intuition (including an inventory of which physical processes the various approximations included and which they did not). This need would be addressed by developing an overarching "theory of theories" that would generate a taxonomy for the various scattering models. This matrix of theories would then be used to fill in the gaps in our knowledge of the problem. In particular, we would be able to apply a given approach to a wide variety of fields and boundary conditions, to develop new approximations, and most importantly to conduct a systematic search for the missing physics.

The basic technique was proposed by Dashen, and I had the opportunity to participate with him in its development and application to wide variety of situations. At the core of the new approach was the realization that for modern 20th century field theories, a clear hierarchy of possible approximate solutions falls out naturally. To this was added the insight that the difference between fields that were discovered in the 19th century and those that were discovered in the 20th century is the approach used to describe them and

[hhhh] An HH polarized electromagnetic wave scattering from a perfect conductor obeys the same Dirichlet boundary condition that as that obeyed by an acoustic field incident on the air-sea interface from below.

not the underlying physics[iiii]. During the 19th century, fields were traditionally described using a "tour de force" of vector calculus and formal mathematical manipulation, while in the 20th century field theories have often been "bootstrapped" from symmetry arguments. Thus, the goal of our effort was to rederive classical field theory using modern techniques.

To be specific, the expression for the scattering amplitude was derived using a symmetry principle: Noether's theorem. Roughly speaking, when a symmetry leads to a conserved current, Noether's theorem associates a source term for the current with the symmetry breaking operation. Time reversal invariance was the symmetry invoked, and the conserved current was defined by Lorentz's lemma. The symmetry was broken by stipulating that the reciprocal problem scatters from a perturbed surface. The associated "source" in the current-conservation equation was the change in the scattering amplitude associated with the perturbation of the scattering surface. The result was a new 2-scale theory (i.e., composite model) that was exact with respect to the reference problem and first order with respect to the perturbation of the scattering surface[iiii]. The result was obtained for acoustic field[135,141], electromagnetic[141] fields, and eventually also for elastodynamic fields[138].

The reciprocal 2-scale theory was then used to spawn a family of approximations. An infinitesimal transformation of this result leads to an exact new manifestly reciprocal expression for the scattering amplitude[73,135,138,141]. Using this result, it is almost trivial to obtain the lowest order (manifestly reciprocal) small slope approximation for a wide variety of fields and boundary conditions[32,135,138]. It was also possible to derive an optimal "local" approximation—the "small curvature" approximation[32]. The formalism also led to shortcuts to higher-order perturbation theory, cleared up the relationship between the various scattering theories mentioned above, and provided a reciprocal scattering amplitude for collections of scatterers near a rough surface (where the distribution of scatterers as a function of the depth follows the surface as it is perturbed)[81].

[iiii] Concerning quantum fields versus classical fields, the measurement problem and the associated issues related to the collapsing wave packet is apparently an exception (although if the proponents of decoherence generated internally to field theory are correct, then even this distinction blurs), but this issue is not (at present) addressed within field theory. What is addressed is the gradual development of the quantum field as a function of time and space, and this is entirely analogous to the development of a classical field. (Quantum fields also often contain rich algebraic structures that are not typically found in classical fields, but this distinction is also irrelevant to the discussion here.)

[iiii] The earlier composite (or 2-scale) model developed in Russia and the United States between 1960's and the early-1980's will henceforth be called the "old" composite model.

Since it is exact with respect to the reference problem, the new 2-scale theory models non-local effects associated with the reference surface. If the perturbation is taken to be the Bragg-scale features and the reference surface is taken to be the "big" waves, then the non-local effects include diffraction as well as effects that in the geometrical acoustics limit become shadowing and multiple scattering. This new 2-scale theory was used by a group at Dynamics Technology[142] to model radar scattering. The related report contained the perceptive observation that the principal advantage of the reciprocal 2-scale result is that it properly models all the paths involved in a scenario where the field scatters twice from the surface in the following manner: once with the wavelength scales somewhat larger than a wavelength (via diffraction or locally-specular scattering) and the other time via Bragg scattering. In reference [73], where the contribution associated with the reference surface was obtained to 2nd order, it was recognized that these (non-local) scattering channels cover the dominant parts of 4th order perturbation theory (for the stochastic cross section), and so the 2-scale result was used to get a serviceable approximation to 4th order perturbation theory (for the Dirichlet boundary conditions).

The reciprocal scattering theory was used in several additional contexts. Dashen *et al*. used it to create a new theory of scattering from finite objects[143]. Small slope approximations developed using the reciprocal scattering formalism[32,138] are currently being used to model scattering from elastic ocean bottoms[144,145] and from the air-sea interface[145].

As the reciprocal theory was developed, other approaches were being successfully implemented elsewhere. Thorsos has worked extensively with 4th order perturbation theory[146,147]. M. Milder designed an operator expansion method that is both elegant and has proven very useful[148,149,150]. Voronovich has developed a non-local version of the small slope approximation[151]. Numerical studies by Thorsos and collaborators have produced an "empirical taxonomy" of approximations based on their observed range of validity as a function of parameters characterizing the scattering surface[134,150,152].

O.3 Shortcomings inherent to perturbative models of rough-surface scattering

Despite all this progress, the theoretical approach has remained incomplete. The issues involved have yet to play any direct role in practical applications in underwater acoustics, and so the topic has remained fairly obscure. However, it is of physical and mathematical interest, and as such one suspects that it will find its way into applications once the related phenomena are understood. The physics that is obscured by the various perturbative approaches in wide use today manifests itself in four ways:

- Energy is not conserved on an order-by-order basis.
- Curvature-induced boundary wave phenomena and the somewhat related effects that depend explicitly on the tilt are relegated to high orders where they become very illusive multiple scattering effects.

- In principle, at some point, the need arises to renormalize these theories. For standard perturbation theory, this is typically at very high orders[119,120,121], but the issue can appear already at first order (e.g., the small curvature or arctangent formulas derived in reference [32]). If uncorrected, the need for renormalization leads to infinities for fractal surfaces and unphysical sensitivity to scales far below a wavelength for self-affine (cutoff fractal) surfaces as well as for any other surfaces whose spectra do not rapidly decay to insignificant levels at scales below the Bragg scale.
- On the other hand, those orders of perturbative scattering theories that do not raise renormalization issues fail to properly account for scattering from surface features that are smaller than the Bragg scale, but could still be physically relevant according to the uncertainty principle. These features constitute a third scale that comes in addition to the two scales usually discussed[119]: the Bragg scale and the "big" scales (> wavelength).

O.3.1 Energy non-conservation and boundary waves

A number of researchers have recognized the connection between the first two manifestations of the phenomenon: energy non-conservation and curvature-induced boundary waves. Thorsos has based his argument on the insight that for 1st order perturbation theory corresponding to the Neumann boundary condition, as the grazing angle goes to zero, the incoming flux goes to zero, but the scattering cross-section does not. This violates energy conservation, and Thorsos has identified boundary waves as the culprits behind this anomaly[82]. Soto-Crespo *et al*.[83] wrote about the same phenomenon in the context of electromagnetic theory. They attributed the failure of energy conservation to what they called polaritons, which are the curvature-induced boundary waves. Tang and Frisk[84] have also noted the existence of curvature-induced boundary waves. On a track parallel to, but outside the framework of modern scattering theory, Biot and Tolstoy have extensively studied curvature-induced boundary waves along bossed surfaces. This work is briefly examined at the end of Subsection 5.3.3.

O.3.2 The third scattering scale and renormalization

Some time ago, Dashen and Orris made the connection between the third and fourth manifestations of this phenomenon[119,120,121]. In this regard, it is worth quoting the abstract from Dashen's talk at the 120th meeting of the Acoustical Society of America in 1990[119]:

"Theoretical work on scattering from rough surfaces is often plagued by an extreme range of scales of surface roughness. In particular, a wide range of scales can make numerical calculations impractical. Roughness on scales longer than a wavelength can be handled by an improved composite model. Scales smaller than a wavelength can, in certain circumstances, cause serious trouble. The cross section can depend explicitly on the cutoff at high wave numbers."

In this talk, Dashen primarily referred to perturbation theory, but the issue of a cutoff also appears in the implementations of Dashen's small curvature formula[32] (also known as the arctangent formula). This too was an early motivating factor for Dashen's attention to the third scattering scale. Among other things, he was looking for a proper way to cutoff approximations, which, like the small curvature formula, addressed the physics of the third scattering scale. (It should be noted that formally the cutoff issue for the small curvature formula was related to the slope $\dot{f}$ and not the curvature $\ddot{f}$. This is ultimately the result of a hidden integration by parts, and the 1st order contribution does indeed originate from the curvature $\ddot{f}$ (see the discussion in Appendix A of reference [32], and in particular equation A22 in the reference).)

Before proceeding, it should also be noted that Voronovich and Zavorotny have recently introduced a small slope approximation that includes the curvature[153]. In this case, the curvature is cutoff at the upper limit of the "big"-wave scale. The physics involved is diffraction and similar issues in physical acoustics, but the third-scale physics with its related renormalization issues does not come up in this work. In this sense, it is a little like the old composite model[127,128,129,130], where the cutoff was imposed on the *slope* at the upper end of the "big"-wave scale (reference [73] includes a look at the process of cutting off the "old" composite model).

The connection between the need for renormalization and the sensitivity to small scales is an intimate one. As noted in the text (see Section 4.4), it comes from the fact that the curvature $\ddot{f}$ and the slope $\dot{f}^2$ are "broad-spectrum" parameters that depend on all scales. They are especially sensitive to the smallest scales. This means that terms proportional to these parameters will not miss the bona fide physical effects associated with the sub-wavelength scale, but it also means that these terms will have trouble accounting for the mechanism that imposes the uncertainty principle on a classical field. The real effects are not clearly delineated from the artifacts. This is why third-scale scattering phenomena are invariably tied up with the issue of renormalization.

The renormalization of full-wave perturbative theories is generally a cumbersome process involving the repeated resummation of the perturbative series. As the orders are remixed, cancellations that used to occur between orders now occur within a given order. Most noticeably, any infinities now properly cancel each other out on an order-by-order basis. Rather than deal with all the complications related to renormalization, one typically throws out the legitimate physical effects associated with subwavelength scales. To change this, we will need a method to bring curvature/tilt-induced third-scale physics (including especially boundary wave phenomena) down to accessibly low orders, and we will also need a relatively workable solution to the renormalization issue.

O.4 The parabolic equation is a good way to examine the issues left unresolved by perturbative theories

The parabolic equation generated by the Foldy-Wouthuysen transformation manifestly accomplishes the first goal listed in the last paragraph of Subsection O.3.2 just above. We have contributions that are 1st order in the curvature ($\mathrm{O}\left(\ddot{f}\right)$) and 2nd order in the slope ($\mathrm{O}\left(\dot{f}^2\right)$). These orders are certainly low. As discussed in Section 4.4, there also exists a rather simple workaround to the issue of renormalization. The surface spectrum is a function of $\underline{k}$, a wavevector in the average plane of the quasi-planar surface (i.e., the x-y plane). (For a 1-dimensional surface, $\underline{k} \to k_x$.) Fourier decomposing the field into plane-wave components, a given component of the surface will more or less excite the component of the field whose wave vector projects to $\underline{k}$ on the x-y plane. This projected wavevector can have any magnitude between 0 and k_0. Thus, we are well justified in mimicking quantum mechanics and choosing our upper spectral cutoff to be k_0. From the uncertainty principle $\Delta k \Delta r_{x\text{-}y} \geq \frac{1}{2}$ ($r_{x\text{-}y}$ is a distance in the x-y plane), this gives us

$$\Delta r_{x\text{-}y} \geq \frac{1}{2\Delta k} = \frac{1}{2k_0} = \frac{\lambda_0}{4\pi}.$$

The field cannot resolve features smaller than about $\frac{1}{12}$ wavelength, and the third scale lies roughly between λ_0 and $\lambda_0/4\pi$.

Using the $\lambda_0/4\pi$ cutoff to calculate the renormalized values of $\ddot{f}$ and $\dot{f}^2$ is adequate as a first guess. Replacing these parameters with their renormalized values is an example of a reduction formula (see reference [76], p. 438). It is completely analogous to the "guess" for a cutoff on the energy spectrum that Bethe used in calculating the Lamb shift (except recall that he already effectively had a problem with $\left\langle f^2 \right\rangle$; see Section 4.4). (Bethe's calculation can be found in reference [76], p. 593.) This issue arose in the context of a low energy approximation that depends on assumptions that are similar to the low-grazing-angle small-backscatter approximation implicit in the parabolic equation. Bethe chose the rest mass m_0 as his high-energy cutoff. Our cutoff k_0 plays the same role in the Helmholtz equation as the rest mass m_0 plays in the Klein-Gordon equation, and k_0 also plays the same role in the parabolic equation as m_0 does in the Schrödinger equation. Thus, Bethe's choice of m_0 as a cutoff is completely analogous to our choice of k_0. Bethe obtained good results with his technique. However, it is good to keep in mind that it is ultimately better to use experimental values for the effective curvature $\ddot{f}_{\text{effective}}$ and effective slope squared $\dot{f}^2_{\text{effective}}$, or better yet, to use the full power of field theory to include higher-order "radiative" corrections (see reference [76], p. 593-594). For now, we will be taking the easy way out, and impose the cutoff k_0.

Note that if we were operating in full-wave theory, we would also have to allow for backscatter and a given component of the surface could also excite a backward traveling wave with wave number $-\underline{k}$. This leads to some contribution for the $-k_0$ to 0 wave number range, but this contribution has to weighted differently than the positive

contribution. There is no obvious way to do so, and so getting the needed reduction formulas is no longer as easy as choosing a single value for the cutoff wave number! Here we have the second big advantage of the parabolic equation. (Recall that the first was that these effects are of low order.)

Thus, the parabolic equation takes a subtle group of physical effects associated with curvature, slope and sub-wavelength scales, and makes them accessible by bringing them to low orders (essentially by stripping off the local component of these effects and separating it out from associated multiple scatter effects). It also offers a serviceable workaround to the renormalization problem.

O.5 Final thoughts

As an interesting side note, we remark that in stochastic scattering theory, the third-scale physics will involve the coherent component proportional to $\left\langle \dot{f}^2 \right\rangle \langle \chi \rangle$ and the incoherent component proportional to $\left\langle \ddot{f} \cdot \delta\chi \right\rangle$. The contribution to the scattering of the incoherent wave is associated with the curvature. This illustrates why most of the attention in the rough surface scattering community (which usually considers the stochastic incoherent field) has focused on curvature-induce boundary waves. Furthermore, as we have seen in the main body of the paper, the tilt-induced contribution $\propto \left\langle \dot{f}^2 \right\rangle \langle \chi \rangle$ disappears entirely when there is no density jump (Section 4.3), and it is a very modest effect when there is a density jump (Subsection 5.3.4). The tilt-induced effect is thus insignificant in the stochastic problem. It is of primary interest in the deterministic problem.

Finally, let us note two interesting phenomena that are *not* covered by the formalism discussed here. Enhanced backscatter is obviously not compatible with the forward-propagating parabolic equation. Whispering gallery waves bear a superficial similarity with the curvature-induced boundary waves introduced here, primarily because they are curvature-induced boundary waves associated with concave hard surfaces. However, they are not a small-scale effect at all. They are usually understood in terms of geometrical acoustics, where rays will bunch up along a concave surface. Furthermore, looking at equation (N.18), we see that this type of curvature induced boundary wave has an e-folding distance of 4 times the radius of curvature, while whispering gallery waves are confined to a fraction of the radius of curvature of the surface that generates them.

Nevertheless, the parabolic equation complete with the "vacuum polarization" set of terms introduced by the Foldy-Wouthuysen transformation holds real promise for casting light on a heretofore poorly understood class of physical effects associated with curvature, slope and sub-wavelength scales.

P Appendix: The acoustic Lamb shift when the density and compressibility *both* jump

This appendix examines the stochastic boundary conditions for the quasi-first order theory of a density/sound speed jump. Section P.1 provides the details of the derivation of the boundary conditions (equation (5.20)), Section P.2 a discussion of the meaning of this result, and Section P.3 a discussion of adjustments to the stepping procedure peculiar to this quasi-first order theory.

P.1 The derivation of the boundary conditions for the stochastic problem

The boundary condition on the field χ is considered in Subsection P.1.1 and the boundary condition involving the first derivative $\partial\chi/\partial z$ is considered in Subsection P.1.2. Subsection P.1.3 provides a lemma used in Subsection P.1.2 and Subsection P.1.4 provides a lemma used in the derivation of both boundary conditions.

Let us start with the deterministic boundary conditions (5.16) valid along the surface $z = f$. These boundary conditions are written here in slightly different form:

$$\begin{aligned} \chi_I\big|_{z=f} - \chi_{II}\big|_{z=f} &= -\dot{f}^2 A\,\overline{\rho\chi}\big|_{z=f} - B\left(\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=f} + \dot{f}^2\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=f}\right) \\ \frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} - \frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\bigg|_{z=f} &= A\left(\ddot{f}\,\overline{\chi}\big|_{z=f} + \dot{f}^2\,\overline{\frac{\partial\chi}{\partial z}}\bigg|_{z=f}\right) \end{aligned}, \qquad \text{(P.1)}$$

where

$$A = \frac{1}{8\rho_{II}}\left(\frac{\delta K}{K_I} - \frac{\delta\rho}{\rho_{II}}\right) = \frac{1}{4\rho_{II}}\left(\underbrace{\frac{K_{II}-K_I}{2K_I}}_{-\mu_{II}} - \underbrace{\frac{\rho_{II}-\rho_I}{2\rho_{II}}}_{\gamma_I}\right) = -\frac{1}{4\rho_{II}}\left(\mu_{II}+\gamma_I\right) \qquad \text{(P.2)}$$

$$B = \frac{\delta\rho}{8k_0^2}$$

The derivation of equation (5.16) depended on the assumptions described by Figure 5.1, and these must continue to hold here. Specifically, we are operating in 2-dimensional x-z space, where space is separated into two regions by a quasi-planar rough surface $z = f(x)$. The positive z-axis points from Region II into Region I, and the average plane of the rough surface is along the line $z = 0$. Now we add one new condition: assume that f defines a random rough surface that obeys Gaussian statistics. As always,

K is the compressibility is and ρ is the density. As before, also assume that $K_I > K_{II}$ and $\rho_I < \rho_{II}$, and that the reference values are chosen to be the larger value. The reference wave number is therefore given by $k_0 = \omega\sqrt{K_I \rho_{II}}$, where ω is a frequency.

Now, follow the stochastic procedure for the cusp (Subsection 3.2.3) and the sound speed jump (Section 4.3), and as in these sections, adapt the technique originally developed by Kuperman[65]. To this end, we will project the boundary conditions at $z = f$ down to the line $z = 0$, break the wave function evaluated at $z = 0$ into coherent and incoherent parts: $\chi|_{z=0} = \langle\chi\rangle(0) + \delta\chi$, and average these boundary conditions.

P.1.1 The boundary condition for the field χ

Thus, we begin with an updated version of equations (3.27) and (4.11).

$$\begin{aligned}\chi_I(0) - \chi_{II}(0) = \chi_I(f) - \chi_{II}(f) - f\left(\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f}\right) \\ + \frac{f^2}{2}\left(\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right)\end{aligned} \quad . \tag{P.3}$$

Now recast the second boundary condition in equation (P.1):

$$-\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} = -\frac{\rho_{II}}{\rho_I}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \rho_{II} A\ddot{f}\,\overline{\chi}|_{z=f} + \mathrm{O}\left(\dot{f}^2\right)$$

to get

$$\begin{aligned}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} &= \underbrace{\left(1 - \frac{\rho_{II}}{\rho_I}\right)}_{\Downarrow}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \rho_{II} A\ddot{f}\,\overline{\chi}|_{z=f} + \mathrm{O}\left(\dot{f}^2\right) \\ &= -\frac{\delta\rho}{\rho_I}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \rho_{II} A\ddot{f}\,\overline{\chi}|_{z=f} + \mathrm{O}\left(\dot{f}^2\right)\end{aligned} \quad . \tag{P.4}$$

Let us symmetrize this result. This time recast the second boundary condition in equation (P.1) this way:

$$\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} = \frac{\rho_I}{\rho_{II}}\left.\frac{\partial\chi_{II}}{\partial z}\right|_{z=f} + \rho_I A\ddot{f}\,\overline{\chi}|_{z=f} + \mathrm{O}\left(\dot{f}^2\right)$$

and get

$$\left.\frac{\partial \chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f} = \underbrace{\left(\frac{\rho_I}{\rho_{II}} - 1\right)}_{\Downarrow} \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f} + \rho_I A\ddot{f}\,\overline{\chi}\big|_{z=f} + \mathrm{O}\left(\dot{f}^2\right)$$
$$= -\frac{\delta\rho}{\rho_{II}} \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f} + \rho_I A\ddot{f}\,\overline{\chi}\big|_{z=f} + \mathrm{O}\left(\dot{f}^2\right). \tag{P.5}$$

Add (P.4) and (P.5) and divide by 2 to get

$$\left.\frac{\partial \chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f} = -\delta\rho\overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]} + A\ddot{f}\,\overline{\rho}\,\overline{\chi}\big|_{z=f} + \mathrm{O}\left(\dot{f}^2\right).$$

Now,

$$\overline{\rho}\cdot\overline{\chi} = \frac{\rho_I\overline{\chi} + \rho_{II}\overline{\chi}}{2} = \frac{\rho_I\chi_I + \rho_{II}\chi_{II}}{2} + \mathrm{O}\left(\ddot{f}\right) = \overline{\rho\chi} + \mathrm{O}\left(\ddot{f}\right) \tag{P.6}$$

and

$$\left.\frac{\partial \chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f} = -\delta\rho\overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]}_{z=f} + A\ddot{f}\,\overline{\rho\chi}\big|_{z=f} + \mathrm{O}\left(\dot{f}^2, \ddot{f}^2\right). \tag{P.7}$$

Now, expanding on each side of the interface independently through 1st order in f, we have

$$\overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]}_{z=f} = \overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]}_{z=0} + f\overline{\left[\frac{1}{\rho}\frac{\partial^2 \chi}{\partial z^2}\right]}_{z=0} + \mathrm{O}\left(f^2\right).$$

Similarly through 0th order in f, we also have $\left.\overline{\rho\chi}\right|_{z=f} = \left.\overline{\rho\chi}\right|_{z=0} + \mathrm{O}(f)$. Substituting these expansions into (P.7) and multiplying by $-f$ gives us

$$-f\left(\left.\frac{\partial \chi_I}{\partial z}\right|_{z=f} - \left.\frac{\partial \chi_{II}}{\partial z}\right|_{z=f}\right) = f\delta\rho\overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]}_{z=0} - A\ddot{f}\cdot f\,\overline{\rho\chi}\big|_{z=0}$$
$$+ f^2\delta\rho\overline{\left[\frac{1}{\rho}\frac{\partial^2 \chi}{\partial z^2}\right]}_{z=0} + \underbrace{\mathrm{O}\left(f\cdot\dot{f}^2, f\cdot\ddot{f}^2, f^3\right)}_{3^{\text{rd}}\text{ order}}. \tag{P.8}$$

Now plugging result (P.8) into (P.3)

$$\chi_I(0) - \chi_{II}(0) = \chi_I(f) - \chi_{II}(f) + f\underbrace{\delta\rho}_{8k_0^2 B}\overline{\left[\frac{1}{\rho}\frac{\partial \chi}{\partial z}\right]}_{z=0} - A\ddot{f}\cdot f\,\overline{\rho\chi}\big|_{z=0}$$
$$+ \underbrace{\frac{f^2}{2}\left(\left(1 + \frac{\cancel{2}}{\cancel{2}}\frac{\delta\rho}{\rho_I}\right)\frac{\partial^2 \chi_I}{\partial z^2} - \left(1 - \frac{\cancel{2}}{\cancel{2}}\frac{\delta\rho}{\rho_{II}}\right)\frac{\partial^2 \chi_{II}}{\partial z^2}\right)}_{\boxed{\text{The } \mathrm{O}\left(f^2\right) \text{ term}}} + \underbrace{\mathrm{O}\left(f\cdot\dot{f}^2, f\cdot\ddot{f}^2, f^3\right)}_{3^{\text{rd}}\text{ order}}. \tag{P.9}$$

Note that the term in (P.8) proportional to $f^2\delta\rho\cdot\left(\partial^2\chi/\partial z^2\right)$ now generates two new terms each marked by a factor of ⅔. We picked up the factor of 2 in the numerator to cancel the overall factor of ½ out in front of the $\mathrm{O}\left(f^2\right)$ term, and we also picked up a factor of 2 in the denominator since we busted apart the average. Also in the $\mathrm{O}\left(f^2\right)$ term, we have dropped the designation identifying the depth coordinate, since the term is already 2nd order, and we will be taking advantage of this to move freely between $z=f$ and $z=0$. To remind ourselves that we are doing this, we will retain the $\mathrm{O}\left(f^3\right)$ error designation.

Let us rework the $\mathrm{O}\left(f^2\right)$ term in equation (P.9). The goal is to symmetrize this term: i.e., get this term into a form involving averages at the interface rather than values on one side or the other. To begin, note that

$$1+\frac{\delta\rho}{\rho_I}=1+\frac{\rho_{II}-\rho_I}{\rho_I}=\frac{\rho_{II}}{\rho_I}\quad;\quad 1-\frac{\delta\rho}{\rho_{II}}=1-\frac{\rho_{II}-\rho_I}{\rho_{II}}=\frac{\rho_I}{\rho_{II}}.$$

Substitute this result into the $\mathrm{O}\left(f^2\right)$ term in equation (P.9):

$$\boxed{\text{The } \mathrm{O}\left(f^2\right) \text{ term}} =$$

$$\frac{f^2}{2}\left(\left(1+\frac{\delta\rho}{\rho_I}\right)\frac{\partial^2\chi_I}{\partial z^2}-\left(1-\frac{\delta\rho}{\rho_{II}}\right)\frac{\partial^2\chi_{II}}{\partial z^2}\right)=\frac{f^2}{2}\left(\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right)+\mathrm{O}\left(f^3\right).$$

Now, to get this into a form involving averages on the interface, we have to continue with the following manipulations:

$$\begin{aligned}\boxed{\text{The } \mathrm{O}\left(f^2\right) \text{ term}} &= \frac{f^2}{4}\left(\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right)+\frac{f^2}{4}\left(\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right)+\mathrm{O}\left(f^3\right)\\ &= \frac{f^2}{4}\left(\left(\frac{\rho_{II}}{\rho_I}-1\right)\frac{\partial^2\chi_I}{\partial z^2}+\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right)\\ &\quad+\frac{f^2}{4}\left(\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\partial^2\chi_{II}}{\partial z^2}+\left(1-\frac{\rho_I}{\rho_{II}}\right)\frac{\partial^2\chi_{II}}{\partial z^2}\right)+\mathrm{O}\left(f^3\right).\end{aligned}$$

Reorganizing these terms as follows:

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} = \frac{f^2}{4}\left[\underbrace{\left(\frac{\rho_{II}}{\rho_I}-1\right)}_{\delta\rho/\rho_I}\frac{\partial^2\chi_I}{\partial z^2}+\underbrace{\left(1-\frac{\rho_I}{\rho_{II}}\right)}_{\delta\rho/\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right]$$
$$+\frac{f^2}{4}\left[\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right]+\frac{f^2}{4}\left[\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\partial^2\chi_{II}}{\partial z^2}\right]+\text{O}\left(f^3\right),$$

the $\text{O}\left(f^2\right)$ term in equation (P.9) becomes:

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} =$$
$$\frac{f^2}{2}\delta\rho\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]+\frac{f^2}{4}\underbrace{\left[\frac{\partial^2\chi_I}{\partial z^2}-\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right]}_{\text{Use Lemma 2}}+\frac{f^2}{4}\underbrace{\left[\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}-\frac{\partial^2\chi_{II}}{\partial z^2}\right]}_{\text{Use Lemma 2}}+\text{O}\left(f^3\right). \quad \text{(P.10)}$$

Now, use Lemma 2 in Section P.1.4 below. Substitute for the last two terms in equation (P.10) using equations (P.34) and (P.35):

$$\boxed{\text{The O}\left(f^2\right)\text{ term}}$$
$$=\frac{f^2}{2}\delta\rho\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]+\frac{f^2}{4}\left(8k_0^2\rho_I A\overline{\chi}\right)+\frac{f^2}{4}\left(8k_0^2\rho_{II}A\overline{\chi}\right)+O\left(f^2\cdot\ddot{f},f^3\right)$$
$$=\frac{f^2}{2}\delta\rho\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]+f^2 4k_0^2\frac{\left(\rho_I+\rho_{II}\right)}{2}A\overline{\chi}+O\left(f^2\cdot\ddot{f},f^3\right)$$
$$=\frac{f^2}{2}\delta\rho\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]+4k_0^2f^2A\overline{\rho}\cdot\overline{\chi}+O\left(f^2\cdot\ddot{f},f^3\right).$$

Now, recall equation (P.6) to replace $\overline{\rho}\cdot\overline{\chi}$ with $\overline{\rho\chi}$. Then use the definition of B, equation (P.2), to get:

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} = 4k_0^2f^2B\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=0}+4k_0^2f^2A\overline{\rho\chi}\Big|_{z=0}+O\left(f^2\cdot\ddot{f},f^3\right). \quad \text{(P.11)}$$

This is the symmetric form we are looking for. Since we are already at 2nd order, we have used our freedom to evaluate χ down at $z=0$.

Finally, to finish our evaluation of equation (P.3), we need to obtain $\chi_I(f)-\chi_{II}(f)$. Use the first boundary condition in equation (P.1), and the usual Taylor series expansion to get

$$\chi_I\big|_{z=f} - \chi_{II}\big|_{z=f} = -\dot{f}^2 A\overline{\rho\chi}\big|_{z=0} - B\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=0} - B\ddot{f}\cdot f\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=0} - B\dot{f}^2\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=0} + 3^{\text{rd}}\text{ order.} \tag{P.12}$$

Thus, take equation (P.9), and substitute results (P.11) and (P.12) to get

$$\begin{aligned}\chi_I(0) - \chi_{II}(0) = &-\left(\dot{f}^2 + \ddot{f}\cdot f\right)A\overline{\rho\chi}\big|_{z=0} - B\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=0} \\ &- B\left(\ddot{f}\cdot f + \dot{f}^2\right)\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=0} + 8k_0^2 f\cdot B\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=0} \\ &+ 4k_0^2 f^2 B\left[\overline{\frac{1}{\rho}\frac{\partial^2\chi}{\partial z^2}}\right]_{z=0} + 4k_0^2 f^2 A\overline{\rho\chi}\big|_{z=0} + 3^{\text{rd}}\text{ order.}\end{aligned} \tag{P.13}$$

Now, again follow Kuperman[65], and Sections 3.2.3 and 4.3. In equation (P.13), set

$$\underbrace{\chi(0) = \langle\chi\rangle\big|_{z=0} + \delta\chi}_{\text{On either side}}$$

and take the average. The result is

$$\begin{aligned}\langle\chi_I\rangle\big|_{z=0} - \langle\chi_{II}\rangle\big|_{z=0} = &\underbrace{-B\left[\overline{\frac{1}{\rho}\left\langle\ddot{f}\frac{\partial(\delta\chi)}{\partial z}\right\rangle}\right]_{z=0} + 8k_0^2\cdot B\left[\overline{\frac{1}{\rho}\left\langle f\frac{\partial(\delta\chi)}{\partial z}\right\rangle}\right]_{z=0}}_{\text{Diffuse (Bragg) scatter terms}} + 4^{\text{th}}\text{ order.} \\ &+ 4k_0^2\langle f^2\rangle B\left[\overline{\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}}\right]_{z=0} + 4k_0^2\langle f^2\rangle A\overline{\rho\langle\chi\rangle}\big|_{z=0}\end{aligned} \tag{P.14}$$

Equation (P.14) indeed provides the first boundary condition of equation (5.20). Note that this result once again mimics the tilted interface with $\dot{f}^2 \to -4k_0^2\langle f^2\rangle$. The error is 4th order in the stochastic problem, because for Gaussian surfaces, the average of odd powers is always zero. Also note that as with the interface where the sound speed (or compressibility) alone jumps, the "vacuum polarization" terms do not survive the averaging process. This will not be true for the second boundary condition, which we derive next.

P.1.2 The boundary condition on the derivative $\partial\chi/\partial z$

Now, as with Sections 3.2.3 and 4.3, let us go on obtain the boundary condition on the first derivative. Modifying equation (3.30) or equivalently (4.14), we have

$$\left.\frac{1}{\rho_I}\frac{\partial \chi_I}{\partial z}\right|_{z=0} - \left.\frac{1}{\rho_{II}}\frac{\partial \chi_{II}}{\partial z}\right|_{z=0} = \left.\frac{1}{\rho_I}\frac{\partial \chi_I}{\partial z}\right|_{z=f} - \left.\frac{1}{\rho_{II}}\frac{\partial \chi_{II}}{\partial z}\right|_{z=f}$$
$$-f\left(\left.\frac{1}{\rho_I}\frac{\partial^2 \chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{1}{\rho_{II}}\frac{\partial^2 \chi_{II}}{\partial z^2}\right|_{z=f}\right)$$
$$+\frac{f^2}{2}\left(\left.\frac{1}{\rho_I}\frac{\partial^3 \chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{1}{\rho_{II}}\frac{\partial^3 \chi_{II}}{\partial z^3}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right).$$

Now use the second boundary condition in (P.1) to replace the first two terms and rearrange the $\mathrm{O}(f)$ term to get:

$$\left.\frac{1}{\rho_I}\frac{\partial \chi_I}{\partial z}\right|_{z=0} - \left.\frac{1}{\rho_{II}}\frac{\partial \chi_{II}}{\partial z}\right|_{z=0} = A\ddot{f}\,\overline{\chi}\big|_{z=f} + A\dot{f}^2\left.\overline{\frac{\partial \chi}{\partial z}}\right|_{z=f}$$
$$-f\left[\frac{1}{2\rho_{II}}\left(\frac{\rho_{II}}{\rho_I}\left.\frac{\partial^2 \chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\partial^2 \chi_{II}}{\partial z^2}\right|_{z=f}\right) + \frac{1}{2\rho_I}\left(\left.\frac{\partial^2 \chi_I}{\partial z^2}\right|_{z=f} - \frac{\rho_I}{\rho_{II}}\left.\frac{\partial^2 \chi_{II}}{\partial z^2}\right|_{z=f}\right)\right] \qquad \text{(P.15)}$$
$$+\frac{f^2}{2}\left(\left.\frac{1}{\rho_I}\frac{\partial^3 \chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{1}{\rho_{II}}\frac{\partial^3 \chi_{II}}{\partial z^3}\right|_{z=f}\right) + \mathrm{O}\left(f^3\right).$$

The first two terms in (P.15) can be Taylor-series expanded to give

$$\begin{aligned} A\ddot{f}\,\overline{\chi}\big|_{z=f} + A\dot{f}^2\left.\overline{\frac{\partial \chi}{\partial z}}\right|_{z=f} &= A\ddot{f}\,\overline{\chi}\big|_{z=0} + A\left(\ddot{f}\cdot f\right)\left.\overline{\frac{\partial \chi}{\partial z}}\right|_{z=0} A\dot{f}^2\left.\overline{\frac{\partial \chi}{\partial z}}\right|_{z=0} + 3^{\text{rd}}\text{ order} \\ &= A\ddot{f}\,\overline{\chi}\big|_{z=0} + A\left(\ddot{f}\cdot f + \dot{f}^2\right)\left.\overline{\frac{\partial \chi}{\partial z}}\right|_{z=0} + 3^{\text{rd}}\text{ order} \end{aligned} \qquad \text{(P.16)}$$

To evaluate the $\mathrm{O}(f)$ term in equation (P.15), use equations (P.34) and (P.35) from Lemma 2:

$$\boxed{\text{The } \mathrm{O}(f) \text{ term}} = -f\left(\frac{1}{2\rho_{II}}\overset{4}{8}k_0^2\rho_{II}A\,\overline{\chi}\big|_{z=f} - \frac{B\ddot{f}\rho_{II}}{2\rho_{II}}\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3 \chi}{\partial z^3}\right]}\right|_{z=f}\right)$$
$$-f\left(\frac{1}{2\rho_I}\overset{4}{8}k_0^2\rho_I A\,\overline{\chi}\big|_{z=f} - \frac{B\ddot{f}\rho_I}{2\rho_I}\left.\overline{\left[\frac{1}{\rho^3}\frac{\partial^3 \chi}{\partial z^3}\right]}\right|_{z=f}\right) + \mathrm{O}\left(f\cdot\dot{f}, f\cdot\ddot{f}, f^3\right)$$
$$= -8k_0^2 f\cdot A\,\overline{\chi}\big|_{z=f} + B\left(f\cdot\ddot{f}\right)\left.\overline{\left[\frac{1}{\rho^3}\frac{\partial^3 \chi}{\partial z^3}\right]}\right|_{z=f} + \mathrm{O}\left(f\cdot\dot{f}, f\cdot\ddot{f}, f^3\right).$$

Now, expand in f on each side of the interface:

$$\boxed{\text{The O}\left(f\right)\text{ term}} = -8k_0^2 f\cdot A\,\overline{\chi}\big|_{z=0} - 8k_0^2 f^2 A\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}$$
$$+B\left(f\cdot\ddot{f}\right)\left.\overline{\left[\frac{1}{\rho^3}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} + \text{O}\left(f\cdot\dot{f}, f\cdot\dddot{f}; f^2\cdot\ddot{f}, f^3\right). \qquad \text{(P.17)}$$

We still need to evaluate the last term in equation (P.15), the $\text{O}\left(f^2\right)$ term. We have

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} = \frac{f^2}{2}\left(\left.\frac{1}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{1}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right)$$
$$= \frac{f^2}{2}\left[\frac{1}{2\rho_{II}}\left(\frac{\rho_{II}}{\rho_I}\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right) + \frac{1}{2\rho_I}\left(\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f} - \frac{\rho_I}{\rho_{II}}\left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right)\right].$$

Now use Lemma 1 in the form of equations (P.25) and (P.26) to get

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} = \frac{f^2}{2}\frac{1}{2\rho_{II}}\left(-\frac{8k_0^2 B}{\rho_{II}}\left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f}\right) + \frac{f^2}{2}\frac{8k_0^2\cancel{\rho_{II}}}{2\cancel{\rho_{II}}}A\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f}$$
$$+\frac{f^2}{2}\frac{1}{2\rho_I}\left(-\frac{8k_0^2 B}{\rho_I}\left.\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f}\right) + \frac{f^2}{2}\frac{8k_0^2\rho_{II}}{2\rho_I}A\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \text{O}\left(f^2\ddot{f}, f^2\dot{f}\right)$$
$$= -4k_0^2 f^2 B\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=f} + 4k_0^2 f^2 A\left(\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \underbrace{\frac{\rho_{II}}{\rho_I}\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f}}_{\partial\chi_{II}/\partial z}\right) + \text{O}\left(f^2\ddot{f}, f^2\dot{f}\right),$$

and so the $\text{O}\left(f^2\right)$ in equation (P.15) is

$$\boxed{\text{The O}\left(f^2\right)\text{ term}} = 4k_0^2 f^2 A\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0} - 4k_0^2 f^2 B\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} + 3^{\text{rd}}\text{ order}. \qquad \text{(P.18)}$$

Since equation (P.18) is already at 2nd order, we have used our freedom to slide χ down to $z=0$.

Now, take equations (P.16), (P.17) and (P.18), and substitute into equation (P.15). This gives us

$$\left.\frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z}\right|_{z=0} - \left.\frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\right|_{z=0} = A\ddot{f}\,\overline{\chi}\big|_{z=0} + A\left(\ddot{f}\cdot f + \dot{f}^2\right)\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}$$
$$-A\cdot 8k_0^2 f\,\overline{\chi}\big|_{z=0} - 8k_0^2 f^2 A\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}$$
$$+B\left(f\cdot\ddot{f}\right)\left.\overline{\left[\frac{1}{\rho^3}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} + 4k_0^2 f^2 A\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}$$
$$-4k_0^2 f^2 B\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} + \mathrm{O}\left(f\cdot\dot{f}, f\cdot\dddot{f}\right) + 3^{\text{rd}}\text{ order},$$

and combining terms

$$\left.\frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z}\right|_{z=0} - \left.\frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\right|_{z=0} = A\ddot{f}\,\overline{\chi}\big|_{z=0} - A\cdot 8k_0^2 f\,\overline{\chi}\big|_{z=0} + A\left(\ddot{f}\cdot f + \dot{f}^2\right)\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0}$$
$$-4k_0^2 f^2 A\left.\overline{\frac{\partial\chi}{\partial z}}\right|_{z=0} - 4k_0^2 f^2 B\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} \qquad \text{(P.19)}$$
$$+B\left(f\cdot\ddot{f}\right)\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}\right|_{z=0} + \mathrm{O}\left(f\cdot\dot{f}, f\cdot\dddot{f}\right) + 3^{\text{rd}}\text{ order}.$$

Now, once again as in Sections 3.2.3 and 4.3 and earlier in this calculation (just above equation (P.14)), follow Kuperman[65]: let $\chi(0) = \langle\chi\rangle\big|_{z=0} + \delta\chi$ and average. This gives us

$$\left.\frac{1}{\rho_I}\frac{\partial\langle\chi_I\rangle}{\partial z}\right|_{z=0} - \left.\frac{1}{\rho_{II}}\frac{\partial\langle\chi_{II}\rangle}{\partial z}\right|_{z=0} = \underbrace{A\left\langle\ddot{f}\,\overline{\delta\chi}\right\rangle_{z=0} - 8k_0^2 A\left\langle f\,\overline{\delta\chi}\right\rangle_{z=0}}_{\text{Diffuse (Bragg) scatter terms}}$$
$$-4k_0^2\left\langle f^2\right\rangle A\left.\overline{\frac{\partial\langle\chi\rangle}{\partial z}}\right|_{z=0} - 4k_0^2\left\langle f^2\right\rangle B\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}\right|_{z=0} \qquad \text{(P.20)}$$
$$+B\left\langle f\cdot\ddot{f}\right\rangle\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}\right|_{z=0} + 4^{\text{th}}\text{ order}.$$

Note that we have used

$$\left\langle f\cdot\dot{f}\right\rangle = 0 \quad ; \quad \left\langle f\cdot\dddot{f}\right\rangle = 0$$

as discussed in Section P.1.4 just below equation (P.28). We have also once again made use of the property of Gaussian functions that $\left\langle f^{\text{odd power}}\right\rangle = 0$.

We can also rewrite the last term as

$$B\left\langle f\cdot\ddot{f}\right\rangle\left[\overline{\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}}\right]_{z=0}=-B\left\langle\dot{f}^2\right\rangle\left[\overline{\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}}\right]_{z=0}.$$

This is the final answer of this section. Result (P.20) indeed provides the second boundary condition of equation (5.20). This boundary condition is further discussed in Section P.2.

P.1.3 Lemma 1: An expression needed to evaluated differences of 3rd derivatives

In this subsection, it will be shown that

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}-\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}=-\frac{8k_0^2B}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}+8k_0^2\rho_{II}A\frac{\partial\chi_I}{\partial z}\bigg|_{z=f}+\mathrm{O}\left(\ddot{f},\dot{f}\right). \quad \text{(P.21)}$$

Note that this result is only good through 0th order in the derivatives of f. That is all that is needed in the context in which it will be used. The results throughout Appendix P are only good through 2nd order in f and its derivatives, and the results of this lemma will be multiplied by a quantity that is already 2nd order in f and its derivatives.

$\frac{1}{\rho}\frac{\partial\chi}{\partial z}$ is continuous to $\mathrm{O}\left(\ddot{f}\right)$, which implies that the transverse derivative of this quantity is also continuous:

$$\hat{t}\cdot\vec{\nabla}\left[\Delta\left(\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right)\right]_{z=f}\equiv\hat{t}\cdot\vec{\nabla}\left[\frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z}\bigg|_{z=f}-\frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\bigg|_{z=f}\right]=0+\mathrm{O}\left(\ddot{f}\right). \quad \text{(P.22)}$$

Since $\hat{t}=\left(\hat{x}+\dot{f}\cdot\hat{z}\right)\Big/\sqrt{1+\dot{f}^2}$, equation (P.22) becomes

$$\frac{\partial}{\partial x}\left[\Delta\left(\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right)\right]_{z=f}=0+\mathrm{O}\left(\ddot{f},\dot{f}\right)$$

Now, use the fact ρ is range-independent in the half-spaces to commute it with $\partial/\partial x$, and then also commute $\partial/\partial x$ and $\partial/\partial z$. Next, use the parabolic equation: $\partial\chi/\partial x=iH\chi$, and this time note that H is independent of z in the half-spaces, and so commutes with $\partial/\partial z$ (recall that the density and compressibility are assumed constant in the half-spaces). This gives us

$$\left[\frac{H_I}{\rho_I}\frac{\partial\chi_I}{\partial z}\right]_{z=f}-\left[\frac{H_{II}}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\right]_{z=f}=0+\mathrm{O}\left(\ddot{f},\dot{f}\right). \quad \text{(P.23)}$$

Now, recall that with our conventions

$$H_I = \frac{\rho_{II}}{\rho_I}\frac{\nabla_T^2}{2k_0} + k_0\gamma_I$$
$$H_{II} = \frac{\nabla_T^2}{2k_0} - k_0\mu_{II} \quad ,$$

and so substituting into (P.23), we have

$$\frac{1}{2k_0}\frac{\rho_{II}}{\rho_I^2}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} + \frac{k_0\gamma_I}{\rho_I}\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} - \frac{1}{2k_0}\frac{1}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} + \frac{k_0\mu_{II}}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\bigg|_{z=f} = 0 + \mathrm{O}\left(\ddot{f},\dot{f}\right),$$

and pulling out $1/(2k_0\rho_I)$

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} - \frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} + 2k_0^2\gamma_I\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} + 2k_0^2\mu_{II}\underbrace{\frac{\rho_I}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\bigg|_{z=f}}_{\partial\chi_I/\partial z} = 0 + \mathrm{O}\left(\ddot{f},\dot{f}\right).$$

This gives us the basic equation

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} - \frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} + 2k_0^2\underbrace{\left(\gamma_I + \mu_{II}\right)}_{-4\rho_{II}A}\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} = 0 + \mathrm{O}\left(\ddot{f},\dot{f}\right). \qquad \text{(P.24)}$$

Now, let us get a couple of useful alternate versions of (P.24). First, start with

$$\underbrace{\left(-1+\frac{\rho_{II}}{\rho_I}\right)}_{\delta\rho/\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} + \frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} - \frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} - 8k_0^2\rho_{II}A\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} = 0 + \mathrm{O}\left(\ddot{f},\dot{f}\right)$$

to get

$$\begin{aligned}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} - \frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} &= -\frac{\delta\rho}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} + 8k_0^2\rho_{II}A\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} + \mathrm{O}\left(\ddot{f},\dot{f}\right) \\ &= -\frac{8k_0^2B}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} + 8k_0^2\rho_{II}A\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} + \mathrm{O}\left(\ddot{f},\dot{f}\right).\end{aligned} \qquad \text{(P.25)}$$

Now, go back to the basic equation (P.24), and rearrange it to get

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f} - \frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} + \underbrace{\left(1-\frac{\rho_I}{\rho_{II}}\right)}_{\delta\rho/\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f} - 8k_0^2\rho_{II}A\frac{\partial\chi_I}{\partial z}\bigg|_{z=f} = 0 + \mathrm{O}\left(\ddot{f},\dot{f}\right),$$

and so

$$\left.\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\right|_{z=f} - \left.\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f} = -\left.\frac{\delta\rho}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f} + 8k_0^2\rho_{II}A\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \mathrm{O}\left(\ddot{f},\dot{f}\right)$$
$$= -\left.\frac{8k_0^2B}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\right|_{z=f} + 8k_0^2\rho_{II}A\left.\frac{\partial\chi_I}{\partial z}\right|_{z=f} + \mathrm{O}\left(\ddot{f},\dot{f}\right). \qquad \text{(P.26)}$$

The second equality is the form of the result quoted in equation (P.21). Both (P.25) and (P.26) are used during the calculation pursued in Subsection P.1.1.

P.1.4 Lemma 2: An expression needed to evaluated differences of second derivatives

In this section, it will be shown that

$$\left.\frac{\partial^2\chi_I}{\partial z^2}\right|_{z=f} - \left.\frac{\rho_I}{\rho_{II}}\frac{\partial^2\chi_{II}}{\partial z^2}\right|_{z=f} = 8k_0^2\rho_I A\,\overline{\chi}\big|_{z=f} - B\ddot{f}\rho_I\left[\overline{\frac{1}{\rho^3}\frac{\partial^3\chi}{\partial z^3}}\right]_{z=f} + \mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right). \qquad \text{(P.27)}$$

Note that this result is valid to 1st order in the even derivatives of f, but only to 0th order in its odd derivatives. For reasons to be discussed below, the accuracy of (P.27) will prove sufficient to eventually produce a stochastic theory good through 2nd order in f and its derivatives. The results throughout Appendix P are only good through this order.

We begin with the first boundary condition in (P.1).

$$\chi_I\big|_{z=f} - \chi_{II}\big|_{z=f} = -B\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=f} + \mathrm{O}\left(\dot{f}^2\right).$$

This implies that

$$\chi_I\big|_{z=f} - \chi_{II}\big|_{z=f} + B\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=f} = 0 + \mathrm{O}\left(\dot{f}^2\right)$$

on the interface. Thus, taking the tangential derivative $\hat{t}\cdot\vec{\nabla} = \partial/\partial x + \dot{f}\cdot\partial/\partial z + \mathrm{O}\left(\dot{f}^2\right)$ of this equation valid on the interface and noting that the density ρ is constant in the half-spaces, we wind up with

$$\left.\frac{\partial\chi_I}{\partial x}\right|_{z=f} - \left.\frac{\partial\chi_{II}}{\partial x}\right|_{z=f} + B\dddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial\chi}{\partial z}}\right]_{z=f} + B\ddot{f}\left[\overline{\frac{1}{\rho}\frac{\partial}{\partial x}\left(\frac{\partial\chi}{\partial z}\right)}\right]_{z=f} = 0 + \mathrm{O}\left(\dot{f},\dot{f}^2\right). \qquad \text{(P.28)}$$

Note that we are already dropping the $\mathrm{O}\left(\dot{f}\right)$ term (proportional to $\partial/\partial z$) in anticipation of the result we now derive. In the context of the calculation presented above in Appendix P, result (P.28) will eventually be multiplied by a quantity proportional to f and averaged. The average of f multiplied by odd derivatives such as $\left\langle f\cdot\dot{f}\right\rangle$ or $\left\langle f\cdot\dddot{f}\right\rangle$ is zero. To see this, consider the autocorrelation function

$$\left\langle f(x_1)f(x_2)\right\rangle=\int_{-\infty}^{\infty}dk\ S(k)e^{ik(x_1-x_2)}.$$

Since f is real, $S(k)$ must be symmetric: $S(k)=S(-k)$. Take $\partial/\partial x_1$, and set $x_1=x_2=x$. This gives us

$$\left\langle \dot{f}\cdot f\right\rangle=\int_{-\infty}^{\infty}dk\ \underbrace{S(k)}_{\text{even}}\underbrace{k}_{\text{odd}}=0\quad;\quad\left\langle \dddot{f}\cdot f\right\rangle=\int_{-\infty}^{\infty}dk\ \underbrace{S(k)}_{\text{even}}\underbrace{k^3}_{\text{odd}}=0.$$

Thus, in the context of the calculation presented in Appendix P, an error in equation (P.28) of 1st order in its odd derivative will still be good enough to eventually yield a result good to 2nd order in f and its derivatives. Since this order is consistent with the accuracy elsewhere in this appendix, let us drop the remaining $\mathrm{O}\left(\ddot{f}\right)$ term right away. Note that equation (P.28) good through 1st order in f and its *even* derivatives is also sufficient to eventually produce the desired 2nd order accuracy.

Now recall that we are an infinitesimal distance into the half-spaces, and so all quantities are effectively constant, and $\partial/\partial x$, $\partial/\partial z$ and the Hamiltonian H freely commute. Use the parabolic equation to replace all $\partial\chi/\partial x$ with $iH\chi$ and divide by i. Equation (P.28) now gives us

$$\begin{aligned}\left[H_I\chi_I\right]_{z=f}-\left[H_{II}\chi_{II}\right]_{z=f}+B\ddot{f}\left[\frac{1}{\rho_I}\left(H_I\frac{\partial\chi_I}{\partial z}\right)_{z=f}+\frac{1}{\rho_{II}}\left(H_{II}\frac{\partial\chi_{II}}{\partial z}\right)_{z=f}\right].\\=0+\mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right)\end{aligned}\qquad\text{(P.29)}$$

Next, as in Section P.1.3 use

$$H_I=\frac{\rho_{II}}{\rho_I}\frac{\nabla_T^2}{2k_0}+k_0\gamma_I$$

$$H_{II}=\frac{\nabla_T^2}{2k_0}-k_0\mu_{II}$$

and multiply through by $2k_0$.

Let us concentrate on the $\mathrm{O}\left(\ddot{f}\right)$ term first:

$$\frac{B\ddot{f}}{2}\left[\frac{\rho_{II}}{\rho_I^2}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}+\frac{1}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}+\frac{2k_0^2\gamma_I}{\rho_I}\frac{\partial\chi_I}{\partial z}\bigg|_{z=f}-2k_0^2\mu_{II}\underbrace{\left(\frac{1}{\rho_{II}}\frac{\partial\chi_{II}}{\partial z}\bigg|_{z=f}\right)}_{\frac{1}{\rho_I}\frac{\partial\chi_I}{\partial z}\Big|_{z=f}+O\left(\ddot{f}\right)}\right]$$

$$\underbrace{\frac{B\ddot{f}}{2\rho_I}\left[\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}+\frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}\right]}_{\text{Consider this term first}}+\frac{B\ddot{f}}{2}\left[2k_0^2\left(\gamma_I-\mu_{II}\right)\left(\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right)\right]+2^{\text{nd}}\text{ order.}$$

Now note that

$$\begin{aligned}\left[\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}+\frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}\right]&=\frac{\rho_I\rho_{II}}{\rho_I\rho_{II}}\left[\frac{\rho_{II}}{\rho_I}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}+\frac{\rho_I}{\rho_{II}}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}\right]\\&=\rho_I\rho_{II}\left[\frac{1}{\rho_I^2}\frac{\partial^3\chi_I}{\partial z^3}\bigg|_{z=f}+\frac{1}{\rho_{II}^2}\frac{\partial^3\chi_{II}}{\partial z^3}\bigg|_{z=f}\right]\\&=2\rho_I\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f},\end{aligned}$$

and we have for the $\mathrm{O}\left(\ddot{f}\right)$ term in equation (P.29) (times $2k_0$):

$$\begin{aligned}&2k_0\cdot B\ddot{f}\left[\frac{1}{\rho_I}H_I\left(\frac{\partial\chi_I}{\partial z}\right)_{z=f}+\frac{1}{\rho_{II}}H_{II}\left(\frac{\partial\chi_{II}}{\partial z}\right)_{z=f}\right]\\&=B\ddot{f}\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}+B\ddot{f}\cdot k_0^2\left(\gamma_I-\mu_{II}\right)\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]+\cdots\ .\end{aligned}\qquad\text{(P.30)}$$

The other term in (P.29) becomes (recall we are multiplying by $2k_0$):

$$2k_0\left(H_I\chi_I-H_{II}\chi_{II}\right)=\frac{\rho_{II}}{\rho_I}\nabla_T^2\chi_I-\nabla_T^2\chi_{II}+2k_0^2\gamma_I\chi_I+2k_0^2\mu_{II}\chi_{II}\,.\qquad\text{(P.31)}$$

Substituting (P.30) and (P.31) into (P.29) (times $2k_0$) gives us

$$0=\frac{\rho_{II}}{\rho_I}\nabla_T^2\chi_I-\nabla_T^2\chi_{II}+2k_0^2\gamma_I\chi_I+2k_0^2\mu_{II}\chi_{II}$$
$$+B\ddot{f}\,\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}+B\ddot{f}\cdot k_0^2\left(\gamma_I-\mu_{II}\right)\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}+\mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right)$$

or

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}\bigg|_{z=f}-\frac{\partial^2\chi_{II}}{\partial z^2}\bigg|_{z=f}=-2k_0^2\gamma_I\,\chi_I\big|_{z=f}-2k_0^2\mu_{II}\,\chi_{II}\big|_{z=f}-B\ddot{f}\,\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}$$
$$-B\ddot{f}\cdot k_0^2\left(\gamma_I-\mu_{II}\right)\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}_{z=f}+\mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right). \tag{P.32}$$

Now, at $z=f$ (the interface), we have from the first boundary condition (P.1)

$$\chi_I=\overline{\chi}+\frac{\chi_I-\chi_{II}}{2}=\overline{\chi}-\frac{B\ddot{f}}{2}\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}+\mathrm{O}\left(\dot{f}^2\right)$$
$$\chi_{II}=\overline{\chi}-\frac{\chi_I-\chi_{II}}{2}=\overline{\chi}+\frac{B\ddot{f}}{2}\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}+\mathrm{O}\left(\dot{f}^2\right),$$

and so at $z=f$ (the interface) we have

$$-2k_0^2\left(\gamma_I\,\chi_I\big|_{z=f}+\mu_{II}\,\chi_{II}\big|_{z=f}\right)=-2k_0^2\left(\gamma_I+\mu_{II}\right)\overline{\chi}\big|_{z=f}$$
$$-\cancel{2}k_0^2\left(-\gamma_I+\mu_{II}\right)\frac{B\ddot{f}}{\cancel{2}}\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}_{z=f}+\mathrm{O}\left(\dot{f}^2\right)$$
$$=-2k_0^2\left(\gamma_I+\mu_{II}\right)\overline{\chi}\big|_{z=f}$$
$$+k_0^2\left(\gamma_I-\mu_{II}\right)B\ddot{f}\overline{\left[\frac{1}{\rho}\frac{\partial\chi}{\partial z}\right]}_{z=f}+\mathrm{O}\left(\dot{f}^2\right). \tag{P.33}$$

Substituting (P.33) into (P.32), we see that the two terms proportional to $\partial\chi/\partial z$ cancel and we are left with

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}\bigg|_{z=f}-\frac{\partial^2\chi_{II}}{\partial z^2}\bigg|_{z=f}=-2k_0^2\underbrace{\left(\gamma_I+\mu_{II}\right)}_{-4\rho_{II}A}\overline{\chi}\big|_{z=f}-B\ddot{f}\,\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}+\mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right)$$

or

$$\frac{\rho_{II}}{\rho_I}\frac{\partial^2\chi_I}{\partial z^2}\bigg|_{z=f}-\frac{\partial^2\chi_{II}}{\partial z^2}\bigg|_{z=f}=8k_0^2\rho_{II}A\,\overline{\chi}\big|_{z=f}-B\ddot{f}\,\rho_{II}\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\chi}{\partial z^3}\right]}_{z=f}+\mathrm{O}\left(\dot{f},\ddot{f},\dot{f}^2\right). \tag{P.34}$$

Multiplying through by ρ_I/ρ_{II}, we reproduce equation (P.27):

$$\left.\frac{\partial^2 \chi_I}{\partial z^2}\right|_{z=f} - \frac{\rho_I}{\rho_{II}}\left.\frac{\partial^2 \chi_{II}}{\partial z^2}\right|_{z=f} = 8k_0^2 \rho_I A \overline{\chi}\big|_{z=f} - B\ddot{f}\rho_I \overline{\left[\frac{1}{\rho^3}\frac{\partial^3 \chi}{\partial z^3}\right]}_{z=f} + \mathrm{O}\left(\dot{f}, \ddot{f}, f^2\right). \quad \text{(P.35)}$$

Both equations (P.34) and (P.35) will be used in the calculations pursued in Sections P.1.1 and P.1.2.

P.2 Discussion of the $\partial\chi/\partial x$ boundary condition

Subsection P.2.1 examines some superficially surprising aspects of the $\partial\chi/\partial x$ boundary condition (equation (P.20)), and Subsection P.2.2 reinforce the veracity of the result. Subsection P.2.3 sums up the discussion.

P.2.1 Unaesthetic aspects of the $\partial\chi/\partial x$ boundary condition for quasi-first order theory

The structure of equation (P.20) seems to suggest that the $\partial\chi/\partial z$ boundary condition in the deterministic result (5.16) (or equivalently (P.1)) is missing a term of the form

$$B\dot{f}^2 \overline{\left[\frac{1}{\rho^2}\frac{\partial^3 \chi}{\partial z^3}\right]}_{z=f}. \quad \text{(P.36)}$$

In the stochastic problem, this term would become

$$B\left\langle \dot{f}^2 \right\rangle \overline{\left[\frac{1}{\rho^2}\frac{\partial^3 \langle\chi\rangle}{\partial z^3}\right]}_{z=f},$$

and when introduced as an additional term into the stochastic boundary condition for $\partial\langle\chi\rangle/\partial z$ (equation (P.20)), it would provide the usual cancellation with the term proportional to $\left\langle f \cdot \ddot{f} \right\rangle$. If present, term (P.36) would also maintain the rule that the transverse (i.e., traditional) Lamb shift (i.e., the part generated by smearing alone) can be obtained by substituting $-4k_0^2\left\langle f^2 \right\rangle$ for $\dot{f}^2$ into the "vacuum polarization" terms (i.e., downrange Lamb shift) for the *deterministic* tilted interface and setting $\ddot{f} = 0$. This rule is essentially equivalent to the assertion that we can naively take the procedure for distorted *volume* given in Subsection 3.2.2, and apply it to an *interface* $z = f$, where f now measures the distortion of a range-independent surface. This procedure involves expanding the Hamiltonian in a Taylor series to get a stochastic roughness-induced term (see equation (3.16) and the related discussion):

$$\frac{\left\langle f^2 \right\rangle}{2} \frac{\partial^2 \langle H \rangle}{\partial z^2} . \tag{P.37}$$

However, expression (P.37) will not generate the term

$$-4k_0^2 \left\langle f^2 \right\rangle B\left[\overline{\frac{1}{\rho^2} \frac{\partial^3 \langle \chi \rangle}{\partial z^3}} \right]_{z=0}$$

that appears in equation (P.20)—for exactly the same reason that term (P.36) is absent. Up to now expression (P.37) has worked even when singularities are present, but this time the absence of the term (P.36) has led to an exception for this rule of thumb.

Furthermore, as it stands equation (P.20) suffers from another rather unaesthetic trait. To demonstrate that the two terms

$$-4k_0^2 \left\langle f^2 \right\rangle B\left[\overline{\frac{1}{\rho^2} \frac{\partial^3 \langle \chi \rangle}{\partial z^3}} \right]_{z=0} \quad \text{and} \quad B\left\langle f \cdot \ddot{f} \right\rangle \left[\overline{\frac{1}{\rho^2} \frac{\partial^3 \langle \chi \rangle}{\partial z^3}} \right]_{z=0}$$

conserve energy, one would have to engage in formal gymnastics: Basically, we would need to add extra δ''' - and $\nabla_T \delta' \nabla_T$ -terms to the Hamiltonian to bring these boundary conditions into our stochastic Hamiltonian as Hermitian contact potentials.

P.2.2 The "unaesthetic" result is nevertheless correct

These two aesthetic shortcomings cause some concern that there might be some subtle error in the reasoning that produced equation (P.20).

The latter concern, namely that the argument establishing energy conservation for the two terms proportional to $\left[\overline{1/\rho^2 \cdot \partial^3 \langle \chi \rangle / \partial z^3} \right]_{z=f}$ turns out to be unusually subtle, might incline us to conclude that these terms were somehow erroneously introduced into equation (P.20). However, there is simply no solid reason to conclude that these terms are artifacts. They clearly fall out of the calculation.

Concerning the first issue, namely the surprising absence from the deterministic result of the term (P.36), it is relatively unlikely that there is some fundamental flaw in our technique, which caused us to accidentally drop this "missing term". The only unusual aspect of the calculation that produced the deterministic result was the use of δ -function bifurcation to evaluate products of distributions (i.e., generalized functions), but this technique only affects terms that are 2nd order in the density jump ($\mathrm{O}\left(\delta\rho^2\right)$) or of higher

than 2nd order in the slope $\dot{f}$, while the missing term $\dot{f}^2 B\overline{\left[1/\rho^2 \cdot \partial^3 \chi/\partial z^3\right]}_{z=f}$ already shows up at 1st order in $\delta\rho$ and at 2nd order in $\dot{f}$ [kkkk].

Thus, we would be well advised to accept equation (P.20) as is, and not allow it to be trumped by some preconceived notion of what it should be. The soundness of this decision is further reinforced by the observation that, in a sense, the missing term is already hidden in our current result. Examining equation (M.12) and the argument leading up to it, we see that $-\ddot{\lambda}/8k_0^2$, the term that generates the "vacuum polarization" contribution to the deterministic result (5.16) (or equivalently (P.1)), contains a hanging (or invisible) contribution:

[kkkk] It is easy to verify that we are not overlooking other terms that are 1st order in $\delta\rho$, 2nd order in f and its derivatives, might involve δ-function bifurcation, and may in some way substitute for the "missing term". For example, in principle δ-function bifurcation can affect terms that are 2nd order in the curvature (i.e., $\mathrm{O}\left(\ddot{f}^2\right)$). However, $\ddot{f}^2$ does not mimic the behavior of $\dot{f}^2$ in either the deterministic or the stochastic problem, so $\mathrm{O}\left(\ddot{f}^2\right)$ terms are not proper substitutes for the missing $O\left(\dot{f}^2\right)$ term. At first glance, terms of $\mathrm{O}\left(\ddot{f} \cdot f\delta\rho\right)$ are more promising substitutes for the $\mathrm{O}\left(\dot{f}^2\delta\rho\right)$ term, since such terms can mimic the each other's behavior in the stochastic problem. However, it is hard to see how terms in the "vacuum polarization" series, where the surface function is pulled out by taking some number of range derivatives of the step function $\Theta\left(z - f\left(x\right)\right)$, could possibly lead to something proportional to $\mathrm{O}\left(\ddot{f} \cdot f\delta\rho\right)$. Thus, this backdoor channel for generating something in the deterministic problem, which later functions like the missing term once we get to the stochastic problem, is not available either. Thus, the problem term is indeed $\mathrm{O}\left(\dot{f}^2\delta\rho\right)$, and not $\mathrm{O}\left(\ddot{f}^2\delta\rho\right)$ or even $\mathrm{O}\left(\ddot{f} \cdot f\delta\rho\right)$. Of course anything $\mathrm{O}\left(\delta\rho^2\right)$ comes in addition to the already problematic $\mathrm{O}\left(\delta\rho\right)$ term. At order $\mathrm{O}\left(\dot{f}^2\delta\rho\right)$, δ-function bifurcation has no relevance, and so it also has no relevance to the "surprising" behavior arising from the absence of the $\mathrm{O}\left(\ddot{f}^2\delta\rho\right)$ term.

$$-\frac{\rho_0 \dot{f}^2 \delta\rho}{16k_0^3}\nabla_T \delta'(z-f)\overline{\left[\frac{1}{\rho^2}\frac{\partial\chi}{\partial z}\right]}_{z=f} = -\frac{\rho_0 \dot{f}^2 B}{2k_0}\delta''(z-f)\overline{\left[\frac{1}{\rho^2}\frac{\partial\chi}{\partial z}\right]}_{z=f}$$

(note that as always ρ_0 is chosen to be ρ_{II}). This term does not contribute to quasi-1st order theory, because it will not contribute to a single or double infinitesimal integration (see Subsection 3.3.3 for the conversion from contact potentials to boundary conditions using infinitesimal integrations). However, in the $\mathrm{O}\left(\lambda^2, \ddot{\lambda}\right)$ theory, it will show up as a boundary condition on $\partial\chi/\partial z$ that is $\mathrm{O}\left(\dot{f}^2\delta\rho\right)$, just like the "missing" term we have been seeking. Indeed, it is easy to show that we now have the cancellation that has been lacking from our formalism[IIII]. The boundary condition that was absent from $\mathrm{O}\left(\lambda, \ddot{\lambda}\right)$ (quasi-1st order) theory has now effectively migrated back into $\mathrm{O}\left(\lambda^2, \ddot{\lambda}\right)$ theory. The effect that was related to its absence in quasi-1st order is still there, but it has shifted up to the boundary condition on the third derivative. We never get rid of it; it just migrates just like any of our effects generated by contact potentials. The effect appears to be real, and it constitutes a "downrange Lamb shift" (i.e., "vacuum polarization") contribution associated with a density jump.

P.2.3 The bottom line

Thus, the bottom line is that the contribution to the stochastic boundary condition on the first derivative (i.e., equation (P.20)) that is proportional to $\left\langle \ddot{f}\cdot f\right\rangle\delta\rho$ is surprising and a

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[IIII] The related term $-\left[\left(\rho_0\ddot{f}\cdot B\right)/\left(2k_0\right)\right]\delta'(z-f)\overline{\left[\left(1/\rho^2\right)\left(\partial\chi/\partial z\right)\right]}_{z=f}$, which contributed to the discontinuity in χ in $\mathrm{O}\left(\lambda, \ddot{\lambda}\right)$ theory, now in $\mathrm{O}\left(\lambda^2, \ddot{\lambda}\right)$ theory directly modifies the boundary condition on the second derivative $\partial^2\chi/\partial z^2$. When we use the usual procedure to evaluate the stochastic boundary condition on $\partial\left\langle\chi\right\rangle/\partial z$, the usual expansion that we use to project down to the $z=0$ line generates a term proportional to $f\left(\partial^2\chi_I/\partial z^2 - \partial^2\chi_{II}/\partial z^2\right)$. The new contribution to the difference between the second derivatives will in turn generate a new term proportional to $f\cdot\ddot{f}\delta\rho$, which once averages are taken provides the long-awaited cancellation with the now-present term proportional to $\dot{f}^2\delta\rho$.

little suspicious, but for now we have to accept it as is, and keep an open mind as future research either confirms or refutes this finding.

When performing a numerical calculation of the Lamb shift for a realistic shallow water environment (Section 5.4), we will employ the following practical strategy: Since it is the most important contribution, and by far the easiest to evaluate, we will concentrate only on the component of the acoustic Lamb shift that involves the wave function χ and its 1st derivative, and drop the terms that involve the 2nd and 3rd derivatives (this includes the "vacuum polarization" term) from our initial assessment of the significance of the acoustic Lamb shift. For future use, Section P.3 discusses the stepping algorithm for the full quasi-1st order stochastic theory that includes the terms that do involve the 2nd and 3rd derivatives (including the "vacuum polarization" effect).

P.3 A downrange stepping procedure of the quasi-1st order result

Here, we consider stochastic quasi-1st order (i.e., $O\left(\lambda,\ddot{\lambda}\right)$) theory as given by boundary conditions (P.14) and (P.20). We either drop the loss terms associated with Bragg scattering and just consider the downrange propagation of the coherent field, or we evaluate these terms by writing the locally generated incoherent field $\delta\chi$ as some constant times the incoherent field (see a brief discussion in Subsection 3.2.2 just below equation (3.16) and also reference [64] for more on this general approach). The stochastic theory is good to 2nd order in the surface height and its derivatives, and at this order, it involves the mean square surface height $\left\langle f^2 \right\rangle$ and the mean square slope $\left\langle \dot{f}^2 \right\rangle$. As throughout this paper, the surface is assumed to be Gaussian.

Only the Hamiltonian away from the interface is directly involved in downrange stepping, and the lead transverse derivative in this Hamiltonian comes from $\langle\lambda\rangle$ and is 2nd order: $\partial^2\langle\chi\rangle/\partial z^2$. The $O\left(\left\langle\ddot{\lambda}\right\rangle\right)$ contribution contributes a term proportional to $\left\langle \dot{f}^2 \right\rangle$ in the boundary conditions at the interface. This and some other terms (associated with downrange smearing) in the stochastic boundary conditions (P.20) are proportional to the 2nd and 3rd-order transverse derivatives of $\langle\chi\rangle$. These terms create tricky issues for the stepping algorithm, and in this section, we will develop a stepping algorithm that

addresses these issues[mmmm]. This procedure will not be used in Section 5.4, since there the terms that involve the 2nd and 3rd derivatives will simply be dropped.

Assume that we have just stepped on side I (above the flat interface), and we have $\langle \chi_I \rangle$ just above the interface (and of course also $\langle \chi \rangle$ at all grid points away from the interface). Now, use the 0th order (in f and its derivatives)[nnnn] boundary conditions to evaluate $\langle \chi \rangle$ on both sides (i.e., $\langle \chi_{II} \rangle = \langle \chi_I \rangle$). Next use finite differences to calculate

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[mmmm] The deterministic problem would proceed in a similar fashion. There is some added complexity, since the interface is tilted and so in general we would need to evaluate $H\chi$ on both sides of the interface. On the other hand, we would benefit from some simplification, since the deterministic problem does not involve 3rd derivatives. It is not worth examining the deterministic case in detail, because it is unlikely that this problem will be solved numerically using quasi-1st order theory. As shown in Section 6.1, $\mathrm{O}\left(\lambda^2\right)$ theory introduces effects that are far more important than the effects introduced by the $\mathrm{O}\left(\ddot{\lambda}\right)$ term. In the $\mathrm{O}\left(\lambda^2\right)$ theory, the wave function χ is continuous and it remains so when the $\mathrm{O}\left(\ddot{\lambda}\right)$ term is added. Furthermore, in the $\mathrm{O}\left(\lambda^2\right)$ theory, the lead order is a 4th derivative, and the 2nd and 3rd derivatives from the $\mathrm{O}\left(\ddot{\lambda}\right)$ raise no special issues. Thus, $\mathrm{O}\left(\lambda^2,\ddot{\lambda}\right)$ theory is perfectly well behaved, and there is no reason to worry about the extra complexities that emerge in $\mathrm{O}\left(\lambda,\ddot{\lambda}\right)$ theory. On the other hand, in stochastic theory, the $\mathrm{O}\left(\lambda\right)$ component already leads to the problems discussed here in Appendix P.3, and we cannot avoid these issues.

[nnnn] Since these terms eventually get multiplied by terms that are already 2nd order in f and its derivatives, 0th order in f and its derivatives is all we need at this stage. In stochastic theory for a Gaussian surface, terms that are 0th order in f and its derivatives come with an error term that is 2nd order in f and its derivatives. The reason is that for a Gaussian surface, the expectation values of odd powers in the surface function (or its derivatives) are zero.

$\partial\langle\chi_{II}\rangle/\partial z$ and then use the 0th order (in f and its derivatives)nnnn boundary condition on $\partial\langle\chi\rangle/\partial z$ to find $\partial\langle\chi_I\rangle/\partial z$:

$$\frac{\partial\langle\chi_I\rangle}{\partial z}=\left(\frac{\rho_I}{\rho_{II}}\right)\left[\frac{\partial\langle\chi_{II}\rangle}{\partial z}\right]+2^{\text{nd}}\text{ order}.$$

Now use finite differences to obtain $\partial^2\langle\chi_I\rangle/\partial z^2$, and a stochastic version of the implicit boundary condition (P.34) to get (to $\mathrm{O}\left(f^0\right)$)nnnn

$$\left.\frac{\partial^2\langle\chi_{II}\rangle}{\partial z^2}\right|_{z=0}=-\frac{\rho_{II}}{\rho_I}\left.\frac{\partial^2\langle\chi_I\rangle}{\partial z^2}\right|_{z=0}-8k_0^2\rho_{II}A\langle\chi\rangle\big|_{z=0}+2^{\text{nd}}\text{ order}.$$

(Recall that at $\mathrm{O}\left(f^0\right)$, $\langle\chi_I\rangle=\langle\chi_{II}\rangle=\langle\chi\rangle$.) Since we now have second derivatives on both sides, we can take the average

$$\left.\overline{\left[\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}\right]}\right|_{z=0}=-4k_0^2A\langle\chi\rangle\big|_{z=0}+2^{\text{nd}}\text{ order}.$$

We can also use finite differences to get $\partial^3\langle\chi_{II}\rangle/\partial z^3$. We still need to evaluate the average

$$\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}\right|_{z=0}.$$

To do so, note that (to $\mathrm{O}\left(f^0\right)$)nnnn

$$\begin{aligned}\left.\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}\right|_{z=0}&=\frac{1}{2}\left[\frac{1}{\rho_I^2}\frac{\partial^3\langle\chi_I\rangle}{\partial z^3}+\frac{1}{\rho_{II}^2}\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right]\\&=\frac{1}{2\rho_{II}^2}\left[\frac{\rho_{II}}{\rho_I}\left(\frac{\rho_{II}}{\rho_I}\frac{\partial^3\langle\chi_I\rangle}{\partial z^3}\right)+\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right]+2^{\text{nd}}\text{ order}.\end{aligned}\qquad\text{(P.38)}$$

Now use the stochastic version of the implicit boundary condition (P.26) projected down to the $z=0$ line. Again, this is valid to 0th order in f nnnn. The boundary condition is:

$$\begin{aligned}\left.\frac{\rho_{II}}{\rho_I}\frac{\partial^3\langle\chi_I\rangle}{\partial z^3}\right|_{z=0}&=\left.\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right|_{z=0}-\left.\frac{8k_0^2B}{\rho_{II}}\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right|_{z=0}+\left.8k_0^2\rho_{II}A\frac{\partial\langle\chi_I\rangle}{\partial z}\right|_{z=0}\\&=\left(1-\frac{8k_0^2B}{\rho_{II}}\right)\left.\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right|_{z=0}+\left.8k_0^2\rho_{II}A\frac{\partial\langle\chi_I\rangle}{\partial z}\right|_{z=0}+2^{\text{nd}}\text{ order}.\end{aligned}$$

Now, substitute it into (P.38):

$$\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}_{z=0}$$

$$=\frac{1}{2\rho_{II}^2}\left[\frac{\rho_{II}}{\rho_I}\left(1-\frac{8k_0^2B}{\rho_{II}}\right)\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\bigg|_{z=0}+8k_0^2\rho_{II}A\underbrace{\frac{\rho_{II}}{\rho_I}\frac{\partial\langle\chi_I\rangle}{\partial z}\bigg|_{z=0}}_{\partial\langle\chi_{II}\rangle/\partial z}+\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\right]$$

$$=\frac{1}{2\rho_{II}^2}\left[\left[1+\frac{\rho_{II}}{\rho_I}\left(1-\frac{8k_0^2B}{\rho_{II}}\right)\right]\underbrace{\frac{\partial^3\langle\chi_{II}\rangle}{\partial z^3}\bigg|_{z=0}}_{\text{known}}+8k_0^2\rho_{II}A\underbrace{\frac{\partial\langle\chi_{II}\rangle}{\partial z}\bigg|_{z=0}}_{\text{known}}\right]+2^{\text{nd}}\text{ order.}$$

Next, plug in our values for

$$\overline{\left[\frac{1}{\rho}\frac{\partial^2\langle\chi\rangle}{\partial z^2}\right]}_{z=0}\quad\text{and}\quad\overline{\left[\frac{1}{\rho^2}\frac{\partial^3\langle\chi\rangle}{\partial z^3}\right]}_{z=0}$$

into boundary condition (P.14) to get $\langle\chi_{II}\rangle$ to $\mathrm{O}(f^2)$ (we already know $\langle\chi_I\rangle$ to this order). Now get $\partial\langle\chi_{II}\rangle/\partial z$ using finite differences, and then use boundary condition (P.20) to get $\partial\langle\chi_I\rangle/\partial z$. Finally, use finite differences to get $\partial^2\langle\chi_I\rangle/\partial z^2$ and so $\langle H_I\rangle\langle\chi_I\rangle$. Now, we can step and start the procedure all over again!

Q Appendix: The boundary conditions for O(λ^2) theory

In this appendix (as throughout this paper when the focus is on the interface itself), we only consider 1-dimensional interfaces embedded in 2-dimensional spaces, where x is the range and z is the depth (as always, the positive z-axis points up into region I). The (now) scalar transverse derivative ∇_T and $\partial/\partial z$ are used interchangeably.

Q.1 The boundary conditions

In this section, we derive equation (6.15). The $\mathrm{O}(\lambda^2)$ equation of motion is given by equation (6.14) rewritten below:

$$-i\frac{\partial\chi}{\partial x}=k_0\left(1-2\gamma+\frac{\lambda}{k_0}-\frac{\lambda^2}{2k_0^2}\right)\chi\,. \qquad \text{(Q.1)}$$

In this section, we let $\Xi \equiv k_0(\gamma - \mu)$, and so

$$\begin{aligned} \lambda &= \frac{\rho_0 \nabla_T \left(\frac{1}{\rho}\right) \nabla_T}{2k_0} + \Xi \\ \lambda^2 &= \frac{\rho_0^2 \cdot \nabla_T \left(\frac{1}{\rho}\right) \nabla_T^2 \left(\frac{1}{\rho}\right) \nabla_T}{4k_0^2} + \frac{\rho_0 \nabla_T \left(\frac{1}{\rho}\right) \nabla_T}{2k_0} \Xi + \Xi \frac{\rho_0 \nabla_T \left(\frac{1}{\rho}\right) \nabla_T}{2k_0} + \Xi^2 \end{aligned} \quad . \qquad \text{(Q.2)}$$

The basic strategy for extracting boundary conditions from equation (Q.1) is as follows. Recalling that for the 2-dimensional problem, $\nabla_T = \partial / \partial z$, we take 0, 1, 2, and 3 indefinite integrations $\int dz \cdots$ followed by an infinitesimal integration at the interface $z = f(x)$:

$$\int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$$

Since the lead order term involves an operator of the form $\nabla_T \left(1/\rho\right) \nabla_T^2 \left(1/\rho\right) \nabla_T$, we will also need to multiply by ρ after the first and third *indefinite* integration. Note that the lead order term is the most important term as far as this procedure is concerned. The difference between the order of this term and the total number of integrations (counting both the indefinite integrations and the definite integrations over infinitesimal intervals that cross the interface) will determine the lead order of the derivatives involved in the resultant boundary condition. Also note that this term will never be collapsed by an explicit internal δ-function. In other words, the final definite integration will *always* involve the integral of a derivative, and so it will always generate the difference between some operator involving the wave function evaluated on the two sides of the interface. Let us proceed and see how all this works in practice.

Performing 3 indefinite integrations followed by 1 definite infinitesimal integration across the interface, the lead order term $\nabla_T \left(1/\rho\right) \nabla_T^2 \left(1/\rho\right) \nabla_T \chi$ gives something proportional to $\chi_I - \chi_{II}$. To get a contribution from elsewhere in equation (Q.1) that survives this battery of 4 integrations, we would need a term that is capable (in principle at least) of generating a $\delta'''(z - f(x))$. By inspection, there are no other terms in $\lambda^2 \chi$, $\lambda \chi$ or $k_0(1 - 2\gamma)$ that will do so[oooo]. Thus, in O(λ^2) as in O(λ) theory, we have the

[oooo] Folded in here is the hidden assumption that a field can at most step at the interface, but it cannot contain δ-functions at the interface. Such field behavior is itself unphysical, and furthermore, consistency with the wave equation would force the field to pick up an even more outrageously unrealistic infinite series of δ^n-functions, with the n standing for derivatives of unbounded order.

boundary condition $\chi_I = \chi_{II}$. Similarly, 2 indefinite integrations followed by one definite integration yields the boundary condition

$$\frac{1}{\rho_I}\frac{\partial \chi_I}{\partial z} = \frac{1}{\rho_{II}}\frac{\partial \chi_{II}}{\partial z}.$$

Now, we need to do 2 (an indefinite and a definite) integrations and 1 (definite) integration to get boundary conditions involving $\partial^2\chi/\partial z^2$ and $\partial^3\chi/\partial z^3$ respectively. In addition to the contribution from the lead order term, non-zero contributions will also come from other terms if they in principle generate $\delta'(z-f)$ and $\delta(z-f)$ functions respectively. Next, we must examine equations (Q.1) and (Q.2), and look for terms that might generate such distributions. Given the boundary conditions we have just obtained for χ and $1/\rho \cdot \partial\chi/\partial z$, it follows that $\nabla_T\left(\frac{1}{\rho}\right)\nabla_T\chi$ has at most a step as do the parameters Ξ and γ. Thus, we see that only one term in addition to the lead order term is capable of generating the needed δ'- and δ- functions. This means we need only perform our two integrations $\int dz \cdots$ on the reduced equation

$$\frac{\rho_0^2 \cdot \nabla_T\left(\frac{1}{\rho}\right)\nabla_T^2\left(\frac{1}{\rho}\right)\nabla_T\chi}{4k_0^2} + \frac{\rho_0 \nabla_T\left(\frac{1}{\rho}\right)\nabla_T}{2k_0}\left(\Xi\chi\right) = 0. \qquad \text{(Q.3)}$$

Including the other terms demanded by equations (Q.1) and (Q.2) would only introduce terms that immediately fall out upon integration.

Thus, we begin by performing a single definite integration $\int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$ on equation (Q.3).

This gives us

$$\frac{\frac{\rho_0^2}{\rho_I^2}\nabla_T^3\chi_I - \frac{\rho_0^2}{\rho_{II}^2}\nabla_T^3\chi_{II}}{4k_0^2} + \frac{\frac{\rho_0}{\rho_I}\Xi_I \cdot \nabla_T\chi_I - \frac{\rho_0}{\rho_{II}}\Xi_{II} \cdot \nabla_T\chi_{II}}{2k_0} = 0.$$

Now, multiply through by $2k_0$ and set $\rho_0 = \rho_{II}$. Define $\alpha_I = \left[\rho_0/\rho\right]_I = \rho_{II}/\rho_I$. Also note that

$$\begin{aligned} \Xi_I &= k_0\left(\gamma_I - \mu_I\right) = k_0\gamma_I \\ \Xi_{II} &= k_0\left(\gamma_{II} - \mu_{II}\right) = -k_0\mu_{II} \end{aligned} \qquad \text{(Q.4)}$$

since $\mu_I = \gamma_{II} = 0$ for our standard conventions. This leaves us with

$$\frac{\alpha_I^2\nabla_T^3\chi_I - \nabla_T^3\chi_{II}}{2k_0} + k_0\alpha_I\gamma_I \cdot \nabla_T\chi_I + k_0\mu_{II} \cdot \nabla_T\chi_{II} = 0. \qquad \text{(Q.5)}$$

This is indeed the first boundary condition in equation (6.15).

Now, we obtain the second boundary condition in equation (6.15). We first perform a single indefinite integration of equation (Q.3). Once again, it is convenient to multiply through by $2k_0$ and divide by ρ_0. This leaves us with

$$\frac{\rho_0 \cdot \frac{1}{\rho}\nabla_T^2\left[\frac{1}{\rho}\nabla_T\chi\right]}{2k_0} + \frac{1}{\rho}\nabla_T\left(\Xi\chi\right) = 0\,.$$

Now, multiply through by ρ and perform the definite integration $\int_{f-\varepsilon}^{f+\varepsilon} dz \cdots$ to obtain

$$\frac{\rho_0\left(\left[\frac{1}{\rho_I}\nabla_T^2\chi_I\right] - \left[\frac{1}{\rho_{II}}\nabla_T^2\chi_{II}\right]\right)}{2k_0} + \left(\Xi_I - \Xi_{II}\right)\chi = 0\,,$$

where use has been made of the fact that the field is continuous: $\chi_I = \chi_{II} = \chi$. Now, set $\rho_0 = \rho_{II}$, and rearrange terms to obtain

$$\frac{\left(\nabla_T^2\chi_I - \nabla_T^2\chi_{II}\right)}{2k_0} - \frac{\left(1-\frac{\rho_{II}}{\rho_I}\right)\nabla_T^2\chi_I}{2k_0} + \left(\Xi_I - \Xi_{II}\right)\chi = 0\,.$$

Note that

$$-\left(1-\frac{\rho_{II}}{\rho_I}\right) = \frac{\rho_{II}}{\rho_I}\left(1-\frac{\rho_I}{\rho_{II}}\right) = 2\alpha_I\gamma_I\,,$$

and recall equation (Q.4) to show that $\Xi_I - \Xi_{II} = k_0\left(\gamma_I + \mu_{II}\right)$. This leaves us with

$$\frac{\left(\nabla_T^2\chi_I - \nabla_T^2\chi_{II}\right)}{2k_0} + \frac{2\alpha_I\gamma_I\nabla_T^2\chi_I}{2k_0} + k_0\left(\gamma_I + \mu_{II}\right)\chi = 0\,, \qquad \text{(Q.6)}$$

which is slightly rearranged version of the second boundary condition in equation (6.15).

We have thus succeeded in reproducing all four boundary conditions in equation (6.15).

Q.2 Separating out the terms that build Bragg-scale vorticity

In equation (6.16), the terms in the first two equalities of equation (6.15) (i.e., those directly related to the O(λ^2) contribution) are rearranged. In this appendix, we demonstrate that the boxed terms in equation (6.16) can indeed be identified with the emergence of Bragg-scale vorticity. Specifically, we demonstrate that contrary to what might be expected based on the 1st order boundary conditions (see equation (Q.7)

below)[pppp], the terms in the boxes modify the boundary conditions on $\nabla_T^n \chi$ ($n \geq 2$) so that the behavior of the auxiliary field χ does not mimic the behavior of the pressure field A. This difference reflects the need to construct Bragg-scale vorticity. The assertions in this paragraph involve some subtlety; so let us take a minute to examine the situation more closely before proceeding.

Q.2.1 What we want our theory to include

At 1st order, the auxiliary field χ has acquired the boundary conditions that would be expected for the pressure field A:

$$\begin{aligned} \tfrac{1}{\rho}\nabla_T \chi_I &= \tfrac{1}{\rho}\nabla_T \chi_{II} \\ \chi_I &= \chi_{II} \end{aligned} \quad . \tag{Q.7}$$

For the sake of this discussion, assume that the problem is range independent and that there is a flat horizontal interface where the density jumps. Note the continuity condition $\chi_I = \chi_{II}$, and recall that χ is a carrier of the downrange flux and not a pressure field. Since the problem is range independent, the operator $H^{-½}$ now commutes with $\partial/\partial x$ and with the Hamiltonian H (to demonstrate $\left[H^{-½}, H\right] = 0$, expand χ in eigenvectors: $\chi = \sum_n c_n \chi_n$ and note that $H^{-½}\chi_n = \chi_n / \sqrt{E_n}$ by definition, where $H\chi_n = E_n \chi_n$).

Therefore, we can now also use the parabolic equation for χ to propagate $u = H^{-½}\chi$ instead. Among other things, this means that u and its transverse derivative $\partial u/\partial x$ are continuous on the interface, as is $(1/\rho)\partial u/\partial z$. Noting that *in the half-spaces*, $\chi = \sqrt{\alpha/k_0} \cdot H^{½} A$ with $\alpha \equiv \rho_0/\rho$ locally constant, we have in the half-spaces $u = \sqrt{\alpha/k_0} \cdot A = \sqrt{\rho_0/(\rho k_0)} \cdot A$, and so we get

$$\begin{aligned} &\frac{A}{\sqrt{\rho}}, \frac{1}{\sqrt{\rho}}\frac{\partial A}{\partial x}, \frac{1}{\rho^{3/2}}\frac{\partial A}{\partial z} \text{ all continuous} \\ &S_x \sim \frac{A}{\rho}\frac{\partial A}{\partial x}, \frac{S_z}{\rho} \sim \frac{A}{\rho^2}\frac{\partial A}{\partial z} \text{ both continuous} \end{aligned} \quad . \tag{Q.8}$$

By contrast, the full wave boundary conditions imply that

[pppp] By the way, these generally survive unchanged in the sets of boundary conditions corresponding to 2nd and higher-order theory. (We just saw this for 2nd order theory.)

$$A, \frac{\partial A}{\partial x}, \frac{1}{\rho}\frac{\partial A}{\partial z} \text{ all continuous}$$
$$S_x \sim \frac{A}{\rho}\frac{\partial A}{\partial x} \text{ not continuous; } S_z \sim \frac{A}{\rho}\frac{\partial A}{\partial z} \text{ continuous} \qquad \text{(Q.9)}$$

The PE conserves energy, but the boundary conditions, and the horizontal and vertical fluxes have been redistributed relative to the full wave result (at least in 1st order theory; this particular result will generalize to higher orders since it turns out that equation (Q.7) remains unchanged in higher-order theory). We could impose continuity on A and consequently on its transverse derivative $\partial A/\partial x$ and restore Bragg-scale vorticity (discontinuity of the transverse velocity $(1/\rho)(\partial A/\partial x)$) by hand. To do so, we add to the 1st order Hamiltonian $H = k_0 - 2\gamma k_0 + \lambda$ an extra (energy conserving) term

$$-\frac{1}{2k_0}\cdot\frac{\rho_0}{\rho}\gamma_I \delta'(z)\chi$$
$$\gamma_I = \frac{\rho_{II}-\rho_I}{2\rho_{II}} = \frac{\rho_0-\rho}{2\rho_0} \text{ with } \rho_0 = \rho_{II}; \rho = \rho_I \qquad \text{(Q.10)}$$

Note that we are following the conventions and definitions outlined below equation (6.15). ρ and now even χ turn out to be discontinuous to 1st order in

$$2\gamma = (\rho_0 - \rho)/\rho_0 = -\Delta\rho/\rho_0 = (\rho_{II} - \rho_I)/\rho_{II} = \delta\rho/\rho_{II},$$

and we should in principle bifurcate $\delta'(z)$ to interpret this term. However, to 0th order the two variables are continuous, and so to 1st order (since we are multiplying by an additional $2\gamma_I$) we can choose either χ_I or χ_{II} and ρ_I or ρ_{II} (or some value in between).

Furthermore, we have

$$\begin{aligned}\lambda &= \frac{\nabla_T \frac{\rho_0}{\rho}\nabla_T}{2k_0}\chi + \text{terms that have no } \delta\text{-functions} \\ &= \frac{\rho_0}{\rho}\frac{\nabla_T^2\chi}{2k_0} + \left[\nabla_T\left(\frac{\rho_0}{\rho}\right)\right]\frac{\nabla_T\chi}{2k_0} + \cdots\end{aligned}$$

The second term on the right hand side of the second line contains a simple δ-function that will not survive an indefinite integration followed by an infinitesimal integration[qqqq]. Thus we drop this term as well as terms that contain no δ-functions. Now, we multiply

[qqqq] Implicitly, we are again either truncating at 1st order, or bifurcating δ-functions when we make this statement.

through by $2k_0 \cdot (\rho/\rho_0)$ and find that the key terms for the discontinuous part of the boundary condition on χ are

$$\nabla_T^2 \chi - \gamma_I \delta'(z) \chi + \cdots,$$

and taking the infinitesimal integration across the interface

$$\chi_I - \chi_{II} - \gamma_I \chi = 0$$

or

$$\begin{aligned} \chi_I &= \chi_{II}\left(1 + \frac{\delta\rho}{2\rho_{II}}\right) \\ &\approx \chi_{II}\left(1 + \frac{\delta\rho}{2\rho_I}\right) + \text{ higher order} \\ &\approx \chi_{II}\sqrt{1 + \frac{\delta\rho}{\rho_I}} \\ &= \chi_{II}\sqrt{\frac{\rho_{II}}{\rho_I}} \end{aligned}$$

or

$$\sqrt{\rho_I}\chi_I = \sqrt{\rho_{II}}\chi_{II}, \qquad \text{(Q.11)}$$

which is indeed the boundary condition we would expect for a quantity that is roughly the square root of the component of the energy flux that is transverse to the interface.

Note that we want a term such as defined in equation (Q.10) to emerge from our theory, and not just to be imposed by hand. The reason is that although the energy is conserved (the term is Hermitian), we have no control over what such a term does to the boundary condition on $\partial\chi/\partial z$ or on the other boundary conditions (i.e., conditions on $\nabla_T^n \chi; n \geq 2$ that are all implicit in 1st order theory). Furthermore, actual jumps in the wavefunction cause problems because now the x-derivative of χ will spawn a δ-function, and this in turn would lead to a very problematic feedback loop in our boundary conditions. Thus, we also want the jump in χ to naturally migrate up to a condition on the higher-order derivatives. This will happen if a term proportional to a δ'-function, such as is given in expression (Q.10), is embedded in a higher-order theory. Therefore, we now examine our O(λ^2) theory and discover how a term of the form (Q.10) is indeed generated by our theory (along with other similar terms).

Q.2.2 For comparison: The boundary conditions on A

Once again, consider a flat horizontal interface (i.e., the range-independent problem). As discussed above equation (Q.8), in this case the WKB amplitude (i.e., the square root of

the Hamiltonian) associated with the transformation between the pressure field A (which obeys the Helmholtz equation) and the auxiliary field χ (which obeys the PE) no longer plays a significant role in the problem since it cancels at the endpoints. In fact, in this case the auxiliary field $u = A/\sqrt{\rho}$, which is χ with the WKB amplitude peeled off, also obeys the parabolic equation (noting that $1/\sqrt{\rho}$ is expressed as a function of the expansion parameter 2γ, expanded and truncated appropriately). Also note that this factor of $1/\sqrt{\rho}$ is associated with Bragg-scale vorticity. Therefore, we have an instance where only the presence of Bragg-scale vorticity distinguishes the solution to the Helmholtz equation and the solution to the PE. Therefore, we will now derive the boundary conditions on the pressure field A, and compare them to the boundary conditions on χ. To facilitate this comparison, the boundary conditions on χ will then be rewritten as the sum of a part that reproduces the boundary conditions on A, and a part that generates Bragg-scale vorticity.

Q.2.2.1 The boundary conditions on A and its first derivative are the same as those on χ and its first derivative

We know that A obeys the 2-fluid boundary conditions

$$\begin{aligned} A_I &= A_{II} \\ \frac{1}{\rho_I}\frac{\partial A_I}{\partial z} &= \frac{1}{\rho_{II}}\frac{\partial A_{II}}{\partial z}. \end{aligned} \tag{Q.12}$$

Since these boundary conditions also apply to χ (see equation (Q.7) and note that it turns out that these conditions apply to higher-order PE's as well), Bragg-scale vorticity must emerge from the higher-order boundary conditions. To observe the emergence of Bragg-scale vorticity, we therefore need to examine the boundary conditions on higher-order derivatives of A and χ, and then note the differences.

For the solution to the Helmholtz equation (with its lead z-derivative 2nd order), these higher-order boundary conditions are implicit, and we will have to derive them using the explicit boundary conditions and the Helmholtz equation itself.

Q.2.2.2 The boundary condition on $\nabla_T^3 A$

Let us proceed to examine the boundary condition on $\nabla_T^3 A$ (still considering the range-independent problem). Take the wave equation in the half-spaces and approach the interface; then multiply by $(1/\rho)\nabla_T$:

$$\begin{aligned}\frac{\nabla_T}{\rho_I}\times\left[\left(\nabla_T^2+k_I^2\right)A_I=-\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}A_I\right)\right]\\ \frac{\nabla_T}{\rho_{II}}\times\left[\left(\nabla_T^2+k_{II}^2\right)A_{II}=-\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}A_{II}\right)\right]\end{aligned}. \qquad \text{(Q.13)}$$

Now, subtract the two equations. Since ρ_I and ρ_{II} are constants, the difference between the two expressions on the right hand side of the "=" signs gives:

$$-\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\left[\frac{1}{\rho_I}\nabla_T A_I-\frac{1}{\rho_{II}}\nabla_T A_{II}\right]\right).$$

Noting that here $\nabla_T=\partial/\partial z$, equation (Q.12) already tells us that

$$\frac{1}{\rho_I}\nabla_T A_I-\frac{1}{\rho_{II}}\nabla_T A_{II}=0$$

everywhere on the interface. Since the interface is horizontal, $\partial/\partial x$ is a tangential derivative relative to the interface (i.e., $\left(1-\hat{n}\hat{n}\right)\cdot\vec{\nabla}=\partial/\partial x$). Thus,

$$\begin{aligned}\frac{\partial}{\partial x}(\text{constant on the interface}) &= 0\\ \text{and also}\quad \frac{\partial^2}{\partial x^2}(\text{constant on the interface}) &= 0.\end{aligned}$$

So the right hand side of the difference of equations (Q.13) is zero. This leaves us with

$$\frac{\nabla_T^3 A_I}{\rho_I}+\frac{k_I^2}{\rho_I}\nabla_T A_I=\frac{\nabla_T^3 A_{II}}{\rho_{II}}+\frac{k_{II}^2}{\rho_{II}}\nabla_T A_{II} \qquad \text{(Q.14)}$$

or

$$\frac{\nabla_T^3 A_I}{\rho_I}-\frac{\nabla_T^3 A_{II}}{\rho_{II}}+\left(k_I^2-k_0^2\right)\frac{\nabla_T A_I}{\rho_I}+\cancel{k_0^2\frac{\nabla_T A_I}{\rho_I}}-\left(k_{II}^2-k_0^2\right)\frac{\nabla_T A_{II}}{\rho_{II}}-\cancel{k_0^2\frac{\nabla_T A_{II}}{\rho_{II}}}=0. \qquad \text{(Q.15)}$$

Note the cancellation. Recall

$$k^2=n^2k_0^2=\frac{c_0^2}{c^2}\cdot\frac{\omega^2}{c_0^2}\quad\text{and}\quad c_0=\sqrt{\frac{1}{K_I\rho_{II}}}$$

and so

$$\begin{aligned} k_I^2 - k_0^2 &= \left(n_I^2 - 1\right)k_0^2 \\ &= \left(\frac{c_0^2}{c_I^2} - 1\right)k_0^2 \\ &= \left(\frac{\rho_I K_I}{\rho_{II} K_I} - 1\right)k_0^2 \\ &= -\left(1 - \frac{\rho_I}{\rho_{II}}\right)k_0^2 \\ &= -2\gamma_I k_0^2 \end{aligned} \quad \left| \quad \begin{aligned} k_{II}^2 - k_0^2 &= \left(n_{II}^2 - 1\right)k_0^2 \\ &= \left(\frac{c_0^2}{c_{II}^2} - 1\right)k_0^2 \\ &= \left(\frac{\rho_{II} K_{II}}{\rho_{II} K_I} - 1\right)k_0^2 \\ &= -\left(1 - \frac{K_{II}}{K_I}\right)k_0^2 \\ &= -2\mu_{II} k_0^2 \end{aligned} \right. . \qquad \text{(Q.16)}$$

Thus, we have

$$\frac{\nabla_T^3 A_I}{\rho_I} - \frac{\nabla_T^3 A_{II}}{\rho_{II}} - 2\gamma_I k_0^2 \frac{\nabla_T A_I}{\rho_I} + 2\mu_{II} k_0^2 \frac{\nabla_T A_{II}}{\rho_{II}} = 0 ,$$

and multiplying through by $\rho_{II}/(2k_0)$

$$\frac{\alpha_I \nabla_T^3 A_I - \nabla_T^3 A_{II}}{2k_0} \underbrace{-}_{\substack{\text{only this sign} \\ \text{will be different in} \\ \text{the } \nabla_T^3 \chi \text{ condition}}} k_0 \alpha_I \gamma_I \nabla_T A_I + k_0 \mu_{II} \nabla_T A_{II} = 0 . \qquad \text{(Q.17)}$$

Note that the sign on the second term is the only difference between this boundary condition on $\nabla^3 A$ and the corresponding boundary condition on $\nabla^3 \chi$ given in (Q.5).

Q.2.2.3 The boundary condition on $\nabla_T^2 A$

Now, let us repeat this for the boundary condition on $\nabla_T^2 A$. Now, consider the Helmholtz equations

$$\left(\nabla_T^2 + k_I^2\right) A_I = -\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} A_I\right)$$
$$\left(\nabla_T^2 + k_{II}^2\right) A_{II} = -\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} A_{II}\right) ,$$

and subtract the second equation from the first. Furthermore, note that $A_I = A_{II}$ on the horizontal interface. This implies that

$$\begin{aligned} \frac{\partial A_I}{\partial x} &= \frac{\partial A_{II}}{\partial x} \\ \underbrace{\frac{\partial}{\partial x}}_{\substack{\text{tangential} \\ \text{derivative}}} \left(\frac{\partial A_I}{\partial x} - \frac{\partial A_{II}}{\partial x}\right) &= 0 . \end{aligned}$$

This leaves us with (noting: $A_I = A_{II} = A$)

$$\begin{aligned} \nabla_T^2 A_I - \nabla_T^2 A_{II} + \left(k_I^2 - k_{II}^2\right) A &= 0 \\ \nabla_T^2 A_I - \nabla_T^2 A_{II} + \left(k_I^2 - k_0^2\right) A - \left(k_{II}^2 - k_0^2\right) A &= 0 \end{aligned}$$

Substituting the results of equation (Q.16) and dividing by $2k_0$ gives us

$$\frac{\nabla_T^2 A_I - \nabla_T^2 A_{II}}{2k_0} \underbrace{\qquad}_{\substack{\text{this sign is the lowest order part of the difference between the } \nabla_T^2 A \text{ and } \nabla_T^2 \chi \\ \text{boundary conditions}}} k_0 \gamma_I A + k_0 \mu_{II} A = 0 . \qquad \text{(Q.18)}$$

Once again, note that the sign on the second term is a difference between this boundary condition on $\nabla^2 A$ and the corresponding boundary condition on $\nabla^2 \chi$ given in equation (Q.6). In the equation for $\nabla^2 \chi$ there is also an additional higher-order term $\left(\alpha_I \gamma_I \nabla_T^2 \chi_I\right)/k_0$. This term too is associated with Bragg-scale vorticity.

Q.2.3 How the distinction between χ and A is reflected in their boundary conditions

Now, let us collect the boundary conditions involving $\nabla_T^3 \chi$ and $\nabla_T^2 \chi$ (as given in equation (6.15); and equivalently in equations (Q.5) and (Q.6)), and the corresponding (implicit) boundary conditions on $\nabla_T^3 A$ and $\nabla_T^2 A$ along a flat (i.e., $f(x,y) = 0$) interface (equations (Q.17) and (Q.18)). Take the two boundary conditions involving χ, and separate out those parts that reproduce the corresponding boundary conditions on the pressure field A, and place the leftover parts in boxes. This gives us equation (6.16) rewritten here as equation (Q.19):

$$\begin{aligned} \tfrac{1}{2k_0}\left[\alpha_I^2 \nabla_T^3 \chi_I - \nabla_T^3 \chi_{II}\right] - k_0 \alpha_I \gamma_I \nabla_T \chi_I + k_0 \mu_{II} \nabla_T \chi_{II} \boxed{+2k_0 \alpha_I \gamma_I \nabla_T \chi_I} &= 0 \\ \tfrac{1}{2k_0}\left[\nabla_T^2 \chi_I - \nabla_T^2 \chi_{II}\right] + k_0 \left(\mu_{II} - \gamma_I\right) \chi \boxed{+2k_0 \gamma_I \chi + \tfrac{\alpha_I \gamma_I}{k_0} \nabla_T^2 \chi_I} &= 0 \end{aligned} . \qquad \text{(Q.19)}$$

Reversing the basic argument that led to equation (Q.11), it is not difficult to show that the δ'-function responsible to 1st order for the extra part of the $\nabla_T^2 \chi$ boundary condition is $\left(-1/2k_0\right) \alpha \gamma_I \delta'(z)$. This is the same as in equation (Q.10). In obtaining equation (Q.19) from this δ'-function, we also picked up an extra factor $-\left(2k_0\right)^2$ that comes from peeling off part of the coefficient in front of the new leading order derivative

$$-\lambda^2/2k_0 = -\left(1/2k_0\right)^2 \left(1/2k_0\right) \nabla_T \left(\rho_0/\rho\right) \nabla_T^2 \left(\rho_0/\rho\right) \nabla_T + \cdots .$$

It is not difficult to show how $(-1/2k_0)\alpha\gamma_I\delta'(z)$ emerges from the two cross-terms in $-\lambda^2/2k_0$:

$$(-1/2k_0)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}(k_0\gamma)\chi \tag{Q.20}$$

and part of

$$(-1/2k_0)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}(-k_0\mu)\chi\,. \tag{Q.21}$$

Let us examine the second term. With our conventions that $K_0 = K_I$ and $\rho_0 = \rho_{II}$ (useful if, for example, medium I is water and medium II is mud), we find

$$\mu \equiv \frac{1}{2}\left(1-\frac{K}{K_0}\right) = \frac{1}{2}\left(1-\frac{K}{K_I}\right),$$

and so in region I, $\mu = 0$ and in region II,

$$\mu = \frac{K_I - K_{II}}{2K_I} = -\frac{\delta K}{2K_I} = -\frac{\Delta K}{2K_I} = \mu_{II}$$

or

$$\mu_{II} = \frac{1}{2}\left(1-\frac{K_{II}\rho_{II}}{K_I\rho_{II}}\right) = \frac{1}{2}\left(1-\frac{c_0^2}{c_{II}^2}\right).$$

Thus, with the positive z-axis pointing into region I:

$$\begin{aligned} -k_0\mu &= -\frac{k_0}{2}\Theta(-z)\left(1-\frac{c_0^2}{c_{II}^2}\right) \\ &= -\frac{k_0}{2}\Theta(-z)\left(1-\frac{c_I^2}{c_{II}^2}\frac{\rho_I}{\rho_{II}}\right) \\ &= -\frac{k_0}{2}\Theta(-z)\left(1-n_{\text{total}}^2\frac{\rho_I}{\rho_{II}}\right) \end{aligned}$$

where n_{total} is the index of refraction between the media and $\Theta(z)$ is the Heaviside step function. Now $n_{\text{total}}^2 = 1-2\mu_{\text{total}}$, where μ_{total} is the familiar parameter measuring the sound speed jump between the media, and

$$\frac{\rho_I}{\rho_{II}} = \frac{\rho_I}{\rho_I+\delta\rho} = \frac{1}{1+\frac{\delta\rho}{\rho_I}} = 1-\frac{\delta\rho}{\rho_I}+\cdots = 1-\frac{\delta\rho}{\rho_{II}}+\cdots$$

to 1st order (recall our conventions $\rho_{II}-\rho_I = \delta\rho = -\Delta\rho$). Thus

$$n_{\text{total}}^2 \frac{\rho_I}{\rho_{II}} = 1 - 2\mu_{\text{total}} - \frac{\delta\rho}{\rho_{II}}$$

to 1st order. This gives us

$$\begin{aligned} -k_0\mu &= -\frac{k_0}{2}\Theta(-z)\left(1-\left(1-2\mu_{\text{total}}-\frac{\delta\rho}{\rho_{II}}\right)\right) \\ &= -\frac{k_0}{2}\Theta(-z)\left(2\mu_{\text{total}}+\frac{\delta\rho}{\rho_{II}}\right) \\ &= -k_0\Theta(-z)\left(\mu_{\text{total}}+\frac{\delta\rho}{2\rho_{II}}\right) \end{aligned} \quad . \qquad \text{(Q.22)}$$

Note that equation (Q.22) also implies that

$$\mu_{II} = \mu_{\text{total}} + \frac{\delta\rho}{2\rho_{II}} = \mu_{\text{total}} + \gamma_I \qquad \text{(Q.23)}$$

to 1st order.

We also have

$$\gamma \equiv \frac{1}{2}\left(1-\frac{\rho}{\rho_0}\right) = \frac{\rho_{II}-\rho}{2\rho_{II}} . \qquad \text{(Q.24)}$$

Thus, $\gamma = 0$ in region II and

$$\gamma = \frac{\rho_{II}-\rho_I}{2\rho_{II}} = \frac{\delta\rho}{2\rho_{II}} = -\frac{\Delta\rho}{2\rho_{II}} = \gamma_I$$

in region I. Thus

$$\gamma = \gamma_I\Theta(z) . \qquad \text{(Q.25)}$$

Combining (Q.22) and (Q.25), we have

$$-k_0\mu + k_0\gamma = -k_0\Theta(-z)\,\mu_{\text{total}} + k_0\gamma_I\left[\Theta(z)-\Theta(-z)\right] \qquad \text{(Q.26)}$$

at 1st order for our standard example $K_0 = K_I$ and $\rho_0 = \rho_{II}$. From equation (Q.23), we have $\mu_{II} - \gamma_I = \mu_{\text{total}}$, and it is straightforward to show that the first term in equation (Q.26) when substituted into the cross-term (Q.21) reproduces the unboxed part of the $\nabla_T^2\chi$ boundary condition in equation (Q.19) (i.e., the part the reproduces the behavior of the pressure wave A, and so does not remove Bragg-scale vorticity). This leaves us with the term $k_0\gamma_I\left[\Theta(z)-\Theta(-z)\right]$. From equations (Q.20) and (Q.21), we see that this gets operated on by

$$(-1/2k_0)\frac{\nabla_T\left(\rho_0/\rho\right)\nabla_T}{2k_0}$$

to form

$$-\frac{1}{2k_0}\frac{\rho_0}{\rho}\frac{1}{2k_0}\cdot k_0\gamma_I\left(\frac{\partial^2\Theta(z)}{\partial z^2}-\frac{\partial^2\Theta(-z)}{\partial z^2}\right).$$

Note that ∇_T operating on $1/\rho$ generates a simple δ-function, which will not survive a double integration across an infinitesimal integral, and so this operation has been dropped from the present calculation. Finally use

$$\frac{\partial^2\Theta(z)}{\partial z^2}=\delta'(z)=-\delta'(-z)=-\frac{\partial^2\Theta(-z)}{\partial z^2}$$

to recover the term (Q.10):

$$-\frac{1}{2k_0}\cdot\frac{\rho_0}{\rho}\gamma_I\delta'(z)\chi\,.$$

R Appendix: The electromagnetic field

The appendix supplies the details behind the results presented in Section 7.1. Appendix R.1 derives equation (7.4), the state space equation for the electromagnetic field. Appendix R.2 derives equation (7.6) (with definition (7.7)), an approximate transformation connecting the familiar full-wave magnetic field $\vec{H}_T$ with the corresponding auxiliary field $\vec{\theta}_T$ that is associated with downrange propagation by the parabolic equation. Together, these two results provide enough information to allow the straightforward mechanical implementation of the formalism.

Appendix R.2 also derives a "minimal version" of equation (7.6) applicable when the grazing angle and the changes in the electric permittivity and magnetic permeability are all small.

R.1 The state space equation for the electromagnetic field

Section R.1.1 sets up the needed formalism for electromagnetic fields, and identifies the conventions used in this calculation. Section R.1.2 identifies the Foldy-Wouthuysen ansatz appropriate for electromagnetic fields. Two lemmas needed in the calculation are derived in Subsection R.1.3, and the resulting state space equation is derived in Section R.1.4

R.1.1 The basic electromagnetic formalism

To derive the state space equation (7.4), we begin with Maxwell's equations (in MKS units):

$$\begin{aligned} \vec{\nabla}\cdot\vec{D} &= \rho_f \\ \vec{\nabla}\cdot\vec{B} &= 0 \\ \vec{\nabla}\times\vec{E} &= -i\omega\mu\vec{H} \\ \vec{\nabla}\times\vec{H} &= i\omega\varepsilon\vec{E} + \vec{J}_f \end{aligned} \quad , \tag{R.1}$$

where $\vec{E}$ is the electric field, $\vec{H}$ the magnetic field, and ρ_f is the free charge. For a linear isotropic medium, the electric displacement $\vec{D}$ is given by $\vec{D} = \varepsilon\vec{E}$, the magnetic induction $\vec{B}$ by $\vec{B} = \mu\vec{H}$ and the free current $\vec{J}_f$ by $\vec{J}_f = \sigma\vec{E}$. The electric permittivity ε is related to some reference value ε_0 by $\varepsilon = \varepsilon_0 + \delta\varepsilon$, while the magnetic permeability is related to its reference value μ_0 by $\mu = \mu_0 + \delta\mu$. The conductivity σ is set to zero in the current context[rrrr], although a nonzero value would involve only modest modifications to the current formalism.

Only the last two of Maxwell's equations (R.1) will be used here in Section R.1. In addition, the second Maxwell equation will be used below in Section R.2, but the first Maxwell equation is not used in our treatment. Thus, technically speaking, our treatment makes no assumption concerning the free charge ρ_f. Furthermore, the treatment here in Section R.1 does not assume that the medium is necessarily linear and isotropic, but the treatment in Section R.2 will assume $\vec{B} = \mu\vec{H}$, a property of a linear isotropic medium.

The energy flux is given by the Poynting vector:

$$\vec{S} \equiv \vec{E}\times\vec{H} = \text{ energy flux vector}.$$

Throughout this work, the physical field is actually the real part of a complex field. Under these circumstances, the time-averaged Poynting vector becomes

$$\vec{S}_{\text{ave}} = \left\langle \text{Re}\left(\vec{E}\right)\times\text{Re}\left(\vec{H}\right)\right\rangle_{\text{ave}} = \frac{1}{2}\text{Re}\left[\vec{E}\times\vec{H}^*\right] = \text{ average energy flux vector}. \tag{R.2}$$

As always, we consider duct-like (i.e., waveguide) propagation, where the x-axis defines the downrange direction. A subscript T on a vector indicates that the vector is embedded in transverse y-z space.

[rrrr] When $\rho_f = 0$ and $\vec{J}_f = 0$, then the medium is a dielectric.

R.1.2 The Foldy-Wouthuysen ansatz for an electromagnetic field

Next, let the discussion at the beginning of Appendix I guide us in constructing an ansatz that will lead to a state space equation that is a suitable starting point for the Foldy-Wouthuysen (FW) transformation. Specifically, start with the basic form

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix}$$

and construct θ and χ from the original field in such a way that $\Phi^\dagger \eta \Phi = |\theta|^2 - |\chi|^2$ is proportional to the (time-averaged) downrange flux $S_x = \vec{S}_{\text{ave}} \cdot \hat{x}$. As noted in Appendix I, this will guarantee that the total energy flux $\Phi^\dagger \eta \Phi$ remains conserved at all values of the range, and this in turn will force the matrix Hamiltonian $\mathcal{H}$ to be pseudo-Hermitian. The Hamiltonian in the state space equation must be either Hermitian or pseudo-Hermitian for the equation to constitute a suitable starting point for the Foldy-Wouthuysen transformation (see the second to last paragraph in Subsection C.2.3.2 or footnote yyy for indications of why this is so).

With these considerations in mind, the suitable ansatz is

$$\underset{\sim}{\Phi} = \begin{pmatrix} \vec{\theta}_T \\ \vec{\chi}_T \end{pmatrix} = \frac{1}{2}\left(\vec{H}_T \pm \sqrt{\frac{\varepsilon_0}{\mu_0}} \cdot \hat{x} \times \vec{E} \right), \tag{R.3}$$

where $\vec{H}_T$ is the projection in (transverse) y-z space of the magnetic field $\vec{H}$. The vector $\underset{\sim}{\Phi}$ is underlined with a tilde to indicate that it now has 4 rather than 2 components. The factor of $\sqrt{\varepsilon_0/\mu_0}$ has been inserted into the ansatz so that the units work out properly. Below, this factor will sometimes be denoted by $a \equiv \sqrt{\varepsilon_0/\mu_0}$. It is easy to verify that $\underset{\sim}{\Phi}^\dagger \eta \underset{\sim}{\Phi}$ indeed represents the uprange/downrange flux:

$$\begin{aligned} \underset{\sim}{\Phi}^\dagger \eta \underset{\sim}{\Phi} = \vec{\theta}_T^* \cdot \vec{\theta}_T - \vec{\chi}_T^* \cdot \vec{\chi}_T &= \text{Re}\left[\vec{H}_T^* \cdot \left(\hat{x} \times \vec{E} \right) \right] \cdot \sqrt{\frac{\varepsilon_0}{\mu_0}} \\ &= \text{Re}\left[\vec{H}^* \cdot \left(\hat{x} \times \vec{E} \right) \right] \cdot \sqrt{\frac{\varepsilon_0}{\mu_0}} \\ &= \text{Re}\left[\hat{x} \cdot \left(\vec{E} \times \vec{H}^* \right) \right] \cdot \sqrt{\frac{\varepsilon_0}{\mu_0}} \\ &= 2\left(\vec{S} \cdot \hat{x} \right) \sqrt{\frac{\varepsilon_0}{\mu_0}} = 2\left[\text{uprange/downrange flux} \right] \cdot \sqrt{\frac{\varepsilon_0}{\mu_0}} \quad . \end{aligned} \tag{R.4}$$

There is one small new twist: this time it is $\vec{\theta}_T$ that represents the downrange flux (and so is of primary interest to us), and $\vec{\chi}_T$ that gives us the uprange flux. (This suggests that in this one case, we should use the $e^{i\omega t}$ convention rather than the usual $e^{-i\omega t}$ convention.)

Also note that we made use of the basic identity that the vector triple product can be rotated (for arbitrary vectors $\vec{A}$, $\vec{B}$ and $\vec{C}$):

$$\vec{A}\cdot\left(\vec{B}\times\vec{C}\right)=\det\begin{pmatrix}\vec{A}\\ \vec{B}\\ \vec{C}\end{pmatrix}=\vec{B}\cdot\left(\vec{C}\times\vec{A}\right)=\vec{C}\cdot\left(\vec{A}\times\vec{B}\right). \tag{R.5}$$

Before proceeding, let us note in passing that we could just as easily chosen the ansatz

$$\underset{\sim}{\Phi}=\begin{pmatrix}\vec{\theta}_T\\ \vec{\chi}_T\end{pmatrix}=\frac{1}{2}\left(\vec{E}_T\pm\sqrt{\frac{\mu_0}{\varepsilon_0}}\cdot\hat{x}\times\vec{H}\right)$$

and the whole derivation below would work just as well.

Next, we prove two lemmas that will be needed later.

R.1.3 Two lemmas

Lemma $\mathcal{A}$ (equation (R.6))

$$H_x=\frac{-i}{\omega a\mu}\vec{\nabla}_T\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right) \tag{R.6}$$

Proof: Start with $\vec{\theta}_T-\vec{\chi}_T=a\left(\hat{x}\times\vec{E}\right)$ and observe that since there is no $\hat{x}$ component to $\vec{\theta}_T$ and $\vec{\chi}_T$, $\vec{\nabla}_T\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)=\vec{\nabla}\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)$. Thus, we have

$$\begin{aligned}\vec{\nabla}_T\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)&=\vec{\nabla}\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)=\vec{\nabla}\cdot\left[a\left(\hat{x}\times\vec{E}\right)\right]\\ &=-a\underbrace{\vec{\nabla}\cdot\left(\vec{E}\times\hat{x}\right)}_{\substack{\text{Rotate the}\\ \text{triple product}}}\\ &=-a\left(\hat{x}\cdot\underbrace{\vec{\nabla}\times\vec{E}}_{\substack{\text{Use Maxwell's}\\ \text{third equation}}}\right)\\ &=-a\left(\hat{x}\cdot\left(-i\omega\mu\right)\vec{H}\right)\\ &=i\omega a\mu H_x\quad\mathbb{QED}\end{aligned}$$

Note that the third Maxwell equation in (R.1) was used. We also made use of the basic vector identity (R.5), now being careful to note that $\hat{x}$ is constant[ssss].

Lemma $\mathcal{B}$ (equation (R.7))

$$\frac{\partial}{\partial x}\frac{1}{\varepsilon}\vec{\nabla}_T H_x - \frac{\partial}{\partial x}\frac{1}{\varepsilon}\frac{\partial}{\partial x}\vec{H}_T = \vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T^i \vec{H}_T - \vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T \vec{H}_T^i + \omega^2 \mu \vec{H}_T \qquad \text{(R.7)}$$

As always, unless explicitly noted otherwise, repeated indices are summed.

Proof: Begin with the fourth Maxwell equation in (R.1)

$$\vec{\nabla}\times\vec{H} = i\omega\varepsilon\vec{E} \quad \text{or} \quad \frac{1}{\varepsilon}\vec{\nabla}\times\vec{H} = i\omega\vec{E}\,,$$

take the curl, and use the third Maxwell equation to simplify:

$$\vec{\nabla}\times\left[\frac{1}{\varepsilon}\vec{\nabla}\times\vec{H}\right] = i\omega\underbrace{\vec{\nabla}\times\vec{E}}_{-i\omega\mu\vec{H}} = \omega^2\mu\vec{H}\,. \qquad \text{(R.8)}$$

Note that equation (R.8) is the wave equation for the magnetic field $\vec{H}$.

Next, use the basic vector identity

$$\vec{A}\times\left(\vec{B}\times\vec{C}\right) = \left(\vec{A}\cdot\vec{C}\right)\vec{B} - \left(\vec{A}\cdot\vec{B}\right)\vec{C} = A^i\vec{B}C^i - \left(\vec{A}\cdot\vec{B}\right)\vec{C} \qquad \text{(R.9)}$$

with $\vec{A} = \vec{\nabla}$; $\vec{B} = \frac{1}{\varepsilon}\vec{\nabla}$; $\vec{C} = \vec{H}$ to obtain[ssss]

$$\vec{\nabla}\times\left[\frac{1}{\varepsilon}\vec{\nabla}\times\vec{H}\right] = \nabla^i\frac{1}{\varepsilon}\vec{\nabla}H^i - \left(\vec{\nabla}\cdot\frac{1}{\varepsilon}\vec{\nabla}\right)\vec{H}\,.$$

Substituting into (R.8), we now have:

$$\nabla^i\frac{1}{\varepsilon}\vec{\nabla}H^i - \left(\vec{\nabla}\cdot\frac{1}{\varepsilon}\vec{\nabla}\right)\vec{H} = \omega^2\mu\vec{H}\,.$$

Taking the transverse projection $\left(\mathbf{1}-\hat{x}\hat{x}\right)\cdot(\ldots)$,

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[ssss] In general, we will continue to use standard vector identities like (R.5) and (R.9) even when some of the vectors are operators, as long as we are sure to keep all vectors being operated on to the right of the operator. To maintain this convention, it will at times prove necessary to express vector products in terms of sums involving the components. In this section, and always throughout this paper unless explicitly noted otherwise, repeated indices are summed.

$$\omega^2\mu\vec{H}_T = \nabla^i \frac{1}{\varepsilon}\vec{\nabla}_T H^i - \left(\vec{\nabla}\cdot\frac{1}{\varepsilon}\vec{\nabla}\right)\vec{H}_T ,$$

and then explicitly making the replacement $\vec{\nabla} = \hat{x}\partial/\partial x + \vec{\nabla}_T$, we have

$$\omega^2\mu\vec{H}_T = \frac{\partial}{\partial x}\frac{1}{\varepsilon}\vec{\nabla}_T H_x - \frac{\partial}{\partial x}\frac{1}{\varepsilon}\frac{\partial}{\partial x}\vec{H}_T + \nabla_T^i \frac{1}{\varepsilon}\vec{\nabla}_T H_T^i - \vec{\nabla}_T\cdot\frac{1}{\varepsilon}\vec{\nabla}_T\vec{H}_T ,$$

and rearranging terms, we have (R.7). $\mathbb{QED}$

R.1.4 The state space equation

Following Sections C.1.1 and I, recall that the derivation of the state space equation requires that we develop two separate intermediate equations, one involving $\partial\left(\vec{\theta}_T - \vec{\chi}_T\right)\big/\partial x$ and being essentially a rewrite of the wave equation, and the second involving $\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)\big/\partial x$ and being a manipulation of the definitions in the ansatz. These two equations will be derived below, the former being equation (R.14) and the latter (R.16). These are derived in Subsections R.1.4.1 and R.1.4.2 respectively. In Subsection R.1.4.3, these two partial differential equations are combined to form a state space equation, which is then streamlined in Subsection R.1.4.4.

R.1.4.1 The equation for $\partial\left(\vec{\theta}_T - \vec{\chi}_T\right)\big/\partial x$

To obtain the equation involving $\partial\left(\vec{\theta}_T - \vec{\chi}_T\right)\big/\partial x$ (equation (R.14)), start with

$$\begin{aligned}\vec{\theta}_T - \vec{\chi}_T &= a\,\hat{x}\times \underbrace{\vec{E}}_{\substack{\text{Replace using}\\ \text{the 4}^{\text{th}}\text{ Maxwell}\\ \text{equation}}} \\ &= \frac{a}{i\omega\varepsilon}\hat{x}\times\left(\vec{\nabla}\times\vec{H}\right)\end{aligned} \quad . \tag{R.10}$$

Again use $\vec{A}\times\left(\vec{B}\times\vec{C}\right) = A^i\vec{B}C^i - \left(\vec{A}\cdot\vec{B}\right)\vec{C}$ this time with $\vec{A} = \hat{x}$; $\vec{B} = \vec{\nabla}$; $\vec{C} = \vec{H}$:

$$\begin{aligned}\hat{x}\times\left(\vec{\nabla}\times\vec{H}\right) &= \vec{\nabla}H_x - \frac{\partial}{\partial x}\vec{H} \\ &= \cancel{\hat{x}\frac{\partial H_x}{\partial x}} + \vec{\nabla}_T H_x - \cancel{\hat{x}\frac{\partial H_x}{\partial x}} - \frac{\partial}{\partial x}\vec{H}_T \\ &= \vec{\nabla}_T H_x - \frac{\partial\vec{H}_T}{\partial x} \quad ,\end{aligned} \tag{R.11}$$

and substitute into (R.10) to get

$$\vec{\theta}_T - \vec{\chi}_T = \frac{a}{i\omega\varepsilon}\left[\vec{\nabla}_T H_x - \frac{\partial \vec{H}_T}{\partial x}\right]. \tag{R.12}$$

Multiplying through by i and taking $\partial/\partial x$, we have

$$i\frac{\partial}{\partial x}\left(\vec{\theta}_T - \vec{\chi}_T\right) = \frac{a}{\omega}\left[\frac{\partial}{\partial x}\frac{1}{\varepsilon}\vec{\nabla}_T H_x - \frac{\partial}{\partial x}\frac{1}{\varepsilon}\frac{\partial \vec{H}_T}{\partial x}\right]. \tag{R.13}$$

Now, substitute Lemma $\mathcal{B}$ (equation (R.7)) into the right hand side of (R.13) to get

$$i\frac{\partial}{\partial x}\left(\vec{\theta}_T - \vec{\chi}_T\right) = \frac{a}{\omega}\left[\vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T^i \vec{H}_T - \vec{\nabla}_T^k \frac{1}{\varepsilon}\vec{\nabla}_T \vec{H}_T^k + \omega^2\mu\vec{H}_T\right]$$

or

$$\begin{aligned} i\frac{\partial}{\partial x}\left(\vec{\theta}_T - \vec{\chi}_T\right)^j &= \frac{a}{\omega}\left[\vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T^i \vec{H}_T^j - \vec{\nabla}_T^k \frac{1}{\varepsilon}\vec{\nabla}_T^j \vec{H}_T^k + \omega^2\mu\vec{H}_T^j\right] \\ &= \underbrace{\frac{a}{\omega}\left[\vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T^i \delta^{jk} - \vec{\nabla}_T^k \frac{1}{\varepsilon}\vec{\nabla}_T^j + \omega^2\mu\delta^{jk}\right]}_{\xi^{jk}} \vec{H}_T^k \\ &= \xi^{jk}\vec{H}_T^k \quad . \end{aligned}$$

Substituting $\vec{\theta}_T + \vec{\chi}_T = \vec{H}_T$, we have successfully recast the wave equation into the desired form:

$$i\frac{\partial}{\partial x}\left(\vec{\theta}_T - \vec{\chi}_T\right)^j = \xi^{jk}\left(\vec{\theta}_T + \vec{\chi}_T\right)^k \quad \text{or} \quad i\frac{\partial}{\partial x}\left(\vec{\theta}_T - \vec{\chi}_T\right) = \vec{\vec{\xi}}\cdot\left(\vec{\theta}_T + \vec{\chi}_T\right), \tag{R.14}$$

with

$$\begin{aligned} \xi^{jk} &\equiv \frac{a}{\omega}\left[\vec{\nabla}_T^i \frac{1}{\varepsilon}\vec{\nabla}_T^i \delta^{jk} - \vec{\nabla}_T^k \frac{1}{\varepsilon}\vec{\nabla}_T^j + \omega^2\mu\delta^{jk}\right] \\ \vec{\vec{\xi}} &\equiv \frac{a}{\omega}\left[\mathbf{1}\vec{\nabla}_T \cdot \frac{1}{\varepsilon}\vec{\nabla}_T + \mathbf{1}\omega^2\mu - \left[\vec{\nabla}_T \frac{1}{\varepsilon}\vec{\nabla}_T\right]^{\text{transpose}}\right]. \end{aligned} \tag{R.15}$$

Note that these operators are properly Hermitian[tttt]. This gives us the first part of the state space equation. The wave equation for $\vec{H}$ is embedded in result (R.15). It entered via equation (R.8) in the proof of Lemma $\mathcal{B}$ (equation (R.7)).

R.1.4.2 The equation for $\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)\big/\partial x$

Next, let us obtain the equation involving $\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)\big/\partial x$ (equation (R.16)). This is the second equation we will need to obtain the state space equation, and it emerges as we manipulate the definitions in the ansatz (R.3). We start by once again invoking equation (R.12), this time written in the form

$$\frac{\omega\varepsilon}{a}\left(\vec{\theta}_T - \vec{\chi}_T\right) + i\vec{\nabla}_T H_x = i\frac{\partial \vec{H}_T}{\partial x}.$$

Now substitute for H_x using Lemma $\mathcal{A}$ (equation (R.6)) and again substitute $\vec{\theta}_T + \vec{\chi}_T = \vec{H}_T$:

$$\frac{\omega\varepsilon}{a}\left(\vec{\theta}_T - \vec{\chi}_T\right) + \vec{\nabla}_T \frac{-i^2}{\omega a \mu}\vec{\nabla}_T \cdot \left(\vec{\theta}_T - \vec{\chi}_T\right) = i\frac{\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)}{\partial x}$$

or

$$i\frac{\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)^j}{\partial x} = \frac{1}{\omega a}\vec{\nabla}_T^j \frac{1}{\mu}\vec{\nabla}_T^k \left(\vec{\theta}_T - \vec{\chi}_T\right)^k + \frac{\omega\varepsilon}{a}\left(\vec{\theta}_T - \vec{\chi}_T\right)^j$$

$$i\frac{\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)^j}{\partial x} = \underbrace{\left[\frac{1}{\omega a}\vec{\nabla}_T^j \frac{1}{\mu}\vec{\nabla}_T^k + \frac{\omega\varepsilon}{a}\delta^{jk}\right]}_{\zeta^{jk}}\left(\vec{\theta}_T - \vec{\chi}_T\right)^k .$$

Thus, the equation involving $\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)\big/\partial x$ is

$$i\frac{\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)^j}{\partial x} = \zeta^{jk}\left(\vec{\theta}_T - \vec{\chi}_T\right)^k \quad \text{or} \quad i\frac{\partial\left(\vec{\theta}_T + \vec{\chi}_T\right)}{\partial x} = \vec{\zeta}\cdot\left(\vec{\theta}_T - \vec{\chi}_T\right), \qquad \text{(R.16)}$$

[tttt] In this case, taking the Hermitian conjugate means taking the transpose, and reversing the order of the differentiations. In principle, we should also perform complex conjugation, but that is not an issue here.

where

$$\zeta^{jk} \equiv \frac{1}{\omega a}\vec{\nabla}_T^j \frac{1}{\mu}\vec{\nabla}_T^k + \frac{\omega\varepsilon}{a}\delta^{jk} \quad ; \quad \vec{\vec{\zeta}} \equiv \frac{1}{\omega a}\vec{\nabla}_T \frac{1}{\mu}\vec{\nabla}_T + \frac{\omega\varepsilon}{a}\mathbf{1}. \tag{R.17}$$

Once again, these operators are Hermitian[tttt]. Equation (R.16) gives us the second part of the state space equation.

R.1.4.3 Combining component partial-differential equations to form a matrix state space equation

Together, equations (R.14) and (R.16) are

$$\begin{aligned} i\frac{\partial}{\partial x}\left(\vec{\theta}_T^j - \vec{\chi}_T^j\right) &= \xi^{jk}\left(\vec{\theta}_T^k + \vec{\chi}_T^k\right) \\ i\frac{\partial\left(\vec{\theta}_T^j + \vec{\chi}_T^j\right)}{\partial x} &= \zeta^{jk}\left(\vec{\theta}_T^k - \vec{\chi}_T^k\right) \end{aligned}. \tag{R.18}$$

Now, let us add and subtract these equations. Adding the two equations and dividing by 2 gives us:

$$i\frac{\partial\vec{\theta}_T^j}{\partial x} = \frac{\left(\xi^{jk}+\zeta^{jk}\right)}{2}\vec{\theta}_T^k + \frac{\left(\xi^{jk}-\zeta^{jk}\right)}{2}\vec{\chi}_T^k, \tag{R.19}$$

while subtracting the first equation in (R.18) from the second and dividing by 2 gives us

$$i\frac{\partial\vec{\chi}_T^j}{\partial x} = -\frac{\left(\xi^{jk}-\zeta^{jk}\right)}{2}\vec{\theta}_T^k - \frac{\left(\xi^{jk}+\zeta^{jk}\right)}{2}\vec{\chi}_T^k. \tag{R.20}$$

Putting these two equations in matrix form gives us

$$\begin{pmatrix} i\frac{\partial\vec{\theta}_T^j}{\partial x} \\ i\frac{\partial\vec{\chi}_T^j}{\partial x} \end{pmatrix} = \left[\frac{\left(\xi^{jk}-\zeta^{jk}\right)}{2}\underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\tilde{\xi}} + \frac{\left(\xi^{jk}+\zeta^{jk}\right)}{2}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta}\right]\begin{pmatrix} \vec{\theta}_T^k \\ \vec{\chi}_T^k \end{pmatrix}. \tag{R.21}$$

Note that as $j = 1,2$, we indeed pick up all 4 components of $i\partial\Phi/\partial x$, although perhaps not in the usual order. Also note that we have once again identified the matrices η and $\tilde{\xi}$ (as first defined in Section 3.1). Temporarily, there is a tilde on top of $\tilde{\xi}$ to distinguish it from the matrix ξ^{jk}. These two matrices are completely different, but they only appear together briefly, since ξ^{jk} will shortly disappear from the scene.

To get a Hamiltonian in standard form $\mathcal{H} \equiv \mathcal{O} + \mathcal{E} + k_0\eta$, we need to pull out a $k_0\eta$ (this time multiplied by the identity matrix δ^{jk}) from the term in (R.21) that is proportional to η:

$$\begin{pmatrix} i\dfrac{\partial \vec{\theta}_T^{\,j}}{\partial x} \\ i\dfrac{\partial \vec{\chi}_T^{\,j}}{\partial x} \end{pmatrix} = \left[\underbrace{\frac{\left(\xi^{jk} - \zeta^{jk}\right)}{2}\tilde{\xi}}_{\mathcal{O}} + \underbrace{\frac{\left(\xi^{jk} + \zeta^{jk} - 2k_0\delta^{jk}\right)}{2}\eta}_{\mathcal{E}} + k_0\eta\cdot\delta^{jk} \right] \begin{pmatrix} \vec{\theta}_T^{\,k} \\ \vec{\chi}_T^{\,k} \end{pmatrix}. \qquad \text{(R.22)}$$

Now, let us define new variables so that the answer (R.22) looks more like the result for the 2-fluid acoustic case. Specifically, define λ^{jk} such that is the coefficient of the matrix $\tilde{\xi}$ and so the primary expansion coefficient. Also define γ^{jk} such that $\lambda^{jk} - 2k_0\gamma^{jk}$ is the coefficient of η in the even operator $\mathcal{E}$. This gives us

$$\lambda^{jk} = \frac{\xi^{jk} - \zeta^{jk}}{2} \quad \text{and} \quad \gamma^{jk} = -\frac{\zeta^{jk}}{2k_0} + \frac{\delta^{jk}}{2}. \qquad \text{(R.23)}$$

Substituting for ξ^{jk} and ζ^{jk} using equations (R.15) and (R.17) respectively, we have

$$\begin{aligned} \lambda^{jk} &= \frac{\xi^{jk} - \zeta^{jk}}{2} \\ &= \frac{a}{2\omega}\vec{\nabla}_T^{\,i}\frac{1}{\varepsilon}\vec{\nabla}_T^{\,i}\delta^{jk} - \frac{a}{2\omega}\vec{\nabla}_T^{\,k}\frac{1}{\varepsilon}\vec{\nabla}_T^{\,j} - \frac{1}{2\omega a}\vec{\nabla}_T^{\,j}\frac{1}{\mu}\vec{\nabla}_T^{\,k} + \frac{1}{2}\left(a\omega\mu - \frac{\omega\varepsilon}{a}\right)\delta^{jk} \end{aligned} \qquad \text{(R.24)}$$

and

$$\gamma^{jk} = -\frac{\zeta^{jk}}{2k_0} + \frac{\delta^{jk}}{2} = -\frac{1}{2k_0\omega a}\vec{\nabla}_T^{\,j}\frac{1}{\mu}\vec{\nabla}_T^{\,k} - \frac{\omega\varepsilon}{a}\frac{\delta^{jk}}{2k_0} + \frac{\delta^{jk}}{2}. \qquad \text{(R.25)}$$

Now, let us streamline equations (R.24) and (R.25). To do so, we obtain four useful identities.

R.1.4.4 A streamlined version of the state space equation

Identities 1 and 2 are closely related. First, recall that $a \equiv \sqrt{\varepsilon_0/\mu_0}$ and

$$\delta\varepsilon \equiv \varepsilon - \varepsilon_0 \quad ; \quad \delta\mu \equiv \mu - \mu_0 .$$

Therefore,

$$\frac{\omega\varepsilon}{a} = \omega\varepsilon\sqrt{\frac{\mu_0}{\varepsilon_0}} = \omega\varepsilon_0\sqrt{\frac{\mu_0}{\varepsilon_0}} + \omega\underbrace{\left(\varepsilon-\varepsilon_0\right)}_{\delta\varepsilon}\sqrt{\frac{\mu_0}{\varepsilon_0}}$$

$$= \omega\sqrt{\varepsilon_0\mu_0} + \omega\delta\varepsilon\sqrt{\frac{\mu_0}{\varepsilon_0}} = \underbrace{\omega\sqrt{\varepsilon_0\mu_0}}_{\omega/c_0=k_0} + \frac{\delta\varepsilon}{\varepsilon_0}\underbrace{\omega\sqrt{\varepsilon_0\mu_0}}_{\omega/c_0=k_0}$$

$$\frac{\omega\varepsilon}{a} = k_0\left(1+\frac{\delta\varepsilon}{\varepsilon_0}\right) \quad ,$$

and similarly

$$a\omega\mu = \sqrt{\frac{\varepsilon_0}{\mu_0}}\omega\mu = \underbrace{\omega\sqrt{\varepsilon_0\mu_0}}_{k_0} + \underbrace{\omega\sqrt{\frac{\varepsilon_0}{\mu_0}}}_{\frac{\omega\sqrt{\varepsilon_0\mu_0}}{\mu_0}=\frac{k_0}{\mu_0}}\underbrace{\left(\mu-\mu_0\right)}_{\delta\mu} \quad .$$

$$a\omega\mu = k_0\left(1+\frac{\delta\mu}{\mu_0}\right)$$

Identities 1 and 2 follow immediately:

$$a\omega\mu - \frac{\omega\varepsilon}{a} = k_0\left(\frac{\delta\mu}{\mu_0} - \frac{\delta\varepsilon}{\varepsilon_0}\right) \quad \boxed{\text{Identity \#1}}$$

$$\frac{\omega\varepsilon}{a} = k_0\left(1+\frac{\delta\varepsilon}{\varepsilon_0}\right) \quad \boxed{\text{Identity \#2}}$$

Identities 3 and 4 are trivial:

$$\frac{a}{\omega} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\frac{1}{\omega} = \frac{\varepsilon_0}{\omega\sqrt{\varepsilon_0\mu_0}} = \frac{\varepsilon_0}{k_0} \quad \boxed{\text{Identity \#3}}$$

$$\frac{1}{a\omega} = \sqrt{\frac{\mu_0}{\varepsilon_0}}\frac{1}{\omega} = \frac{\mu_0}{\omega\sqrt{\varepsilon_0\mu_0}} = \frac{\mu_0}{k_0} \quad \boxed{\text{Identity \#4}}$$

Identities 1 through 4 are then substituted into equation (R.24) to get:

$$\lambda^{jk} = \underbrace{\frac{1}{2k_0}\vec{\nabla}_T^i\frac{\varepsilon_0}{\varepsilon}\vec{\nabla}_T^i\delta^{jk}}_{\text{Used Identity \#3}} - \underbrace{\frac{1}{2k_0}\vec{\nabla}_T^k\frac{\varepsilon_0}{\varepsilon}\vec{\nabla}_T^j}_{\text{Used Identity \#3}} - \underbrace{\frac{1}{2k_0}\vec{\nabla}_T^j\frac{\mu_0}{\mu}\vec{\nabla}_T^k}_{\text{Used Identity \#4}} + \underbrace{\frac{k_0}{2}\left(\frac{\delta\mu}{\mu_0}-\frac{\delta\varepsilon}{\varepsilon_0}\right)}_{\text{Used Identity \#1}}\delta^{jk} \quad \text{(R.26)}$$

and into equation (R.25) to get:

$$\gamma^{jk} = \underbrace{-\frac{1}{2k_0^2}\vec{\nabla}_T^j \frac{\mu_0}{\mu}\vec{\nabla}_T^k}_{\text{Used Identity \#4}} \underbrace{- k_0\left(1+\frac{\delta\varepsilon}{\varepsilon_0}\right)}_{\text{Used Identity \#2}} \frac{\delta^{jk}}{2k_0} + \frac{\delta^{jk}}{2}$$
$$= -\frac{1}{2k_0^2}\vec{\nabla}_T^j \frac{\mu_0}{\mu}\vec{\nabla}_T^k - \frac{\delta\varepsilon}{2\varepsilon_0}\delta^{jk} \qquad \text{(R.27)}$$

Keeping in mind definitions (R.23), equation (R.22) becomes

$$\begin{pmatrix} i\dfrac{\partial\vec{\theta}_T^j}{\partial x} \\ i\dfrac{\partial\vec{\chi}_T^j}{\partial x} \end{pmatrix} = \left[\underbrace{\lambda^{jk}\tilde{\xi}}_{\mathcal{O}} + \underbrace{\left(\lambda^{jk} - 2k_0\gamma^{jk}\right)}_{\mathcal{E}}\eta + k_0\eta\cdot\delta^{jk} \right] \begin{pmatrix} \vec{\theta}_T^k \\ \vec{\chi}_T^k \end{pmatrix}. \qquad \text{(R.28)}$$

This is the state space equation (7.4). Equations (R.26) and (R.27) recover equation (7.3) .

R.2 The transformation tying the parabolic equation field $\vec{\theta}_T$ to the transverse magnetic induction $\vec{H}_T$

Appendix R.2 derives equation (7.6) (with definition (7.7)), an approximate transformation connecting the familiar full-wave magnetic field $\vec{H}_T$ with the corresponding auxiliary field $\vec{\theta}_T$ that is associated with downrange propagation by the parabolic equation. At the end of this appendix, we also derive a "minimal version" of equation (7.6) applicable when the grazing angle is very modest.

This relatively crude look at the "endpoint transformation" makes a number of assumptions. Here in Appendix R.2, propagation must be in the downrange direction only (i.e., the carrier of uprange flux $\vec{\chi}_T$ is zero). The material must be linear and isotropic so that $\vec{B} = \mu\vec{H}$, and it must not conduct (i.e., the free current $\vec{J}_f$ must be zero). As with the endpoint transformation for a variable-density acoustic field, it is further assumed that the environmental parameters (in this case the electric permittivity and magnetic permeability) are slowly varying in the immediate vicinity of the coordinates where the transformation between $\vec{H}_T$ and $\vec{\theta}_T$ is to be applied.

R.2.1 Deducing the basic form of the carrier of the downrange flux: $\vec{\theta}_T \propto \sqrt{\vec{\vec{A}}}\cdot\vec{H}_T$

The derivation of equation (7.6) begins with the basic form of the downrange flux given by equation (R.4) with the uprange flux set equal to zero (i.e., $\vec{\chi}_T = 0$):

$$2S_x = \sqrt{\frac{\mu_0}{\varepsilon_0}} \cdot \left|\vec{\theta}_T\right|^2 .$$

From the structure of the Foldy-Wouthuysen procedure, we know that a linear transformation between $\vec{H}_T$ and $\vec{\theta}_T$ exists, and therefore some dyadic operator which we write as $\sqrt{\ddot{A}}$ must exist such that $\sqrt{\ddot{A}} \cdot \vec{H}_T \propto \vec{\theta}_T$. Now we have

$$2S_x = \sqrt{\frac{\mu_0}{\varepsilon_0}} \cdot \left|\vec{\theta}_T\right|^2 = \vec{H}_T^* \cdot \left(\sqrt{\ddot{A}}^\dagger \cdot \sqrt{\ddot{A}}\right) \cdot \vec{H}_T = \vec{H}_T^* \cdot \ddot{A} \cdot \vec{H}_T . \tag{R.29}$$

Note that

$$\ddot{A} \equiv \sqrt{\ddot{A}}^\dagger \cdot \sqrt{\ddot{A}}$$

implies that $\ddot{A}$ is Hermitian.

Now, as in equation (R.4) (based on the basic equation for a time-averaged flux (R.2) and the vector identity (R.5), and noting that $\hat{x} \times \vec{E}$ is in the transverse direction), we have

$$2S_x = \mathrm{Re}\left[\hat{x} \cdot \vec{E} \times \vec{H}^*\right] = \mathrm{Re}\left[\vec{H}^* \cdot \hat{x} \times \vec{E}\right] = \mathrm{Re}\left[\vec{H}_T^* \cdot \hat{x} \times \vec{E}\right] = \sqrt{\frac{\mu_0}{\varepsilon_0}} \cdot \left|\vec{\theta}_T\right|^2 .$$

Using the fourth Maxwell equation in (R.1) (with the free current $\vec{J}_f = 0$), we get

$$\left|\vec{\theta}_T\right|^2 = \sqrt{\frac{\varepsilon_0}{\mu_0}}\,\mathrm{Re}\left[\vec{H}_T^* \cdot \hat{x} \times \vec{E}\right] = \sqrt{\frac{\varepsilon_0}{\mu_0}}\,\mathrm{Re}\left[\vec{H}_T^* \cdot \hat{x} \times \left(\frac{1}{i\omega\varepsilon}\vec{\nabla} \times \vec{H}\right)\right]$$

or using (R.11)

$$\left|\vec{\theta}_T\right|^2 = \sqrt{\frac{\varepsilon_0}{\mu_0}}\,\mathrm{Re}\left[\vec{H}_T^* \cdot \frac{1}{i\omega\varepsilon}\left(\vec{\nabla}_T H_x - \frac{\partial \vec{H}_T}{\partial x}\right)\right]. \tag{R.30}$$

Now, we need to recast H_x in terms of $\vec{H}_T$. To do so, we use the second Maxwell equation given in (R.1) along with the assumption that $\vec{B} = \mu\vec{H}$ (i.e., a linear and isotropic medium). As has been standard, we also neglect the *local* range dependence of μ at the endpoints. All this gives us:

$$\begin{aligned} \vec{\nabla} \cdot \left(\mu\vec{H}\right) &= 0 \\ \mu\frac{\partial H_x}{\partial x} &= -\vec{\nabla}_T\left(\mu\vec{H}_T\right) \\ \frac{\partial H_x}{\partial x} &= -\frac{1}{\mu}\vec{\nabla}_T\left(\mu\vec{H}_T\right) \end{aligned} \tag{R.31}$$

$$H_x = \left[-\frac{1}{\partial/\partial x} \cdot \frac{1}{\mu} \cdot \vec{\nabla}_T^i \mu \right] \vec{H}_T^i . \tag{R.32}$$

Now,

$$\frac{1}{i\omega\varepsilon}\left(\vec{\nabla}_T H_x - \frac{\partial \vec{H}_T}{\partial x} \right)^k = -\frac{1}{i\omega\varepsilon}\left[\vec{\nabla}_T^k \frac{1}{\partial/\partial x} \cdot \frac{1}{\mu} \cdot \vec{\nabla}_T^j \mu + \delta^{jk} \frac{\partial}{\partial x} \right] \vec{H}_T^j$$

or using dyadic notation

$$\begin{aligned} \frac{1}{i\omega\varepsilon}\left(\vec{\nabla}_T H_x - \frac{\partial \vec{H}_T}{\partial x} \right) &= -\frac{1}{i\omega\varepsilon}\left[\vec{\nabla}_T \frac{1}{\partial/\partial x} \frac{1}{\mu} \vec{\nabla}_T \mu + \frac{\partial}{\partial x} \right] \cdot \vec{H}_T \\ &= \frac{1}{\omega\varepsilon}\left[i\frac{\partial}{\partial x} - \vec{\nabla}_T \frac{1}{i\partial/\partial x} \frac{1}{\mu} \vec{\nabla}_T \mu \right] \cdot \vec{H}_T \end{aligned} . \tag{R.33}$$

Substituting (R.33) into (R.30), we have

$$\left| \vec{\theta}_T \right|^2 = \sqrt{\frac{\varepsilon_0}{\mu_0}} \operatorname{Re}\left[\vec{H}_T^* \cdot \frac{1}{\omega\varepsilon}\left[i\frac{\partial}{\partial x} - \vec{\nabla}_T \frac{1}{i\partial/\partial x} \frac{1}{\mu} \vec{\nabla}_T \mu \right] \cdot \vec{H}_T \right] . \tag{R.34}$$

Now note by setting ε and μ locally equal to constants, the operator between $\vec{H}_T^*$ and $\vec{H}_T$ becomes Hermitian, and we can drop the "real part" operator to get:

$$\left| \vec{\theta}_T \right|^2 = \sqrt{\frac{\varepsilon_0}{\mu_0}} \vec{H}_T^* \cdot \frac{1}{\omega\varepsilon}\left[i\frac{\partial}{\partial x} - \vec{\nabla}_T \frac{1}{i\partial/\partial x} \vec{\nabla}_T \right] \cdot \vec{H}_T . \tag{R.35}$$

Or taking the square root – i.e., reading off $\sqrt{\vec{\vec{A}}} \cdot \vec{H}_T$ by comparing equations (R.29) and (R.35):

$$\vec{\theta}_T = \left(\frac{\varepsilon_0}{\mu_0} \right)^{1/4} \frac{1}{(\omega\varepsilon)^{1/2}} \left[i\frac{\partial}{\partial x} - \vec{\nabla}_T \frac{1}{i\partial/\partial x} \vec{\nabla}_T \right]^{1/2} \cdot \vec{H}_T . \tag{R.36}$$

Note that if we did not want to make the assumption that ε and μ are locally constant, then we would have to symmetrize result (R.34)[uuuu]. To keep things reasonably straightforward, we will not consider this case here.

R.2.2 Getting rid of the $\partial/\partial x$ operator in $\sqrt{\ddot{A}}$

Next, we need to evaluate the operator $i\partial/\partial x$ acting on $\vec{H}_T$. To do so, we again neglect (local) range dependence (at the endpoints), and exploit the fact that (as with the variable density acoustic equation), in the absence of range dependence we can directly take the square root of the wave equation for $\vec{H}_T$. The parabolic equation derived in this way is different from the one obtained using the Foldy-Wouthuysen transformation. As in the variable density acoustic case, the parabolic equation for $\vec{H}_T$ does not generalize to the range-*in*dependent case.

Let us begin with Lemma $\mathcal{B}$ of Section R.1 (equation (R.7)). This result is a reworked form of the wave equation for $\vec{H}$, and it is the wave equation for $\vec{H}_T$. It is repeated here for in slightly modified form:

$$\frac{\partial}{\partial x}\frac{1}{\varepsilon}\frac{\partial}{\partial x}\vec{H}_T+\left(\vec{\nabla}_T\cdot\frac{1}{\varepsilon}\vec{\nabla}_T\right)\vec{H}_T-\frac{\partial}{\partial x}\frac{1}{\varepsilon}\vec{\nabla}_T H_x-\vec{\nabla}_T^i\frac{1}{\varepsilon}\vec{\nabla}_T\vec{H}_T^i+\frac{k^2}{\varepsilon}\vec{H}_T=0\,.$$

Neglecting (local) range dependence of ε, this becomes

$$\frac{1}{\varepsilon}\frac{\partial^2\vec{H}_T}{\partial x^2}+\left(\vec{\nabla}_T\cdot\frac{1}{\varepsilon}\vec{\nabla}_T\right)\vec{H}_T-\frac{1}{\varepsilon}\vec{\nabla}_T\frac{\partial H_x}{\partial x}-\vec{\nabla}_T^i\frac{1}{\varepsilon}\vec{\nabla}_T\vec{H}_T^i+\frac{k^2}{\varepsilon}\vec{H}_T=0\,. \qquad \text{(R.37)}$$

Now, substitute (R.31) into (R.37) to get

$$\frac{1}{\varepsilon}\frac{\partial^2\vec{H}_T^k}{\partial x^2}+\left(\vec{\nabla}_T\cdot\frac{1}{\varepsilon}\vec{\nabla}_T\right)\vec{H}_T^k+\frac{1}{\varepsilon}\vec{\nabla}_T^k\left[\frac{1}{\mu}\vec{\nabla}_T\cdot\left(\mu\vec{H}_T\right)\right]-\vec{\nabla}_T^i\frac{1}{\varepsilon}\vec{\nabla}_T^k\vec{H}_T^i+\frac{k^2}{\varepsilon}\vec{H}_T^k=0\,.$$

Multiply by ε and take the square root of the operators acting on $\vec{H}_T$:

[uuuu] One would have to write the real part as a sum of the function and its complex conjugate, and then carefully reverse the order to recover the proper form with $\vec{H}_T^*$ on the left and $\vec{H}_T$ on the right. This procedure would involve integration by parts, and it would essentially run the analysis in Appendix A in reverse.

$$i\frac{\partial \vec{H}_T^k}{\partial x} = \sqrt{\varepsilon\left(\vec{\nabla}_T \cdot \frac{1}{\varepsilon}\vec{\nabla}_T\right)\delta^{jk} + \vec{\nabla}_T^k \frac{1}{\mu}\vec{\nabla}_T^j \mu - \varepsilon\vec{\nabla}_T^j \frac{1}{\varepsilon}\vec{\nabla}_T^k + k^2\delta^{jk}} \cdot \vec{H}_T^j \qquad \text{(R.38)}$$

Now, to make this result compatible with (R.36), also neglect the (local) dependence of ε and μ:

$$i\frac{\partial \vec{H}_T^k}{\partial x} = \sqrt{\nabla_T^2 + k^2} \cdot \vec{H}_T^k .$$

Thus,

$$i\frac{\partial}{\partial x} = \sqrt{\nabla_T^2 + k^2} = k_0\sqrt{\frac{\nabla_T^2}{k_0^2} + \frac{k^2}{k_0^2}} . \qquad \text{(R.39)}$$

Now,

$$\begin{aligned} k &= \omega\sqrt{\varepsilon\mu} = \omega\sqrt{(\varepsilon_0 + \delta\varepsilon)(\mu_0 + \delta\mu)} \\ &= \underbrace{\omega\sqrt{\varepsilon_0\mu_0}}_{k_0}\sqrt{\left(1 + \frac{\delta\varepsilon}{\varepsilon_0}\right)\left(1 + \frac{\delta\mu}{\mu_0}\right)} \end{aligned} \quad . \qquad \text{(R.40)}$$

Substituting (R.40) into (R.39), we have

$$i\frac{\partial}{\partial x} = k_0\sqrt{\frac{\nabla_T^2}{k_0^2} + 1 + \frac{\delta\varepsilon}{\varepsilon_0} + \frac{\delta\mu}{\mu_0} + \frac{\delta\varepsilon}{\varepsilon_0}\frac{\delta\mu}{\mu_0}} = k_0\sqrt{1 + \frac{2\hat{\lambda}}{k_0}} , \qquad \text{(R.41)}$$

where

$$\hat{\lambda} \equiv \frac{\nabla_T^2}{2k_0} + \frac{k_0}{2}\left(\frac{\delta\varepsilon}{\varepsilon_0}\frac{\delta\mu}{\mu_0} + \frac{\delta\varepsilon}{\varepsilon_0} + \frac{\delta\mu}{\mu_0}\right). \qquad \text{(R.42)}$$

Substituting (R.41) into (R.36), we have

$$\vec{\theta}_T = \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} \frac{1}{\sqrt{\varepsilon_0\left(1 + \frac{\delta\varepsilon}{\varepsilon_0}\right)\omega}}\left[k_0\sqrt{1 + \frac{2\hat{\lambda}}{k_0}} - \vec{\nabla}_T \frac{1}{k_0\sqrt{1 + \frac{2\hat{\lambda}}{k_0}}}\vec{\nabla}_T\right]^{1/2} \cdot \vec{H}_T . \qquad \text{(R.43)}$$

Equations (R.43) and (R.42) recover equation (7.6) and definition (7.7) respectively.

R.2.3 The "minimal" correction

Finally, to get a "minimal" correction, assume the grazing angle is very small. Then, equation (R.43) becomes

$$\vec{\theta}_T = \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} \frac{1}{\sqrt{\varepsilon\omega}} \left[k_0 \sqrt{1 + \frac{\delta\varepsilon}{\varepsilon_0}\frac{\delta\mu}{\mu_0} + \frac{\delta\varepsilon}{\varepsilon_0} + \frac{\delta\mu}{\mu_0}} \right]^{1/2} \vec{H}_T$$

$$= \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} \frac{1}{\sqrt{\varepsilon\omega}} \left[\omega\sqrt{\varepsilon_0\mu_0} \sqrt{\left(1 + \frac{\delta\varepsilon}{\varepsilon_0}\right)\left(1 + \frac{\delta\mu}{\mu_0}\right)} \right]^{1/2} \vec{H}_T$$

$$= \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} \frac{1}{\sqrt{\varepsilon}} [\varepsilon\mu]^{1/4} \vec{H}_T = \left(\frac{\mu}{\mu_0}\right)^{1/4} \left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/4} \vec{H}_T$$

Dropping irrelevant constants that cancel at the endpoints, the "minimal correction" is $\vec{\theta}_T = (\mu/\varepsilon)^{1/4} \vec{H}_T + \mathrm{O}\left(\nabla_T^2 / k_0^2\right)$.

S Appendix: The elastodynamic field

This appendix supplies the details behind the results presented in Section 7.2. Appendix S.1 derives the state space equation for the elastodynamic field, equation (7.13) (with definitions (7.11) and (7.12)). Appendix S.2 derives an approximate transformation connecting the familiar full-wave displacement vector $\vec{u}$ with the corresponding auxiliary field $\vec{\chi}$ that is associated with downrange propagation by the parabolic equation. The transformation is given by equation (7.15) (with definitions (7.16) and (7.17)). This problem is more difficult than the electromagnetic case, and so equation (7.15) is only good to first order in $\vec{\nabla}_T$. Together, these two results provide enough information to allow the straightforward mechanical implementation of the formalism.

S.1 The state space equation for the elastodynamic field

Subsection S.1.1 derives the state space equation (7.13), and Subsection S.1.2 examines several interesting aspects of this result.

S.1.1 The calculation

To begin the derivation of the state space equation for an elastodynamic field (7.13), Subsection S.1.1.1 outlines the basic formalism for an elastic solid and states the Foldy-Wouthuysen ansatz for this problem. Subsection S.1.1.2 evaluates the three constituent partial differential equations of the matrix state space equation that are relatively easy to evaluate. Subsection S.1.1.3 evaluates the hard one. While the Hamiltonian in the state space equation is pseudo-Hermitian, the operators in the constituent partial differential equations should be Hermitian. This is not manifestly apparent for some of the terms that appear, but Subsection S.1.1.4 shows that these terms indeed properly contribute to

Hermiticity for the overall operator. Subsection S.1.1.5 combines the four component partial differential equations to form a state space operator. The combined operator should be manifestly pseudo-Hermitian, but once again this is not manifestly apparent. Subsection S.1.1.6 verifies that the derived Hamiltonian in the state space equation is indeed pseudo-Hermitian. Subsection S.1.1.7 takes the state space equation and converts it into a standard form that resembles the state space equations for the acoustic and electromagnetic fields. Finally, Subsection S.1.1.8 obtains workable expressions for the associated partial differential operators that appeared in the state space equation derived in Subsection S.1.1.7.

S.1.1.1 The basic formalism and the ansatz for the elastodynamic field

Once again as in Appendix R.1, let the discussion at the beginning of Appendix I guide us in constructing an ansatz that will lead to a state space equation that is a suitable starting point for the Foldy-Wouthuysen (FW) transformation. Specifically, start with the basic form

$$\Phi = \begin{pmatrix} \theta \\ \chi \end{pmatrix}$$

and construct θ and χ from the original field in such a way that $\Phi^\dagger \eta \Phi = |\theta|^2 - |\chi|^2$ is proportional to the downrange flux S_x. As noted in Appendix I, this is enough to guarantee that the associated state space equation constitutes a suitable starting point for the Foldy-Wouthuysen transformation.

The appropriate ansatz is

$$\underset{\sim}{\Phi} \equiv \begin{pmatrix} \vec{\theta} \\ \vec{\chi} \end{pmatrix} = \frac{1}{2}\left(\vec{u} \pm ia\hat{x} \cdot \vec{\tau}\right) \tag{S.1}$$

where $\vec{u}$ is the displacement vector, the stress energy tensor $\vec{\tau}$ is

$$\vec{\tau}^{ij} = \lambda\left(\vec{\nabla} \cdot \vec{u}\right)\delta^{ij} + \mu\left(\nabla^i u^j + \nabla^j u^i\right), \tag{S.2}$$

and a is a constant included for dimensional reasons. $\underset{\sim}{\Phi}$ is a 6-dimensional vector.

The elastodynamic wave equation is

$$\vec{\nabla} \cdot \vec{\tau} = -\rho\omega^2 \vec{u} \tag{S.3}$$

and the associated (time-averaged) downrange flux is (e.g., see equation 2.3 on p. 154 from reference [154]):

$$S_x = \frac{1}{2}\mathrm{Im}\left[\vec{u}^* \cdot \vec{\tau} \cdot \hat{x}\right]. \tag{S.4}$$

Note that

$$\vec{\theta}\cdot\vec{\theta}-\vec{\chi}\cdot\vec{\chi}=\frac{-a}{2}\mathrm{Im}\left[\vec{u}^{*}\cdot\vec{\tau}\cdot\hat{x}\right]=-aS_x\propto S_x\,, \tag{S.5}$$

and so our ansatz indeed generates carriers of the downrange flux.

Now we proceed to construct the state space equations. Once again, following Sections C.1.1, I and R.1, recall that the derivation of the state space equation requires that we develop two separate intermediate equations: one involving $\partial\left(\vec{\theta}-\vec{\chi}\right)\big/\partial x$ and the second involving $\partial\left(\vec{\theta}+\vec{\chi}\right)\big/\partial x$. Treating the downrange and transverse components of $\vec{\theta}+\vec{\chi}$ and $\vec{\theta}-\vec{\chi}$ separately, this becomes four equations. We develop these four equations next.

S.1.1.2 The "easy" part: equations for $\partial(\theta_x-\chi_x)/\partial x$, $\partial(\theta_x+\chi_x)/\partial x$ and $\partial\left(\vec{\theta}_T+\vec{\chi}_T\right)\big/\partial x$

<u>Equation #1</u> (equation (S.7))—for $\partial\left(\theta_x-\chi_x\right)\big/\partial x$

Take the divergence of $\left(\vec{\theta}-\vec{\chi}\right)\big/(ia)=\vec{\tau}\cdot\hat{x}$ and then use the wave equation (S.3):

$$\frac{\vec{\nabla}\cdot\left(\vec{\theta}-\vec{\chi}\right)}{ia}=\vec{\nabla}\cdot\vec{\tau}\cdot\hat{x}=-\rho\omega^2\underbrace{u_x}_{\theta_x+\chi_x}=-\rho\omega^2\left(\theta_x+\chi_x\right), \tag{S.6}$$

and so $i\vec{\nabla}\cdot\left(\vec{\theta}-\vec{\chi}\right)=\rho\omega^2 a\left(\theta_x+\chi_x\right)$ or

$$i\frac{\partial\left(\theta_x-\chi_x\right)}{\partial x}=-i\vec{\nabla}_T\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)+\rho\omega^2 a\left(\theta_x+\chi_x\right). \tag{S.7}$$

We will save the equation involving $\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)\big/\partial x$ for last.

<u>Equations #2 and #3</u> (equations (S.10) and (S.11))—for $\partial\left(\theta_x+\chi_x\right)\big/\partial x$ and $\partial\left(\vec{\theta}_T+\vec{\chi}_T\right)\big/\partial x$

Again subtract the two components of (S.1), but this time use definition (S.2) to substitute for $\vec{\tau}$:

$$\vec{\theta}-\vec{\chi}=ia\vec{\tau}\cdot\hat{x}=ia\left[\lambda\left(\vec{\nabla}\cdot\vec{u}\right)\hat{x}+\mu\left(\frac{\partial\vec{u}}{\partial x}+\vec{\nabla}u_x\right)\right]$$

or

$$\frac{\vec{\theta}-\vec{\chi}}{ia}=\vec{\tau}\cdot\hat{x}=(\lambda+2\mu)\frac{\partial u_x}{\partial x}\hat{x}+\lambda\left(\vec{\nabla}_T\cdot\vec{u}_T\right)\hat{x}+\mu\vec{\nabla}_T u_x+\mu\frac{\partial\vec{u}_T}{\partial x}. \tag{S.8}$$

First, we will develop the equation for $\partial\left(\theta_x+\chi_x\right)/\partial x$ (Equation #2) by projecting equation (S.8) into the x-direction:

$$\frac{\hat{x}\cdot\left(\vec{\theta}-\vec{\chi}\right)}{ia}=\frac{\theta_x-\chi_x}{ia}=(\lambda+2\mu)\frac{\partial u_x}{\partial x}+\lambda\left(\vec{\nabla}_T\cdot\vec{u}_T\right),$$

and so

$$\begin{aligned}(\lambda+2\mu)\frac{\partial u_x}{\partial x}&=-\lambda\left(\vec{\nabla}_T\cdot\vec{u}_T\right)+\frac{\theta_x-\chi_x}{ia}\\ i\frac{\partial u_x}{\partial x}&=-i\frac{\lambda}{\lambda+2\mu}\left(\vec{\nabla}_T\cdot\vec{u}_T\right)+\frac{\theta_x-\chi_x}{a(\lambda+2\mu)}\end{aligned}. \tag{S.9}$$

And using $\vec{u}=\vec{\theta}+\vec{\chi}$, we have Equation #2

$$i\frac{\partial\left(\theta_x+\chi_x\right)}{\partial x}=-i\left(\frac{\lambda}{\lambda+2\mu}\right)\vec{\nabla}_T\cdot\left(\vec{\theta}_T+\vec{\chi}_T\right)+\frac{\theta_x-\chi_x}{a(\lambda+2\mu)}. \tag{S.10}$$

Now, let us develop the equation for $\partial\left(\vec{\theta}_T+\vec{\chi}_T\right)/\partial x$ (Equation #3) by taking the transverse projection of equation (S.8) (i.e., $\left(\mathbf{1}-\hat{x}\hat{x}\right)\cdot\ldots$):

$$\begin{aligned}\frac{\vec{\theta}_T-\vec{\chi}_T}{ia}&=\mu\vec{\nabla}_T u_x+\mu\frac{\partial\vec{u}_T}{\partial x}\\ i\frac{\partial\vec{u}_T}{\partial x}&=-i\vec{\nabla}_T u_x+\frac{\vec{\theta}_T-\vec{\chi}_T}{a\mu}\end{aligned}.$$

Next, using $\vec{u}_T=\vec{\theta}_T+\vec{\chi}_T$ and $u_x=\theta_x+\chi_x$ we obtain Equation #3:

$$i\frac{\partial\left(\vec{\theta}_T+\vec{\chi}_T\right)}{\partial x}=-i\vec{\nabla}_T\left(\theta_x+\chi_x\right)+\frac{1}{a\mu}\left(\vec{\theta}_T-\vec{\chi}_T\right). \tag{S.11}$$

S.1.1.3 The "hard" part: the equation for $\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)/\partial x$

Equation #4 (equation (S.20)) — for $\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)/\partial x$

The remaining equation needed to derive the state space equation is the most difficult to obtain.

Recall that to derive Equation #1 (equation (S.7)), we used the x-component of the wave equation (S.3). To develop Equation #4 (equation (S.20) below) start with previously unused transverse components of the wave equation:

$$\vec{\nabla}\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)=-\rho\omega^2\vec{u}_T\,, \tag{S.12}$$

and break apart the gradient operator:

$$\frac{\partial}{\partial x}\left[\hat{x}\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)\right]=-\vec{\nabla}_T\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)-\rho\omega^2\vec{u}_T\,. \tag{S.13}$$

Now, set this result aside, and note that

$$\vec{\theta}_T-\vec{\chi}_T=ia\left[\hat{x}\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)\right]. \tag{S.14}$$

Operating on (S.14) with $i\partial/\partial x$, we get

$$i\frac{\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)}{\partial x}=-a\frac{\partial}{\partial x}\left[\hat{x}\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)\right]. \tag{S.15}$$

Substitute (S.13) into (S.15) to get

$$i\frac{\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)}{\partial x}=a\vec{\nabla}_T\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)+\rho\omega^2a\vec{u}_T\,. \tag{S.16}$$

We are not quite finished, because we still need to evaluate $\vec{\nabla}_T\cdot\vec{\tau}\cdot\left(\mathbf{1}-\hat{x}\hat{x}\right)$. Let us begin with the transverse projection of the definition of the stress-energy tensor, equation (S.2):

$$\begin{aligned}\vec{\tau}_T^{ij}&=\lambda\left(\vec{\nabla}\cdot\vec{u}\right)\underbrace{\delta_T^{ij}}_{\begin{pmatrix}0&0&0\\0&1&0\\0&0&1\end{pmatrix}}+\mu\left(\nabla_T^iu_T^j+\nabla_T^ju_T^i\right)\\&=\lambda\underbrace{\frac{\partial u_x}{\partial x}}_{\substack{\text{we know}\\\text{this}}}\delta_T^{ij}+\lambda\left(\vec{\nabla}_T\cdot\vec{u}_T\right)\delta_T^{ij}+\mu\left(\nabla_T^iu_T^j+\nabla_T^ju_T^i\right)\quad.\end{aligned}$$

Now, substitute for $\partial u_x/\partial x$ using equation (S.9) (divided by i):

$$\begin{aligned}\vec{\tau}_T^{ij}=\lambda&\left(-\frac{\lambda}{\lambda+2\mu}\left(\vec{\nabla}_T\cdot\vec{u}_T\right)+\frac{\theta_x-\chi_x}{ai\left(\lambda+2\mu\right)}\right)\delta_T^{ij}+\lambda\left(\vec{\nabla}_T\cdot\vec{u}_T\right)\delta_T^{ij}\\&+\mu\left(\nabla_T^iu_T^j+\nabla_T^ju_T^i\right)\end{aligned}\,. \tag{S.17}$$

Also note that

$$-\frac{\lambda^2}{\lambda+2\mu}+\lambda=-\frac{\lambda^2}{\lambda+2\mu}+\frac{\lambda(\lambda+2\mu)}{\lambda+2\mu}=\frac{2\mu\lambda}{\lambda+2\mu},$$

so that (S.17) becomes

$$\begin{aligned}\vec{\tau}_T^{ij} &= \frac{2\lambda\mu}{\lambda+2\mu}\left(\vec{\nabla}_T\cdot\vec{u}_T\right)\delta_T^{ij}+\mu\left(\nabla_T^i u_T^j+\nabla_T^j u_T^i\right)+\frac{\lambda(\theta_x-\chi_x)}{ai(\lambda+2\mu)}\delta_T^{ij}\\ &= \frac{2\lambda\mu}{\lambda+2\mu}\vec{\nabla}_T\cdot\left(\vec{\theta}_T+\vec{\chi}_T\right)\delta_T^{ij}+\mu\left(\nabla_T^i\left(\theta_T^j+\chi_T^j\right)+\nabla_T^j\left(\theta_T^i+\chi_T^i\right)\right)+\frac{\lambda(\theta_x-\chi_x)}{ai(\lambda+2\mu)}\delta_T^{ij} \quad \text{(S.18)}\\ &= \left[\frac{2\lambda\mu}{\lambda+2\mu}\delta_T^{ij}\nabla_T^k+\mu\left(\nabla_T^i\delta_T^{jk}+\nabla_T^j\delta_T^{ik}\right)\right]\left(\vec{\theta}_T+\vec{\chi}_T\right)^k+\delta_T^{ij}\left(\frac{\lambda}{ai(\lambda+2\mu)}\right)(\theta_x-\chi_x).\end{aligned}$$

Thus,

$$\begin{aligned}\vec{\nabla}_T\cdot\vec{\tau}\cdot(\mathbf{1}-\hat{x}\hat{x}) &= \vec{\nabla}_T\cdot\vec{\tau}_T\\ &= \nabla_T^j\left[\frac{2\lambda\mu}{\lambda+2\mu}\vec{\nabla}_T^k\left(\vec{\theta}_T+\vec{\chi}_T\right)^k\right]+\\ &\quad+\nabla_T^i\mu\nabla_T^i\delta_T^{jk}\left(\vec{\theta}_T+\vec{\chi}_T\right)^k+\nabla_T^k\mu\nabla_T^j\left(\vec{\theta}_T+\vec{\chi}_T\right)^k\\ &\quad+\nabla_T^j\left(\frac{\lambda}{ai(\lambda+2\mu)}\right)(\theta_x-\chi_x)\quad,\end{aligned} \tag{S.19}$$

and substituting into (S.16) gives us

$$\begin{aligned}i\frac{\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)^j}{\partial x} &= a\left[\nabla_T^j\frac{2\lambda\mu}{\lambda+2\mu}\vec{\nabla}_T^k+\nabla_T^i\mu\nabla_T^i\delta_T^{jk}+\nabla_T^k\mu\nabla_T^j\right]\left(\vec{\theta}_T+\vec{\chi}_T\right)^k\\ &\quad+\nabla_T^j\left(\frac{\lambda}{ai(\lambda+2\mu)}\right)(\theta_x-\chi_x)+\rho\omega^2 a\underbrace{\vec{u}_T^j}_{\left(\vec{\theta}_T+\vec{\chi}_T\right)^j}.\end{aligned} \tag{S.20}$$

Equation (S.20) is Equation #4.

S.1.1.4 A note on Hermiticity

Note the second to the last terms in equation (S.20) and in (S.10). Individually, it looks like they will violate Hermiticity, but taken together they give a structure of the basic form

$$\begin{pmatrix}0 & i\vec{\nabla}_T f\\ if\vec{\nabla}_T & 0\end{pmatrix}. \tag{S.21}$$

If we take the transpose and the complex conjugate of this matrix, we wind up with

$$\begin{pmatrix} 0 & -if\vec{\nabla}_T \\ -i\vec{\nabla}_T f & 0 \end{pmatrix},$$

and then integrating by parts we get back to (S.21). Thus, the matrices of the form (S.21) are perfectly good Hermitian matrices. It is also worth noting that one finds a similar set of operators that initially seem to violate Hermiticity in equations 4, 5 and 6 of reference [155].

S.1.1.5 Combining the component partial differential equations to form the state space equation

Combining the four equations (S.7), (S.10), (S.11) and (S.20), we have

$$\begin{aligned}
\frac{\partial\left(\vec{\theta}_T-\vec{\chi}_T\right)^j}{\partial x} &= \overbrace{a\left[\vec{\nabla}_T^j\frac{2\lambda\mu}{\lambda+2\mu}\vec{\nabla}_T^k\left(\vec{\theta}_T+\vec{\chi}_T\right)^k+\nabla_T^i\mu\nabla_T^i\delta_T^{jk}+\nabla_T^k\mu\nabla_T^j\right]}^{b}\left(\vec{\theta}_T+\vec{\chi}_T\right)^k \\
&\quad \underbrace{-i\nabla_T^j\left(\frac{\lambda}{a\left(\lambda+2\mu\right)}\right)}_{c}\left(\theta_x-\chi_x\right)+\underbrace{\rho\omega^2 a}_{d}\left(\vec{\theta}_T+\vec{\chi}_T\right)^j \\
i\frac{\partial\left(\theta_x-\chi_x\right)}{\partial x} &= \underbrace{-i\vec{\nabla}_T}_{e}\cdot\left(\vec{\theta}_T-\vec{\chi}_T\right)+\underbrace{\rho\omega^2 a}_{f}\left(\theta_x+\chi_x\right) \qquad \text{(S.22)} \\
i\frac{\partial\left(\vec{\theta}_T+\vec{\chi}_T\right)}{\partial x} &= \underbrace{-i\vec{\nabla}_T}_{g}\left(\theta_x+\chi_x\right)+\underbrace{\frac{1}{a\mu}}_{h}\left(\vec{\theta}_T-\vec{\chi}_T\right) \\
i\frac{\partial\left(\theta_x+\chi_x\right)}{\partial x} &= \underbrace{-i\left(\frac{\lambda}{\lambda+2\mu}\right)\vec{\nabla}_T}_{p}\cdot\left(\vec{\theta}_T+\vec{\chi}_T\right)+\underbrace{\frac{1}{a\left(\lambda+2\mu\right)}}_{q}\theta_x-\chi_x \quad .
\end{aligned}$$

Note that a vector with a subscript T is a 2-dimensional vector in the (transverse) y-z plane. An ordinary vector without the subscript also adds a third dimension: the downrange direction x, and so the subscript x denotes a component of the vector in the downrange direction.

Now, the indices $j\in\{1,2\}$ denote y and z components, while the indices $j=0$ and $k=0$ denotes an x-component. Then, with the following definitions:

$$
\begin{aligned}
b^{jk} &= a\left[\nabla_T^j \frac{2\lambda\mu}{\lambda+2\mu}\nabla_T^k + \nabla_T^i \mu \nabla_T^i \underbrace{\delta_T^{jk}}_{\delta^{jk}-\delta^{j0}\delta^{k0}} + \nabla_T^k \mu \nabla_T^j\right] \\
c^{jk} &= -i\nabla_T^j\left(\frac{\lambda}{(\lambda+2\mu)}\right)\delta^{k0} \quad ; \quad d^{jk} = \rho\omega^2 a \underbrace{\delta_T^{jk}}_{\delta^{jk}-\delta^{j0}\delta^{k0}} \\
e^{jk} &= -i\delta^{j0}\nabla_T^k \quad ; \quad f^{jk} = \delta^{j0}\delta^{k0}\rho\omega^2 a \quad ,
\end{aligned}
\tag{S.23}
$$

the first two equations in (S.22) combine to form

$$
i\frac{\partial\left(\vec{\theta}-\vec{\chi}\right)^j}{\partial x} = \left(b^{jk}+d^{jk}+f^{jk}\right)\left(\vec{\theta}+\vec{\chi}\right)^k + \left(c^{jk}+e^{jk}\right)\left(\vec{\theta}-\vec{\chi}\right)^k . \tag{S.24}
$$

Note that $d^{jk}+f^{jk} = \rho\omega^2 a\delta^{jk}$.

Similarly, with the definitions

$$
\begin{aligned}
g^{jk} &= -i\nabla_T^j\delta^{k0} \quad ; \quad h^{jk} = \frac{1}{a\mu}\underbrace{\delta_T^{jk}}_{\delta^{jk}-\delta^{j0}\delta^{k0}} \\
p^{jk} &= -i\left(\frac{\lambda}{\lambda+2\mu}\right)\nabla_T^k\delta^{j0} \quad ; \quad q^{jk} = \frac{1}{a(\lambda+2\mu)}\delta^{j0}\delta^{k0} \quad ,
\end{aligned}
\tag{S.25}
$$

the third and fourth equations in (S.22) combine to form

$$
i\frac{\partial\left(\vec{\theta}+\vec{\chi}\right)^j}{\partial x} = \left(g^{jk}+p^{jk}\right)\left(\vec{\theta}+\vec{\chi}\right)^k + \left(h^{jk}+q^{jk}\right)\left(\vec{\theta}-\vec{\chi}\right)^k . \tag{S.26}
$$

With the definitions (suppressing the indices j,k)

$$
\begin{aligned}
A &\equiv b+d+f \quad ; \quad B \equiv c+e \\
C &= g+p \quad ; \quad D \equiv h+q \quad ,
\end{aligned}
\tag{S.27}
$$

equations (S.24) and (S.26) become

$$
\begin{aligned}
i\frac{\partial\left(\vec{\theta}-\vec{\chi}\right)^j}{\partial x} &= A^{jk}\left(\vec{\theta}+\vec{\chi}\right)^k + B^{jk}\left(\vec{\theta}-\vec{\chi}\right)^k \\
i\frac{\partial\left(\vec{\theta}+\vec{\chi}\right)^j}{\partial x} &= C^{jk}\left(\vec{\theta}+\vec{\chi}\right)^k + D^{jk}\left(\vec{\theta}-\vec{\chi}\right)^k
\end{aligned} \quad .
\tag{S.28}
$$

Below, it will be understood that A,B,C and D are 3×3 matrices, and that the vectors $\vec{\theta}$ and $\vec{\chi}$ can be understood as 3×1 column matrices. Then, (S.28) becomes

$$\begin{aligned} i\frac{\partial\left(\vec{\theta}-\vec{\chi}\right)}{\partial x} &= A\left(\vec{\theta}+\vec{\chi}\right)+B\left(\vec{\theta}-\vec{\chi}\right) \\ i\frac{\partial\left(\vec{\theta}+\vec{\chi}\right)}{\partial x} &= C\left(\vec{\theta}+\vec{\chi}\right)+D\left(\vec{\theta}-\vec{\chi}\right) \end{aligned} . \tag{S.29}$$

To get the state space equation, we will add and subtract the equations in (S.29). Adding and dividing by 2, we get

$$i\frac{\partial\vec{\theta}}{\partial x}=\frac{1}{2}\left(A+B+C+D\right)\vec{\theta}-\frac{1}{2}\left(A-B+C-D\right)\vec{\chi}\,.$$

Subtracting the first from the second and dividing by two, we get

$$i\frac{\partial\vec{\theta}}{\partial x}=\frac{1}{2}\left(-A-B+C+D\right)\vec{\theta}-\frac{1}{2}\left(-A+B+C-D\right)\vec{\chi}$$

or

$$i\begin{pmatrix}\dfrac{\partial\vec{\theta}}{\partial x}\\[2ex] \dfrac{\partial\vec{\chi}}{\partial x}\end{pmatrix}=\frac{1}{2}\begin{pmatrix}A+B+C+D & A-B+C-D\\ -A-B+C+D & -A+B+C-D\end{pmatrix}\begin{pmatrix}\vec{\theta}\\ \vec{\chi}\end{pmatrix}.$$

Thus,

$$i\frac{\partial\underset{\sim}{\Phi}}{\partial x}=\left\{\begin{array}{l}\overbrace{\dfrac{1}{2}\left(A+D\right)\underbrace{\begin{pmatrix}1&0\\0&-1\end{pmatrix}}_{\eta}+\dfrac{1}{2}\left(A-D\right)\underbrace{\begin{pmatrix}0&1\\-1&0\end{pmatrix}}_{\xi}}^{\text{Standard terms just like in Acoustics and E+M}}\\[2ex] \underbrace{\dfrac{1}{2}\left(C+B\right)\begin{pmatrix}1&0\\0&1\end{pmatrix}+\dfrac{1}{2}\left(C-B\right)\begin{pmatrix}0&1\\1&0\end{pmatrix}}_{\text{New terms not previously encountered}}\end{array}\right\}\underset{\sim}{\Phi}=\mathcal{H}\underset{\sim}{\Phi}\,. \tag{S.30}$$

S.1.1.6 Verifying pseudo-Hermiticity

Note that in the matrix Hamiltonian $\mathcal{H}$ we now get new terms of a sort not previously encountered in the acoustic and electromagnetic problems. Before proceeding, let us take a closer look at these terms. The matrix operators $\eta\xi$ and $\mathbf{1}$ have not appeared before in our state space equation, but the most interesting new feature lies in the nature of the coefficients of these matrices. For example, expressing $C+B$ in terms of the definitions in (S.27) and rearranging terms a little, we have

$$
\begin{aligned}
C+B &= (c+p)+(e+g) \\
&= \left[-i\nabla_T^j \left(\frac{\lambda}{(\lambda+2\mu)} \right) \delta^{k0} + -i \left(\frac{\lambda}{\lambda+2\mu} \right) \nabla_T^k \delta^{j0} \right] \\
&\quad + \left(-i\delta^{j0}\nabla_T^k - i\nabla_T^j \delta^{k0} \right) \quad ,
\end{aligned}
\tag{S.31}
$$

and let

$$
\begin{aligned}
\alpha &= (C+B) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \left\{ \begin{aligned} &\left[-i\nabla_T^j \left(\frac{\lambda}{(\lambda+2\mu)} \right) \delta^{k0} - i \left(\frac{\lambda}{\lambda+2\mu} \right) \nabla_T^k \delta^{j0} \right] \\ &+ \left(-i\delta^{j0}\nabla_T^k - i\nabla_T^j \delta^{k0} \right) \end{aligned} \right\} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .
\end{aligned}
\tag{S.32}
$$

Let us verify that the term (S.32) is pseudo-Hermitian. Recall that some operator α is defined to be pseudo-Hermiticitian if $(\alpha\eta)^\dagger = \alpha\eta$ or equivalently $\eta\alpha^\dagger = \alpha\eta$. Therefore, to verify pseudo-Hermiticity, we need to find $\alpha^\dagger$ and commute it with η.

To find $\alpha^\dagger$, we need to:

1. Take the Hermitian conjugate of the differential operators. This means integrate by parts, and take the complex conjugate. This amounts to $\vec{\nabla}_T f \to -f\vec{\nabla}_T$ for a real function f and $i \to -i$.
2. Exchange indices: $j \to k$ and $k \to j$. This exchanges rows and columns in the 3×3 matrices.
3. Take the Hermitian conjugate of the 2×2 matrix in our outer product: exchange rows and columns and take the complex conjugate. (The unit matrix in the example in (S.32) is, of course, its own Hermitian conjugate.)

Then to verify pseudo-Hermiticity, take $\eta\alpha$ and $\alpha^\dagger\eta$, and verify that they are the same. This constitutes step 4.

Let us do this for example (S.32).

(1) Hermitian conjugation of the operators:

$$
\begin{aligned}
C+B \to &\left[-i \left(\frac{\lambda}{(\lambda+2\mu)} \right) \nabla_T^j \delta^{k0} - i\nabla_T^k \left(\frac{\lambda}{\lambda+2\mu} \right) \delta^{j0} \right] \\
&+ \left(-i\nabla_T^k \delta^{j0} - i\nabla_T^j \delta^{k0} \right)
\end{aligned}
$$

(2) Exchange indices to get

$$C+B\rightarrow\left[-i\left(\frac{\lambda}{(\lambda+2\mu)}\right)\nabla_T^k\delta^{j0}-i\nabla_T^j\left(\frac{\lambda}{\lambda+2\mu}\right)\delta^{k0}\right]$$
$$+\left(-i\nabla_T^j\delta^{k0}-i\nabla_T^k\delta^{j0}\right)$$

which from equation (S.31) is equal to $C+B$.

(3) and (4) Taking the complex conjugate of the unit vector and multiplying it with itself are trivial.

Thus, this term is indeed pseudo-Hermitian, as it should be given that the construction of the state space equation guaranteed that it would be so. However, for the first time, the pseudo-Hermiticity was not obvious by casual examination.

Now, let us do the same for the term

$$\frac{1}{2}(C-B)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

Again assign it the label α. Demonstrating that this term is pseudo-Hermitian is trickier than for our previous example.

To begin with, we have (using definitions (S.23), (S.25) and (S.27))

$$C-B=\left(g^{jk}-e^{jk}\right)+\left(p^{jk}-c^{jk}\right)$$
$$=\left(-i\nabla_T^j\delta^{k0}+i\nabla_T^k\delta^{j0}\right)+\left(-i\left(\frac{\lambda}{\lambda+2\mu}\right)\nabla_T^k\delta^{j0}+i\nabla_T^j\left(\frac{\lambda}{(\lambda+2\mu)}\right)\delta^{k0}\right)\quad .$$

Then, we again follow the 3-step procedure to take the Hermitian conjugate of α:

(1) Hermitian conjugate these differential operators to get
$C-B\rightarrow$

$$\left(-i\nabla_T^j\delta^{k0}+i\nabla_T^k\delta^{j0}\right)+\left(-i\nabla_T^k\left(\frac{\lambda}{\lambda+2\mu}\right)\delta^{j0}+i\left(\frac{\lambda}{(\lambda+2\mu)}\right)\nabla_T^j\delta^{k0}\right)$$

(2) Exchange indices:
$C-B\rightarrow$

$$\left(-i\nabla_T^k\delta^{j0}+i\nabla_T^j\delta^{k0}\right)+\left(-i\nabla_T^j\left(\frac{\lambda}{\lambda+2\mu}\right)\delta^{k0}+i\left(\frac{\lambda}{(\lambda+2\mu)}\right)\nabla_T^k\delta^{j0}\right)$$
$$=-(C-B)$$

(3) Taking the Hermitian conjugate of the 2×2 matrix

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we just get it back.

Thus,

$$\alpha^\dagger = -\frac{1}{2}(C-B)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\alpha$$

and

$$\eta\alpha^\dagger = -\frac{1}{2}(C-B)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\frac{1}{2}(C-B)\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{2}(C-B)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Now,

$$\alpha\eta = \frac{1}{2}(C-B)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}(C-B)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

and $\eta\alpha^\dagger = (\alpha\eta)^\dagger = \alpha\eta$, and we have explicitly seen that now the second "new" term in (S.30) is also pseudo-Hermitian.

Thus, the third and fourth terms in (S.30) are properly pseudo-Hermitian. The first and second terms are completely standard and quite obviously pseudo-Hermitian as well. Thus, we have indeed explicitly verified that the matrix Hamiltonian $\mathcal{H}$ is pseudo-Hermitian, and consequently that our formalism properly conserves energy. (From our construction, we knew things should turn out this way, but it is nice to see that it really worked out.)

S.1.1.7 Standard form of the state space equation

Next, let us put the matrix Hamiltonian $\mathcal{H}$ into standard form. We do not yet know what the constant k_0 will turn out to be (because we have not yet chosen a in ansatz (S.1)), but we do know that we will need to pull out a term of the form $k_0\delta^{jk}\eta$ (or in matrix notation $k_0\mathbf{1}_{3\times 3}\otimes\eta$) from the Hamiltonian $\mathcal{H}$ in equation (S.30). Thus, we have (as above, suppressing the explicit outer product sign $\otimes$ to keep things from getting too cluttered)

$$\underset{\sim}{\mathcal{Q}} = \frac{1}{2}(A-D)\underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\xi} + \frac{1}{2}(C-B)\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\tau}$$
$$\underset{\sim}{\mathcal{E}} = \frac{1}{2}(A+D-2k_0\mathbf{1})\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\eta} + \frac{1}{2}(C+B)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \tag{S.33}$$

where $\underset{\sim}{\mathcal{H}} = \underset{\sim}{\mathcal{Q}} + \underset{\sim}{\mathcal{E}} + k_0\mathbf{1}_{3\times 3}\eta$. The tildes underneath serve to remind us that the matrices are 6×6.

Note that $\underset{\sim}{\mathcal{Q}}\eta = -\eta\underset{\sim}{\mathcal{Q}}$ (the fact that $\{\eta,\tau\}=0$ is crucial here), $\underset{\sim}{\mathcal{E}}\eta = \eta\underset{\sim}{\mathcal{E}}$, $\eta^2 = 1$. Also, we have closure under multiplication[vvvv] (as we must since the four matrices $\eta,\xi,\tau,\mathbf{1}$ span the set of 2×2 matrices). We know from reference [1] (or equivalently Appendix C.2.3.2) that the conditions outlined in this paragraph, and the basic form in the previous paragraph is enough to ensure that the Foldy-Wouthuysen procedure will apply.

Before we go on to write out the coefficients in equations (S.33), let us examine one more important issue. As it stands, the coefficients in equations (S.33), which are in a sense expansion parameters, contain terms that are not yet "small". Such terms appear in both $\underset{\sim}{\mathcal{Q}}$ and $\underset{\sim}{\mathcal{E}}$, but let us examine their appearance in $\underset{\sim}{\mathcal{Q}}$, where it will most directly affect the expansion parameter.

In $\underset{\sim}{\mathcal{Q}}$, the term appears in the coefficient of $\xi/2$:

[vvvv] The identities $\xi\tau = \eta = -\tau\xi$ and $\eta\xi = \tau = -\xi\eta$ serve to explicitly remind that us that the expanded set of four matrices that now appear in the matrix Hamiltonian $\mathcal{H}$ are indeed closed.

$$A-D=\left(\begin{array}{c} b+\underbrace{d+f}_{\substack{\rho\omega^2 a\delta^{jk}= \\ \rho\omega^2 a\mathbf{1}}} \end{array}\right)-\underbrace{\left(h+q\right)}_{\frac{1}{a}\begin{pmatrix}\frac{1}{\lambda+2\mu} & 0 & 0\\ 0 & \frac{1}{\mu} & 0\\ 0 & 0 & \frac{1}{\mu}\end{pmatrix}}$$

$$=b+\underbrace{\begin{pmatrix}\rho\omega^2 a-\dfrac{1}{a\left(\lambda+2\mu\right)} & 0 & 0\\ 0 & \rho\omega^2 a-\dfrac{1}{a\mu} & 0\\ 0 & 0 & \rho\omega^2 a-\dfrac{1}{a\mu}\end{pmatrix}}_{\text{Since } b \text{ is already small, this needs to be small too}}.$$

The components of the matrix above must be made small. The first step is to add zero in the form $-\rho_0\omega a+\rho_0\omega a$ to all three terms, $1/\left(\lambda_0+2\tilde{\mu}_0\right)-1/\left(\lambda_0+2\tilde{\mu}_0\right)$ to the top term, and $1/\left(a\mu_0\right)-1/\left(a\mu_0\right)$ to the bottom two terms[wwww]. This will give us a matrix whose terms involve only the deviations from the reference values of the parameters ρ, $\lambda+2\mu$ and μ. This action also generates an additional matrix that we examine next.

Once this first step is done, we are still left with a "problem term" of the form:

$$\begin{pmatrix}\rho_0\omega^2 a-\dfrac{1}{a\left(\lambda_0+2\mu_0\right)} & 0 & 0\\ 0 & \rho_0\omega^2 a-\dfrac{1}{a\mu_0} & 0\\ 0 & 0 & \rho_0\omega^2 a-\dfrac{1}{a\mu_0}\end{pmatrix}.$$

This term has an interesting property that is a little different from anything encountered previously in our study of acoustic and electromagnetic fields. To see this unique property, let us examine the following thought experiment. Consider a 1-dimensional (plane) wave in a completely homogeneous environment, with the reference parameters all chosen to be the same as the medium's parameters, which are all assumed to be

[wwww] Note that $\tilde{\mu}_0$ does not in principle have to be the same as μ_0. In fact, $\rho_0, \lambda_0+2\tilde{\mu}_0$ and μ_0 could refer to different spots in the medium, or some set of reference values that is not associated with any point in physical space. However, usually $\tilde{\mu}_0$ will be chosen to be the same as μ_0.

globally constant. Even in this most basic case, there is nothing to make this term disappear under these circumstances. This is the property that is a little different from any encountered previously in our study of acoustic and electromagnetic fields. To be specific, recall that during our study of the electromagnetic and acoustic fields, we never encountered such a property at all in the odd terms (i.e., off diagonal in the 2×2 state space), and when we observed such terms in the even terms (i.e., the terms that are diagonal in the 2×2 state space), they eventually disappeared except for the ever-present $k_0\eta$ term. Fortunately, we can <u>almost</u> make these terms disappear with a judicious choice of the free parameter a.

Choose

$$a=\frac{1}{\omega\rho_0 c_0^s}\quad;\quad c_0^s\equiv\sqrt{\frac{\mu_0}{\rho_0}}\quad;\quad c_0^p\equiv\sqrt{\frac{\lambda_0+2\tilde{\mu}_0}{\rho_0}}\,, \tag{S.34}$$

so that (with $k_0^s\equiv\omega/c_0^s$)

$$\rho_0\omega^2 a=\frac{\rho_0\omega^2}{\omega\rho_0 c_0^s}=\frac{\omega}{c_0^s}=k_0^s\,,$$

$$\frac{1}{a\left(\lambda_0+2\tilde{\mu}_0\right)}=\frac{\omega\rho_0 c_0^s}{\lambda_0+2\tilde{\mu}_0}=\frac{\omega}{c_0^s}\frac{1}{\left(c_0^p\right)^2}\left(c_0^s\right)^2=k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2, \tag{S.35}$$

and similarly

$$\frac{1}{a\mu_0}=k_0^s\,. \tag{S.36}$$

Now our "problem term" reduces to

$$k_0^s\begin{pmatrix}1-\left(c_0^s/c_0^p\right)^2 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}. \tag{S.37}$$

Note that

$$1-\left(\frac{c_0^s}{c_0^p}\right)^2=1-\frac{\mu_0}{\lambda_0+2\tilde{\mu}_0}=\frac{\lambda_0+2\tilde{\mu}_0-\mu_0}{\lambda_0+2\tilde{\mu}_0}$$

or with $\tilde{\mu}_0=\mu_0$,

$$1-\left(\frac{c_0^s}{c_0^p}\right)^2=\frac{\lambda_0+\mu_0}{\lambda_0+2\mu_0}\,.$$

Provided λ_0 and μ_0 are physical values evaluated at the same location, then this expansion parameter varies from 1 down to ¼ (as λ varies from infinity down to $-2\mu/3$; this range of allowed values is determined by the requirement that the bulk modulus $\lambda + \frac{2}{3}\mu$ be positive[156]). Since it is always smaller than 1, this is a legitimate expansion parameter.

So, we are still left with a new intrinsic expansion parameter $1-\left(c_0^s/c_0^p\right)^2$. While unprecedented, after a little thought, this will not turn out to be too surprising. Let us first proceed to write out the state space equation and then return to this issue in Appendix S.1.2.2 (and in Section 7.2 of the main text as well), when we are better prepared to examine it in detail.

For now, we have a perfectly good state space equation provided that $a = 1/\left(\omega\rho_0 c_0^s\right)$ (as given in equation (S.34)):

$$i\frac{\partial \underset{\sim}{\Phi}}{\partial x} = \left(\underbrace{\underset{\sim}{\mathcal{Q}} + \underset{\sim}{\mathcal{E}}}_{\substack{6\times 6 \text{ matrices made up of outer products of } (3\times 3)\otimes(2\times 2) \text{ matrices}}} + \underbrace{k_0 \mathbf{1}_{3\times 3}\otimes\eta}_{\substack{\text{or equivalently} \\ k_0\delta^{jk}\eta}} \right) \underbrace{\underset{\sim}{\Phi}}_{\substack{6\text{-component vector} \\ \begin{pmatrix}\vec{\theta}\\ \vec{\chi}\end{pmatrix}}} \tag{S.38}$$

with (using (S.33))

$$\begin{aligned} \underset{\sim}{\mathcal{Q}} &= \overbrace{\frac{1}{2}(A-D)}^{\lambda=\lambda^{jk}=3\times 3 \text{ matrix}}\ \xi + \overbrace{\frac{1}{2}(C-B)}^{\kappa}\tau \\ \underset{\sim}{\mathcal{E}} &= \underbrace{\frac{1}{2}\left(A+D-2k_0\mathbf{1}_{3\times 3}\right)}_{\substack{\lambda-2\gamma \\ \gamma\equiv\frac{1}{2}(k_0-D)}}\eta + \underbrace{\frac{1}{2}(C+B)}_{\substack{\kappa-2\beta \\ \beta\equiv-\frac{1}{2}B}}\mathbf{1}_{2\times 2} \quad . \end{aligned} \tag{S.39}$$

So now, we need to evaluate λ, κ, γ and β.

S.1.1.8 Evaluating the operators λ, κ, γ and β

To begin our calculation of the operators λ, κ, γ and β, we will evaluate the following lemma.

Lemma: evaluate "$-h-q$" (which shows up in λ and γ)

We make the usual choice $a = 1/\left(\omega\rho_0 c_0^s\right)$ (but we will not at this point restrict ourselves to $\tilde{\mu}_0 = \mu_0$), and use definitions (S.25):

$$-h-q = \underbrace{-\frac{1}{a\mu}\delta^{jk} + \frac{1}{a\mu}\delta^{j0}\delta^{k0}}_{-h} \underbrace{-\frac{1}{a\left(\lambda+2\mu\right)}\delta^{j0}\delta^{k0}}_{-q}. \tag{S.40}$$

Now, using (S.35) and (S.36) respectively, we have:

$$\begin{aligned} &\frac{1}{a\left(\lambda+2\mu\right)} = \frac{\lambda_0+2\tilde{\mu}_0}{\lambda+2\mu}\cdot k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2, \\ &\frac{1}{a\mu} = \frac{\mu_0}{\mu}k_0^s \end{aligned} \tag{S.41}$$

and so combining (S.40) and (S.41)

$$\begin{aligned} -h-q &= -\frac{\mu_0}{\mu}k_0^s\delta^{jk} + \frac{\mu_0}{\mu}k_0^s\delta^{j0}\delta^{k0} - \frac{\lambda_0+2\tilde{\mu}_0}{\lambda+2\mu}k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2\delta^{j0}\delta^{k0} \\ &= -\frac{\mu_0}{\mu}k_0^s\delta^{jk} + \underbrace{k_0^s\delta^{jk} - k_0^s\delta^{jk}}_{\text{zero}} \\ &\quad + \frac{\mu_0}{\mu}k_0^s\delta^{j0}\delta^{k0}\underbrace{-k_0^s\delta^{j0}\delta^{k0}}_{\swarrow\text{zero}} \\ &\quad + \overbrace{k_0^s\delta^{j0}\delta^{k0}}^{\text{zero}\nearrow}\underbrace{-k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2\delta^{j0}\delta^{k0}}_{\swarrow\text{zero}} \\ &\quad + \overbrace{k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2\delta^{j0}\delta^{k0}}^{\text{zero}\nearrow} - \frac{\lambda_0+2\tilde{\mu}_0}{\lambda+2\mu}k_0^s\left(\frac{c_0^s}{c_0^p}\right)^2\delta^{j0}\delta^{k0}, \end{aligned}$$

and so

$$\begin{aligned} -h-q = &-k_0^s\delta^{jk} + k_0^s\delta^{jk}\left(1-\frac{\mu_0}{\mu}\right) - k_0^s\delta^{j0}\delta^{k0}\left(1-\frac{\mu_0}{\mu}\right) \\ &+k_0^s\delta^{j0}\delta^{k0}\left(\frac{c_0^s}{c_0^p}\right)^2\left(1-\frac{\lambda_0+2\tilde{\mu}_0}{\lambda+2\mu}\right) \\ &+k_0^s\delta^{j0}\delta^{k0}\left(1-\left(\frac{c_0^s}{c_0^p}\right)^2\right). \end{aligned}$$

Now,

$$n_s = c_0^s/c^s \quad ; \quad n_p = c_0^p/c^p \quad ; \quad n_0^{sp} = c_0^s/c_0^p, \tag{S.42}$$

and so

$$\frac{\mu_0}{\mu}=\frac{\mu_0/\rho_0}{\mu/\rho}\cdot\frac{\rho_0}{\rho}=\left(\frac{c_0^s}{c^s}\right)^2\cdot\frac{\rho_0}{\rho}=n_s^2\,\frac{\rho_0}{\rho}$$

$$\frac{\lambda_0+2\tilde{\mu}_0}{\lambda+2\mu}=\frac{\lambda_0+2\tilde{\mu}_0/\rho_0}{\lambda+2\mu/\rho}\cdot\frac{\rho_0}{\rho}=\left(\frac{c_0^p}{c^p}\right)^2\cdot\frac{\rho_0}{\rho}=n_p^2\,\frac{\rho_0}{\rho}\quad ,$$

and

$$\begin{aligned}-h-q=&-k_0^s\delta^{jk}+k_0^s\left(\delta^{jk}-\delta^{j0}\delta^{k0}\right)\left(1-n_s^2\frac{\rho_0}{\rho}\right)\\&+k_0^s\delta^{j0}\delta^{k0}\left(n_0^{sp}\right)^2\left(1-n_p^2\frac{\rho_0}{\rho}\right)\\&+k_0^s\delta^{j0}\delta^{k0}\left(1-\left(n_0^{sp}\right)^2\right)\end{aligned}\quad .\qquad\text{(S.43)}$$

(Note that $n_{sp}^2=\left(c_0^s/c_0^p\right)^2=\mu_0/\left(\lambda+2\tilde{\mu}_0\right)$ is less than 1 for the usual choice $\mu_0=\tilde{\mu}_0$.)

Equation (S.43) is the lemma. $\mathbb{QED}$

Now, we are ready to evaluate λ,γ,κ and β.

From equations (S.23), (S.25), (S.27), (S.39), (S.43) (the lemma) and recalling the usual choice $a=1/\left(\omega\rho_0c_0^s\right)$, we have

$$\begin{aligned}\lambda^{jk}=&\frac{1}{2}\left(b+\underbrace{d+f}_{\substack{\text{Combine into}\\ \rho\omega^2a\delta^{jk}=\\ \rho/\rho_0 k_0^s\delta^{jk}}}\underbrace{-h-q}_{\text{use the lemma}}\right)\\=&\frac{1}{2\omega\rho_0c_0^s}\left[\vec{\nabla}_T^j\frac{2\lambda\mu}{\lambda+2\mu}\vec{\nabla}_T^k\left(\vec{\theta}_T+\vec{\chi}_T\right)^k+\nabla_T^i\mu\nabla_T^i\underbrace{\delta_T^{jk}}_{\delta^{jk}-\delta^{j0}\delta^{k0}}+\nabla_T^k\mu\nabla_T^j\right]\\&\underbrace{+\frac{\rho}{\rho_0}\frac{k_0^s}{2}\delta^{jk}-k_0^s\delta^{jk}}_{-\left(1-\rho/\rho_0\right)\frac{k_0^s}{2}\delta^{jk}}+\frac{k_0^s}{2}\underbrace{\left(\delta^{jk}-\delta^{j0}\delta^{k0}\right)}_{\delta_T^{jk}}\left(1-n_s^2\frac{\rho_0}{\rho}\right)\\&+\frac{k_0^s}{2}\delta^{j0}\delta^{k0}\left(n_0^{sp}\right)^2\left(1-n_p^2\frac{\rho_0}{\rho}\right)+\frac{k_0^s}{2}\delta^{j0}\delta^{k0}\left(1-\left(n_0^{sp}\right)^2\right)\end{aligned}\qquad\text{(S.44)}$$

We also have

$$\gamma_{jk} = \frac{1}{2}\left(\underbrace{k_0}_{\substack{\text{Still}\\ \text{unassigned}}} \quad \delta^{jk} \quad \underbrace{-h-q}_{\text{use the lemma}} \right)$$

$$= \frac{1}{2}\left(\underbrace{k_0\delta^{jk} - k_0^s\delta^{jk}}_{\substack{\text{These terms do not automatically get small. Use our freedom to choose}\\ k_0 = k_0^s \text{ to get the needed cancellation.}}} + k_0^s\left(\delta^{jk} - \delta^{j0}\delta^{k0}\right)\left(1 - n_s^2\frac{\rho_0}{\rho}\right) \right)$$

$$+ \frac{1}{2}\left(k_0^s\delta^{j0}\delta^{k0}\left(n_0^{sp}\right)^2\left(1 - n_p^2\frac{\rho_0}{\rho}\right) + k_0^s\delta^{j0}\delta^{k0}\left(1 - \left(n_0^{sp}\right)^2\right) \right) \quad ,$$

and so

$$\gamma_{jk} = \frac{1}{2}\left(\begin{array}{l} k_0^s\left(\delta^{jk} - \delta^{j0}\delta^{k0}\right)\left(1 - n_s^2\frac{\rho_0}{\rho}\right) + k_0^s\delta^{j0}\delta^{k0}\left(n_0^{sp}\right)^2\left(1 - n_p^2\frac{\rho_0}{\rho}\right) \\ + k_0^s\delta^{j0}\delta^{k0}\left(1 - \left(n_0^{sp}\right)^2\right) \end{array} \right). \qquad \text{(S.45)}$$

In equations (S.43) and (S.45), recall that (using definitions (S.34) (and its generalizations) and (S.42)):

$$n_s^2\frac{\rho_0}{\rho} = \frac{\mu_0}{\mu} \quad ; \quad n_p^2\frac{\rho_0}{\rho} = \frac{\lambda_0 + 2\tilde{\mu}_0}{\lambda + 2\mu} \quad ; \quad \left(n_0^{sp}\right)^2 = \frac{\mu_0}{\lambda_0 + 2\tilde{\mu}_0} .$$

We also need (using (S.23), (S.25) and (S.27))

$$\kappa = \frac{1}{2}(C - B)$$

$$= \frac{1}{2}\big((g+p) - (c+e)\big) = \frac{1}{2}\big((g-e) + (p-c)\big)$$

$$\kappa^{jk} = \frac{1}{2}\left[-i\nabla_T^j\delta^{k0} + i\nabla_T^k\delta^{j0}\right] + \frac{1}{2}\left[-i\left(\frac{\lambda}{\lambda+2\mu}\right)\nabla_T^k\delta^{j0} + i\nabla_T^j\left(\frac{\lambda}{(\lambda+2\mu)}\right)\delta^{k0}\right], \qquad \text{(S.46)}$$

and (using (S.23) and the definition of β noted in equation (S.39))

$$\beta = -\frac{1}{2}B = -\frac{1}{2}(c+e)$$

$$\beta^{jk} = \frac{1}{2}\left(i\nabla_T^j\left(\frac{\lambda}{(\lambda+2\mu)}\right)\delta^{k0} + i\delta^{j0}\nabla_T^k \right) \quad . \qquad \text{(S.47)}$$

Recall that equations (S.44)-(S.47) are to be substituted into the state space equation

$$\begin{aligned}
\underset{\sim}{\mathcal{Q}}^{jk} &= \lambda^{jk}\underset{\sim}{\xi} + \kappa^{jk}\tau \\
\underset{\sim}{\mathcal{E}}^{jk} &= \left(\lambda^{jk} - 2\gamma^{jk}\right)\eta + \left(\kappa^{jk} - 2\beta^{jk}\right)\mathbf{1} \\
\mathcal{H}^{jk} &= \underset{\sim}{\mathcal{Q}}^{jk} + \underset{\sim}{\mathcal{E}}^{jk} + k_0^s\delta^{jk}\eta \quad ,
\end{aligned} \tag{S.48}$$

where

$$k_0^s = \frac{\omega}{c_0^s} = \omega\sqrt{\frac{\rho_0}{\mu_0}} \quad ; \quad \eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad ; \quad \underset{\sim}{\xi} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad ; \quad \tau = \eta\underset{\sim}{\xi} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

These results are also presented in equations (7.11)-(7.13) of Section 7.2.

S.1.2 A few comments

Subsection S.1.2.1 discusses a change a variable from the Lamé parameters μ and λ to their reciprocals. This is to facilitate δ-function bifurcation in cases where an interface is present. Subsection S.1.2.2 discusses the expansion parameter associated with equations (S.37) and (S.44). This expansion parameter is intrinsic to the parabolic equation for an elastic solid, since there is no choice of reference parameters that will make it disappear.

S.1.2.1 The correct variables to use if δ-function bifurcation is needed

When an interface is present, we will need to rework this result as follows. In order to be able to use δ-function bifurcation without imposing Taylor series expansions of the sort discussed in Appendix K.2.3, we will need to convert the terms sandwiched between ∇_T in the lead-order derivative (which comes from powers of the leading-order terms in λ) to a form where multiplication by a "clean step" frees up the lead-order derivative for further integration. To do so, define $K_2 = 1/\mu$ and $K_1 = 1/\lambda$. Thus,

$$\frac{\lambda\mu}{\lambda + 2\mu} = \frac{1}{K_1 K_2\left(\dfrac{1}{K_1} + \dfrac{2}{K_2}\right)} = \frac{1}{K_2 + 2K_1}.$$

It is not really necessary, but we could also define $\tilde{K} \equiv K_2 + 2K_1 = (\lambda + 2\mu)/(\lambda\mu)$. Either way, the leading-order derivatives that appear in λ are now

$$\nabla_T \frac{1}{\tilde{K}} \nabla_T = \nabla_T \frac{1}{K_2 + 2K_1} \nabla_T \quad ; \quad \nabla_T \frac{1}{K_2} \nabla_T \, .$$

This is a form where δ-function bifurcation can be applied without further ado. Also note that in λ, κ, γ and β we get terms such as

$$\frac{\lambda}{\lambda+2\mu}=\frac{K_2}{\tilde{K}} \quad ; \quad n_s^2\frac{\rho_0}{\rho}\propto K_2 \quad ; \quad n_p^2\frac{\rho_0}{\rho}\propto\frac{K_1K_2}{\tilde{K}}.$$

These terms never appear in the lead-order derivative, so they are of no concern as far as the issue of δ-function bifurcation is concerned.

S.1.2.2 A new kind of expansion parameter

Now, let us return to examine the "built-in" expansion parameter contained in (S.44) (it made its first appearance in equation (S.37)):

$$\frac{1}{2}\left(1-\left(\frac{c_0^s}{c_0^p}\right)^2\right).$$

This term turns out to be very closely related to the term $\mu=\left(1-n^2\right)/2=\left(1-{}^{c_0^2}/_{c^2}\right)/2$ in a constant density (i.e., $\delta\rho=0$) fluid (as well as to similar terms that are proportional to $\delta\rho/\rho_0$, $\delta\varepsilon/\varepsilon_0$ and $\delta\mu/\mu_0$). Both the μ (or $k_0\mu$) term and the $\left(1-\left(c_0^s/c_0^p\right)^2\right)/2$ (or $k_0\left(1-\left(c_0^s/c_0^p\right)^2\right)/2$) term are caused by a discrepancy between the "fundamental wave number" of the parabolic equation (i.e., k_0) and the wavelength of a given physical wave. What varies in these various cases is the *source* of the discrepancy, but not the discrepancy itself.

This deserves a closer look. Recall that we long ago established that the parabolic equation selects out a preferred axis in space: the downrange axis. To incorporate waves that have components in the (non-preferred) transverse direction, the expansion has to "work hard" and produce a power series in the expansion parameter ∇_T^2/k_0^2 (or more generally $i\vec{\nabla}_T/k_0$). It is just a little more obscure, but the parabolic equation also selects out a preferred wave number k_0. Components of the overall field with characteristic wave numbers that differ from the preferred value k_0 are once again properly brought back into the problem via an expansion.

In the constant-density acoustic problem, we have a true physical wave number $k=nk_0=\left({}^{c_0}/_{c}\right)k_0$, and in this case, the corresponding expansion parameter is indeed 2μ [xxxx] (as mentioned above). On the other hand, in an elastic solid we have a field with two characteristic wave numbers: k_p and k_s. No matter which we choose as our reference wave number (or equivalently sound speed), we will have a non-favored wave

[xxxx] The factor of 2 results because the parabolic equation looks like an expansion of $\sqrt{1+{}^{2\lambda}/_{k_0}}$.

number, and its related expansion parameter $\left(1-{}^{c_0^2}\!/_{c^2}\right)$ will appear in the parabolic equation. For example, had we chosen $a=1/\left(\omega\rho_0 c_0^p\right)$, then k_0^p would become the reference wave number, and now we would pick up the expansion parameter $1-\left(c_0^p/c_0^s\right)^2$ [yyyy].

Thus, we see that we have encountered a new attribute that must appear in any parabolic equation (PE) that models a field that has multiple characteristic wavelengths. Such parabolic equations will pick up intrinsic expansion parameters that are connected to the need for the PE to adjust for the difference between its reference wave number and one or more of the actual physical wave numbers.

Finally, let us consider a numerical example. For granite and limestone, $c_s \approx c_p/1.9$ typically, and the expansion parameter $1-\left(c_0^s/c_0^p\right)^2 = 1-(1/1.9)^2 = 0.723$. Thus, we have an intrinsic expansion parameter that is fairly close to 1. Its presence explains why the parabolic equation for elastic solids will generally require fairly high orders.

S.2 The transformation tying the parabolic equation field $\vec{\chi}$ to the displacement $\vec{u}$

This appendix derives a transformation first order in $\vec{\nabla}_T$ that connects the familiar full-wave displacement vector $\vec{u}$ with the downrange propagating field $\vec{\chi}$ associated with the parabolic equation. The transformation as recorded in Section 7.2 by equation (7.15) (with definitions (7.16) and (7.17)) is derived below.

There will be an intermediate result. Consider the Hamiltonian for the propagation of the displacement vector $\vec{u}$ when all environmental parameters (λ, μ, ρ) are constant. We discover that even in this elementary example, a fundamental distinction exists between the parabolic equation for $\vec{u}$ and that for the auxiliary field $\vec{\chi}$ (which unlike $\vec{u}$ will continue to propagate according to a parabolic equation even when range dependence is

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[yyyy] Note that since $c^p > c^s$ at a given location, we run a very real risk that this expansion parameter could become greater than 1. Generally, the expansion parameter will be bounded by 1 if we choose the smallest s-wave speed as the reference wave speed (and so $a=1/\left(\omega\rho_0 c_0^s\right)$). Also note that at a fluid-elastic interface, the smallest s-wave speed will go to zero, and our expansion parameters go to 1. This is much like the Dirichlet or Neumann limit in acoustics, and it indicates that it will be quite tricky to adapt the parabolic equation derived here to the fluid-solid interface.

added). The Hamiltonian corresponding to $\vec{u}$ is the desired intermediate result, and it will be derived in Section S.2.1.

This intermediate result will then lead to our final result, an expression for $\sqrt{i\vec{\vec{A}}}$, where $\vec{\chi} \propto \sqrt{i\vec{\vec{A}}} \cdot \vec{u}$. The transformation is given by equation (S.65) (with definitions (S.64) and (S.61)). It is derived in Section S.2.2.

S.2.1 The Hamiltonian for the displacement vector $\vec{u}$

Below in Subsection S.2.1, it is shown that, neglecting range dependence as usual and now also even the local transverse (e.g., vertical) dependence of the environmental parameters λ, μ (Lamé parameters) and ρ (density), we can take the square root of the wave equation for the displacement vector $\vec{u}$, and get a parabolic equation for $\vec{u}$ (see equations (S.50), (S.53) and (S.55)). This derivation is carried out in Subsections S.2.1.3, S.2.1.5, and S.2.1.6. Subsection S.2.1.3 performs the formal square root operation, Subsection S.2.1.5 evaluates a dyadic that appears in the result. The full Hamiltonian contains $\partial/\partial x$ operators multiplied by the expansion parameter $\vec{\nabla}_T$ and so the $\partial/\partial x$ operators can be eliminated by iteration. Subsection S.2.1.6 performs the first iteration.

The derivation of the Hamiltonian for the displacement $\vec{u}$ is supplemented three subsections. Subsection S.2.1.1 previews an important finding that emerges as a byproduct of the derivation: The displacement vector $\vec{u}$ and the carrier of downrange flux $\vec{\chi}$ obey different conservation rules and so their Hamiltonians differ in an important aspect–the Hermiticity property. Subsection S.2.1.4 analyzes this finding the context in which it arises. Subsection S.2.1.2 introduces the aspects of the elastic wave formalism that will be used in the derivation of the Hamiltonian for $\vec{u}$.

S.2.1.1 An important difference between the displacement $\vec{u}$ and the carrier of flux $\vec{\chi}$

During the derivation of the Hamiltonian for $\vec{u}$, it will be noted (in Subsection S.2.1.4) that we cannot use this Hamiltonian as the Hamiltonian for the Foldy-Wouthuysen field $\vec{\chi}$. The immediate reason is that the transformation operator from $\vec{u}$ to $\vec{\chi}$, $\sqrt{i\vec{\vec{A}}}$ (i.e., where $\vec{\chi} \propto \sqrt{i\vec{\vec{A}}} \cdot \vec{u}$) does not commute with $\vec{\vec{H}}_{\vec{\chi}}$ (the standard parabolic equation for $\vec{\chi}$), even given all our stringent simplifying assumptions about the local environment (i.e., $\left[\vec{\vec{H}}_{\vec{\chi}}, \sqrt{i\vec{\vec{A}}}\right] \neq 0$ even at locations where none of the environmental parameters are varying). A profound property associated with the fact that the transformation operator $\sqrt{i\vec{\vec{A}}}$ does not commute with the Hamiltonian (even in the most trivial of cases) is that the magnitude of the carrier of downrange flux $\vec{\chi}^* \cdot \vec{\chi}$ must be conserved, while the

magnitude of the displacement vector $\vec{u}^* \cdot \vec{u}$ is not (ultimately because of beats between the pressure and the shear waves), and so the Hamiltonian for the former $\vec{\vec{H}}_{\vec{\chi}}$ must be Hermitian, while the Hamiltonian for the latter $\vec{\vec{H}}_{\vec{u}}$ need not be! Thus, the transformation from one vector to the other cannot commute with either of the Hamiltonians involved! (Or more precisely, $\sqrt{i\vec{\vec{A}}}$ cannot commute with $\vec{\vec{H}}_{\vec{u}}$, and $\sqrt{i\vec{\vec{A}}}^{-1}$ cannot commute with $\vec{H}_{\vec{\chi}}$.)

Recall that making simplifying assumptions about the variability of the environmental parameters to produce a parabolic equation that is valid for the physical wave function, but not for the carrier of flux, has a precedent in the acoustic case. At the beginning of the discussion of the stair step technique in Section 6.2.2, we found that for the range-*in*dependent variable density ($\delta\rho \neq 0$) scenario,

$$\left[\frac{\partial^2}{\partial x^2} + \rho\nabla_T \tfrac{1}{\rho}\nabla_T + k^2\right] A = 0 \Rightarrow$$

$$-i\frac{\partial A}{\partial x} = \sqrt{k_0^2 + \rho\nabla_T \tfrac{1}{\rho}\nabla_T - k_0^2\left(1-n^2\right)} \cdot A \quad .$$

(As always in this study, the square root operator is understood as an expansion, this time in $\rho\nabla_T \frac{1}{k_0^2\rho}\nabla_T - \left(1-n^2\right)$.) This equation does not generalize to the range-dependent case. To incorporate range dependence, we must consider the carrier of flux χ, which propagates according to the somewhat different parabolic equation generated by the Foldy-Wouthuysen transformation. The differences between the propagation equations reflect differences in the two fields' conservation properties. $|A|^2$ is conserved relative to the metric $d^2\underline{R}_T/\rho$, while $|\chi|^2$ is conserved relative to the metric $d^2\underline{R}_T$ (see Section 6.2.2). All this forms a prototype for the properties of the elastic field as outlined immediately above in the first paragraph of this section.

S.2.1.2 The elastic wave equation

Let us therefore proceed to fully develop the corresponding scenario for the elastic wave. As noted above, the first step is to obtain the parabolic equation for the displacement vector $\vec{u}$. We begin with equation (S.3): $\vec{\nabla}\cdot\vec{\tau} = -\rho\omega^2\vec{u}$, substitute the definition of $\vec{\tau}$ (equation (S.2)), and locally neglect all spatial dependence of λ and μ to get

$$\lambda\vec{\nabla}\left(\vec{\nabla}\cdot\vec{u}\right) + \mu\nabla^2\vec{u} + \mu\vec{\nabla}\left(\vec{\nabla}\cdot\vec{u}\right) = -\rho\omega^2\vec{u}$$

$$\left(\lambda+\mu\right)\vec{\nabla}\left(\vec{\nabla}\cdot\vec{u}\right) + \mu\nabla^2\vec{u} + \rho\omega^2\vec{u} = 0 \quad ,$$

and expanding the gradients

$$\left[(\lambda+\mu)\left(\hat{x}\frac{\partial}{\partial x}+\vec{\nabla}_T\right)\left(\hat{x}\frac{\partial}{\partial x}+\vec{\nabla}_T\right)+\mathbf{1}\mu\left(\frac{\partial^2}{\partial x^2}+\nabla_T^2\right)+\rho\omega^2\mathbf{1}\right]\cdot\vec{u}=0$$

$$\left[\begin{array}{c}(\lambda+\mu)\hat{x}\hat{x}\frac{\partial^2}{\partial x^2}+(\lambda+\mu)\vec{\nabla}_T\hat{x}\frac{\partial}{\partial x}+(\lambda+\mu)\hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T+(\lambda+\mu)\vec{\nabla}_T\vec{\nabla}_T\\ +\mathbf{1}\mu\frac{\partial^2}{\partial x^2}+\mathbf{1}\mu\nabla_T^2+\mathbf{1}\rho\omega^2\end{array}\right]\cdot\vec{u}=0 \quad .$$

$$\left[\begin{array}{c}\left[(\lambda+\mu)\hat{x}\hat{x}+\mathbf{1}\mu\right]\frac{\partial^2}{\partial x^2}+(\lambda+\mu)\left(\vec{\nabla}_T\frac{\partial}{\partial x}\hat{x}+\hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right)+(\lambda+\mu)\vec{\nabla}_T\vec{\nabla}_T\\ +\mathbf{1}\mu\nabla_T^2+\mathbf{1}\rho\omega^2\end{array}\right]\cdot\vec{u}=0$$

Now,

$$\left[(\lambda+\mu)\hat{x}\hat{x}+\mathbf{1}\mu\right]=\begin{pmatrix}\lambda+2\mu & 0 & 0\\ 0 & \mu & 0\\ 0 & 0 & \mu\end{pmatrix}\equiv\vec{E}$$

is a 3×3 diagonal matrix that is invertible provided $\mu\neq0$. Also note that $\lambda+2\mu>0$ (use $\lambda>-\frac{2}{3}\mu$ from reference [156]) and $\mu>0$[zzzz]. Note that for this diagonal matrix, we can take powers and reciprocals simply by taking powers and reciprocals of the components along the diagonal.

Thus we have the wave equation for the displacement vector $\vec{u}$:

$$\left[\vec{E}\frac{\partial^2}{\partial x^2}+(\lambda+\mu)\left(\vec{\nabla}_T\frac{\partial}{\partial x}\hat{x}+\hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right)+(\lambda+\mu)\vec{\nabla}_T\vec{\nabla}_T+\mathbf{1}\mu\nabla_T^2+\mathbf{1}\rho\omega^2\right]\cdot\vec{u}=0 \quad .(S.49)$$

[zzzz] It is interesting to consider the limit $\mu=0$. We have

$\left[\lambda\hat{x}\hat{x}\,\partial^2/\partial x^2+\lambda\left(\vec{\nabla}_T\,\partial/\partial x\,\hat{x}+\hat{x}\,\partial/\partial x\,\vec{\nabla}_T\right)+\lambda\vec{\nabla}_T\vec{\nabla}_T+\mathbf{1}\rho\omega^2\right]\cdot\vec{u}=0$ and taking components:

$\hat{x}\left[\lambda\frac{\partial^2}{\partial x^2}u_x+\lambda\frac{\partial}{\partial x}\left(\vec{\nabla}_T\cdot\vec{u}_T\right)+\rho\omega^2u_x\right]=0$; $\lambda\vec{\nabla}_T\frac{\partial}{\partial x}u_x+\lambda\vec{\nabla}_T\left(\vec{\nabla}_T\cdot\vec{u}_T\right)+\rho\omega^2\vec{u}_T=0$ or

$\hat{x}\left[\frac{\partial}{\partial x}\left(\vec{\nabla}\cdot\vec{u}\right)+\frac{\rho\omega^2}{\lambda}u_x\right]=0$ and $\left[\vec{\nabla}_T\left(\vec{\nabla}\cdot\vec{u}\right)+\frac{\rho\omega^2}{\lambda}\vec{u}_T\right]=0$, and so (using $k^2=\frac{\rho\omega^2}{\lambda}$) we have

$\left[\vec{\nabla}\left(\vec{\nabla}\cdot\vec{u}\right)+k^2\vec{u}\right]=0$. Now, noting $\vec{u}=\vec{\nabla}A/\left(\rho\omega^2\right)$ and multiplying through by the constant $\rho\omega^2$, we have $\vec{\nabla}\left(\vec{\nabla}\cdot\left(\vec{\nabla}A/\rho\right)+\left(k^2/\rho\right)A\right)=0$, which is just the gradient of the (time-independent) acoustic wave equation.

S.2.1.3 Formally taking the "square root" of the elastic wave equation

Next, we will "get rid" of $\ddot{E}$, the operator sitting to the left of $\partial^2/\partial x^2$, by multiplying this equation from the left by $\ddot{E}^{-1}$.

However, before doing so, let us address an important issue. In a superficially similar situation that will come up shortly, we will take pains to do this type of thing in as symmetric a way as possible. In the present case, the analogous action would be to multiply (S.49) by $\ddot{E}^{-½}$ from the right and then also from the left. Let us try to do this, and see what happens. Multiply the equation above by $\ddot{E}^{-½}$ from the right. For the diagonal parts of (S.49), it is trivial to see that multiplying from the right is automatically the same as multiplying from the left. In this case, it turns out that a similar thing happens when we multiply the non-diagonal part of (S.49) by $\ddot{E}^{-½}$ from the right:

$$\begin{aligned}\left[\left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right)\cdot\vec{u}\right]\cdot\ddot{E}^{-½} &= \left(\vec{\nabla}_T^j \frac{\partial}{\partial x}\hat{x}^i u^i + \hat{x}^j \frac{\partial}{\partial x}\nabla_T^i u^i\right)\left[\ddot{E}^{-½}\right]^{jk} \\ &= \left[\ddot{E}^{-½}\right]^{jk}\left(\nabla_T^j \frac{\partial}{\partial x}\hat{x}^i u^i + \hat{x}^j \frac{\partial}{\partial x}\nabla_T^i u^i\right) \\ &= \left[\ddot{E}^{-½}\right]^{kj}\left(\nabla_T^j \frac{\partial}{\partial x}\hat{x}^i + \hat{x}^j \frac{\partial}{\partial x}\nabla_T^i\right)u^i \\ &= \ddot{E}^{-½}\cdot\left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right)\cdot\vec{u}\end{aligned}$$

Thus, the formalism simply kicks $\ddot{E}^{-½}$ over to the left. Basically, this is because $\ddot{E}^{-½}$ is diagonal and because the only free index against which to perform matrix multiplication is on the left. Thus, we are in this case forced to eliminate the coefficient of $\partial^2/\partial x^2$ in (S.49) $\ddot{E}$ by multiplying the equation by $\ddot{E}^{-1}$ from the left.

Multiplying (S.49) from the left by $\ddot{E}^{-1}$, we have

$$\left[\frac{\partial^2}{\partial x^2} + (\lambda+\mu)\ddot{E}^{-1}\cdot\left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right) + (\lambda+\mu)\ddot{E}^{-1}\cdot\vec{\nabla}_T\vec{\nabla}_T + \mu\nabla_T^2\ddot{E}^{-1} + \rho\omega^2\ddot{E}^{-1}\right]\cdot\vec{u} = 0,$$

or formally taking the square root of this equation (with the sign chosen to reflect downrange propagation)

$$-i\frac{\partial\vec{u}}{\partial x} = \underbrace{\sqrt{\begin{array}{c}\rho\omega^2\ddot{E}^{-1} + (\lambda+\mu)\ddot{E}^{-1}\cdot\left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T\right) \\ +(\lambda+\mu)\ddot{E}^{-1}\cdot\vec{\nabla}_T\vec{\nabla}_T + \mu\nabla_T^2\ddot{E}^{-1}\end{array}}}_{\ddot{H}_{\vec{u}}}\cdot\vec{u} = \ddot{H}_{\vec{u}}\cdot\vec{u}\,. \qquad \text{(S.50)}$$

Formally speaking, this is the parabolic equation for $\vec{u}$ with the Hamiltonian $\ddot{H}_{\vec{u}}$.

S.2.1.4 The Hamiltonian for $\vec{u}$ is neither Hermitian nor is it the same as the Hamiltonian for $\vec{\chi}$

Before proceeding, we need to stop and consider a point alluded to earlier. By multiplying the non-diagonal operator $\left(\vec{\nabla}_T \partial/\partial x \hat{x} + \hat{x} \partial/\partial x \vec{\nabla}_T\right)$ from the left by $\vec{E}^{-1}$, we have created a non-symmetric and more importantly non-Hermitian operator. In other words, the Hamiltonian for the propagation of $\vec{u}$ is non-Hermitian—even where λ, μ, ρ are all constants. This implies that the quantity $\int \left(\vec{u}^* \cdot \vec{u}\right) d^2 \underline{R}_T$ is not conserved during downrange propagation. To get an intuitive feel for this result, break a basic plane wave $\vec{u}$ into components that are pressure and shear waves: $\vec{u} = \vec{u}_p + \vec{u}_s = \vec{u}_{p_0} e^{i\vec{k}_p \cdot \vec{x}} + \vec{u}_{s_0} e^{i\vec{k}_s \cdot \vec{x}}$ (where the time dependence $e^{-i\omega t}$ has been taken out). Now,

$$\vec{u}^* \cdot \vec{u} = \left|\vec{u}_p\right|^2 + \left|\vec{u}_s\right|^2 + 2\,\mathrm{Re}\left(\vec{u}^*_{p_0} \cdot \vec{u}_{s_0} e^{i\left(\vec{k}_p - \vec{k}_s\right)\cdot \vec{x}}\right)$$

or taking $\int d^2 \underline{R}_T$, we get something proportional to

$$\mathrm{Re}\left[\delta\left(\vec{k}_{pT} - \vec{k}_{sT}\right) e^{i\left(k_{px} - k_{sx}\right)x}\right] + \ldots = \delta\left(\vec{k}_{pT} - \vec{k}_{sT}\right) \cos\left(\left(k_{px} - k_{sx}\right)x\right) + \ldots$$

where the ellipses stand for terms that do not vary with the range (they are infinite, but that does not matter; also note that $k_{px} - k_{sx} \neq 0$ even though the transverse components are equal because the sound speeds are different). Thus, we pick up beats between the pressure and shear waves, and $\vec{u}^* \cdot \vec{u}$ is not a conserved quantity—even for a plane wave where λ, μ, ρ are all constants! That is the reason why the Hamiltonian $\ddot{H}_{\vec{u}}$ cannot be Hermitian.

This allows us to anticipate a very interesting result. At least for constant λ, μ, ρ, there exists a parabolic equation to propagate $\vec{u}$, but it cannot be the same parabolic equation as that for $\vec{\chi}$, because for one-way propagation, $\vec{\chi}^* \cdot \vec{\chi}$ is conserved, and so its corresponding Hamiltonian $\ddot{H}_{\vec{\chi}}$ must be Hermitian. As noted above, the fact that $\vec{\chi}$ does not obey the parabolic equation for $\vec{u}$ also implies that as we consider the transformation $\vec{\chi} \propto \sqrt{i\ddot{A}} \cdot \vec{u}$, we will have $\left[\ddot{H}_{\vec{u}}, \sqrt{i\ddot{A}}\right] \neq 0$. Finally, note that $\ddot{H}_{\vec{\chi}}, \sqrt{i\ddot{A}}$ will be Hermitian, although $\ddot{H}_{\vec{u}}$ is not.

S.2.1.5 Evaluating the dyadic $\ddot{E}$ in the Hamiltonian for $\vec{u}$

Now, let us proceed to evaluate the Hamiltonian $\vec{\vec{H}}_{\vec{u}}$ given in equation (S.50). We have

$$-i\frac{\partial \vec{u}}{\partial x} = \sqrt{\rho\omega^2 \vec{\vec{E}}^{-1}} \cdot \sqrt{1 + \underbrace{\frac{\lambda+\mu}{\rho\omega^2}}_{\substack{\frac{\lambda+2\mu-\mu}{\rho\omega^2} = \\ 1/k_p^2 - 1/k_s^2}} \left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T \right) + \underbrace{\frac{\lambda+\mu}{\rho\omega^2}}_{1/k_p^2 - 1/k_s^2} \vec{\nabla}_T\vec{\nabla}_T + \underbrace{\frac{\mu}{\rho\omega^2}}_{1/k_s^2} \nabla_T^2} \cdot \vec{u} \quad , \text{(S.51)}$$

where the square root is understood as a Taylor series expansion.

Now,

$$\rho\omega^2 \vec{\vec{E}}^{-1} = \begin{pmatrix} \dfrac{\rho\omega^2}{\lambda+2\mu} & 0 & 0 \\ 0 & \dfrac{\rho\omega^2}{\mu} & 0 \\ 0 & 0 & \dfrac{\rho\omega^2}{\mu} \end{pmatrix} = \begin{pmatrix} k_p^2 & 0 & 0 \\ 0 & k_s^2 & 0 \\ 0 & 0 & k_s^2 \end{pmatrix},$$

and noting that we can take powers of a diagonal matrix by taking powers of its non-zero components, we have

$$\sqrt{\rho\omega^2 \vec{\vec{E}}^{-1}} = \begin{pmatrix} k_p & 0 & 0 \\ 0 & k_s & 0 \\ 0 & 0 & k_s \end{pmatrix} = \vec{\vec{k}} = k_p \hat{x}\hat{x} + k_s\left(\hat{y}\hat{y} + \hat{z}\hat{z}\right). \qquad \text{(S.52)}$$

Substituting (S.52) into (S.51), we have

$$-i\frac{\partial \vec{u}}{\partial x} = \vec{\vec{k}} \cdot \sqrt{1 + \left(\frac{1}{k_p^2} - \frac{1}{k_s^2}\right)\left(\vec{\nabla}_T \frac{\partial}{\partial x}\hat{x} + \hat{x}\frac{\partial}{\partial x}\vec{\nabla}_T \right) + \left(\frac{1}{k_p^2} - \frac{1}{k_s^2}\right)\vec{\nabla}_T\vec{\nabla}_T + \frac{\nabla_T^2}{k_s^2}} \cdot \vec{u} \quad . \text{(S.53)}$$

This parabolic equation contains an explicit $\partial/\partial x$ in the square root operator (i.e., the Hamiltonian $\vec{\vec{H}}_{\vec{u}}$)—even when we remove all spatial dependence on the environmental parameters λ, μ and ρ. This differs from what we found in the acoustic and electromagnetic cases ($\partial/\partial x$ may appear in the transformation between the physical and Foldy-Wouthuysen fields, but until now not in the Hamiltonian). Fortunately, $\partial/\partial x$ is multiplied by the "small" expansion parameter $\vec{\nabla}_T$, and so we can iterate this equation and still generate a series that forms a parabolic equation for $\vec{u}$. This series will be an expansion in a parameter of the basic form $\vec{\nabla}_T/k$, which is a typical expansion parameter

to find in a parabolic equation. The key thing is that the $\partial/\partial x$ is not in the 0th order term, where it would pose insurmountable problems.

S.2.1.6 The 0th-order Hamiltonian for $\vec{u}$

Now, our 0th-order (in $\vec{\nabla}_T$) result is $\vec{\vec{H}}_{\vec{u}} = \vec{\vec{k}} \quad \Rightarrow \quad \mathbf{1}\dfrac{\partial}{\partial x} = \dfrac{\vec{\vec{k}}}{-i}$ and

$$\hat{x}\cdot\mathbf{1}\frac{\partial}{\partial x} = \hat{x}\frac{\partial}{\partial x} = \hat{x}\cdot\frac{\vec{\vec{k}}}{-i} = ik_p\hat{x}\,.$$

Thus, one iteration of (S.53) gives us

$$\begin{aligned}\vec{\vec{H}}_{\vec{u}} &= \vec{\vec{k}}\cdot\sqrt{1+\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)\left(\vec{\nabla}_T ik_p\hat{x}+ik_p\hat{x}\vec{\nabla}_T\right)} + 2^{\text{nd}}\text{ order}\\ &= \vec{\vec{k}}\cdot\left[1+\frac{1}{2}\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)k_p\left(i\vec{\nabla}_T\hat{x}+\hat{x}i\vec{\nabla}_T\right)\right]+\mathrm{O}\left(\nabla_T^2\right)\quad .\end{aligned} \tag{S.54}$$

Now, note that $\vec{\vec{k}}\cdot\left(i\vec{\nabla}_T\hat{x}+\hat{x}i\vec{\nabla}_T\right) = ik_s\vec{\nabla}_T\hat{x}+ik_p\hat{x}\vec{\nabla}_T$, so that

$$\vec{\vec{H}}_{\vec{u}} = \vec{\vec{k}} + i\frac{1}{2}\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)k_p\left(k_s\vec{\nabla}_T\hat{x}+k_p\hat{x}\vec{\nabla}_T\right)+\mathrm{O}\left(\nabla_T^2\right). \tag{S.55}$$

Recall that this is the Hamiltonian for the displacement vector $\vec{u}$ (where the environmental parameters are locally held constant.). Now, we are ready to use this result to examine $\sqrt{i\vec{\vec{A}}}$ where recall $\vec{\chi} \propto \sqrt{i\vec{\vec{A}}}\cdot\vec{u}$.

S.2.2 Using the Hamiltonian for $\vec{u}$ to obtain the endpoint correction for $\vec{\chi}$

Now we use the result of Appendix S.2.1 to obtain the transformation between the displacement vector $\vec{u}$ and the parabolic equation field $\vec{\chi}$. Subsection S.2.2.1 shows that the vector fields are connected by an equation of the form $\vec{\chi} = \sqrt{a}\sqrt{i\vec{\vec{A}}}\cdot\vec{u}$. Subsection S.2.2.2 evaluates the dyadic $i\vec{\vec{A}}$ and Subsection S.2.2.3 deduces its square root. Finally, Subsection S.2.2.4 considers the "minimal connection" between $\vec{u}$ and $\vec{\chi}$.

S.2.2.1 The basic formalism that connects the carrier of flux $\vec{\chi}$ with the displacement $\vec{u}$

Recall equation (S.4): $S_x = \frac{1}{2}\mathrm{Im}\left[\vec{u}^* \cdot \vec{\tau} \cdot \hat{x}\right]$. Next, we want to write this in terms of a "central operator" $\vec{A}\left(\partial/\partial x, \vec{\nabla}_T; \lambda, \mu, \rho\right)$ so that (to within an integration by parts)

$$S_x = \frac{1}{2}\mathrm{Im}\left[\vec{u}^* \cdot \vec{A} \cdot \vec{u}\right]. \tag{S.56}$$

From (S.5) with $\vec{\theta} = 0$ (i.e., one-way downrange propagation), we know that $\vec{\chi}^* \cdot \vec{\chi} = aS_x$ (where a is a free parameter in ansatz (S.1); for reasons discussed in Section S.1.1, it is usually chosen to be $a = 1/\left(\omega\rho_0 c_0^s\right)$). The expression for the downrange flux given in (S.56) then implies that

$$\vec{\chi} = \sqrt{a}\sqrt{i\vec{A}} \cdot \vec{u}\ . \tag{S.57}$$

To see this, begin with $\frac{1}{a}\vec{\chi}^* \cdot \vec{\chi} = \left(\sqrt{i\vec{A}} \cdot \vec{u}\right)^* \cdot \sqrt{i\vec{A}} \cdot \vec{u}$, and note that $\sqrt{i\vec{A}}$ invariably turns out to be Hermitian (at least if we as usual neglect range dependence locally at the endpoints). This means that we can take the product and break it into halves and apply Hermiticity (i.e., integrate by parts, complex conjugate, transpose matrices) in different directions to get[aaaaa]

$$\begin{aligned}\frac{1}{a}\vec{\chi}^* \cdot \vec{\chi} &= \left(\sqrt{i\vec{A}} \cdot \vec{u}\right)^* \cdot \sqrt{i\vec{A}} \cdot \vec{u} = \frac{1}{2}\left[\left(i\vec{A} \cdot \vec{u}\right)^* \cdot \vec{u} + \vec{u}^* \cdot i\vec{A} \cdot \vec{u}\right] \\ &= \frac{i}{2}\left[\vec{u}^* \cdot \vec{A} \cdot \vec{u} - \vec{u} \cdot \left(\vec{A} \cdot \vec{u}\right)^*\right] \\ &= \mathrm{Im}\left[\vec{u}^* \cdot \vec{A} \cdot \vec{u}\right] = 2S_x\end{aligned}\ , \tag{S.58}$$

which indeed agrees with equation (S.56). Note that the operation in equation (S.58) reflects the procedure pursued for the acoustic field in Appendix A. It is also worth noting that in (R.29), roughly speaking the analogous equation for the electromagnetic field, there was no "i" (i.e., in Appendix R.2, $\sqrt{\vec{A}}$ was the relevant Hermitian operator rather than $\sqrt{i\vec{A}}$), because there we needed the real part in order to obtain the time-averaged Poynting vector. (In that case, it also happened to be quite easy to dispense with the need to *explicitly* consider only the real part at this stage.)

[aaaaa] Note that since the Hermiticity property for differential operators is used, this result assumes an implicit integration in the transverse space.

S.2.2.2 Evaluating the dyadic $i\vec{\vec{A}}$

Now, to find $i\vec{\vec{A}}$ and so $\sqrt{i\vec{\vec{A}}}$, we start with $i\vec{\tau}\cdot\hat{x}$, and rewrite it as $i\vec{\vec{A}}\cdot\vec{u}$. We begin with a modified form of equation (S.8):

$$i\vec{\tau}\cdot\hat{x} = (\lambda+2\mu)\hat{x}\underbrace{i\frac{\partial u_x}{\partial x}}_{\hat{x}\cdot\vec{\vec{H}}_{\vec{u}}\cdot\vec{u}} + \lambda i\hat{x}\left(\vec{\nabla}_T\cdot\underbrace{\vec{u}_T}_{\substack{\text{can}\\ \text{replace}\\ \text{with }\vec{u}}}\right) + \mu i\vec{\nabla}_T u_x + \mu\underbrace{i\frac{\partial\vec{u}_T}{\partial x}}_{(1-\hat{x}\hat{x})\cdot\vec{\vec{H}}_{\vec{u}}\cdot\vec{u}}$$
$$= \underbrace{\left[(\lambda+2\mu)\hat{x}\hat{x}\cdot\vec{\vec{H}}_{\vec{u}} + \lambda i\hat{x}\vec{\nabla}_T + \mu i\vec{\nabla}_T\hat{x} + \mu(1-\hat{x}\hat{x})\cdot\vec{\vec{H}}_{\vec{u}}\right]}_{i\vec{\vec{A}}}\cdot\vec{u} \quad ,$$

and so

$$i\vec{\vec{A}} = (\lambda+2\mu)\hat{x}\left(\hat{x}\cdot\vec{\vec{H}}_{\vec{u}}\right) + i\left(\lambda\hat{x}\vec{\nabla}_T + \mu\vec{\nabla}_T\hat{x}\right) + \mu(1-\hat{x}\hat{x})\cdot\vec{\vec{H}}_{\vec{u}} .$$

Now from equation (S.55), we have

$$\vec{\vec{H}}_{\vec{u}} = \vec{\vec{k}} + i\alpha\left(k_s\vec{\nabla}_T\hat{x} + k_p\hat{x}\vec{\nabla}_T\right) + \mathrm{O}\left(\nabla_T^2\right)$$

where

$$\alpha \equiv \frac{1}{2}\left(\frac{1}{k_p^2} - \frac{1}{k_s^2}\right)k_p . \tag{S.59}$$

Thus

$$\hat{x}\hat{x}\cdot\vec{\vec{H}}_{\vec{u}} = k_p\hat{x}\hat{x} + \alpha i k_p\hat{x}\vec{\nabla}_T + \mathrm{O}\left(\nabla_T^2\right)$$
$$(\mathbf{1}-\hat{x}\hat{x})\cdot\vec{\vec{H}}_{\vec{u}} = k_s(\mathbf{1}-\hat{x}\hat{x}) + \alpha i k_s\vec{\nabla}_T\hat{x} + \mathrm{O}\left(\nabla_T^2\right) ,$$

and so

$$i\vec{\vec{A}} = (\lambda+2\mu)k_p\hat{x}\hat{x} + (\lambda+2\mu)\alpha i k_p\hat{x}\vec{\nabla}_T + \lambda i\hat{x}\vec{\nabla}_T$$
$$+\mu k_s(\mathbf{1}-\hat{x}\hat{x}) + \mu\alpha i k_s\vec{\nabla}_T\hat{x} + \mu i\vec{\nabla}_T\hat{x} + \mathrm{O}\left(\nabla_T^2\right)$$
$$= \overbrace{(\lambda+2\mu)k_p\hat{x}\hat{x} + \mu k_s(\mathbf{1}-\hat{x}\hat{x})}^{0^{\text{th}}\text{ order}} + \left[(\lambda+2\mu)\alpha k_p + \lambda\right]i\hat{x}\vec{\nabla}_T$$
$$+\left[\mu\alpha k_s + \mu\right]i\vec{\nabla}_T\hat{x} + \mathrm{O}\left(\nabla_T^2\right) .$$

Now, the 0^{th} order term is

$$(\lambda+2\mu)k_p\hat{x}\hat{x}+\mu k_s(\mathbf{1}-\hat{x}\hat{x})=\begin{pmatrix}(\lambda+2\mu)\underbrace{\sqrt{\frac{\rho\omega^2}{\lambda+2\mu}}}_{k_p} & 0 & 0\\ 0 & \mu k_s & 0\\ 0 & 0 & \mu\underbrace{\sqrt{\frac{\rho\omega^2}{\mu}}}_{k_s}\end{pmatrix},$$

and so

$$\begin{aligned}(\lambda+2\mu)k_p\hat{x}\hat{x}+\mu k_s(\mathbf{1}-\hat{x}\hat{x}) &= \rho\omega^2\begin{pmatrix}\sqrt{\frac{\lambda+2\mu}{\rho\omega^2}} & 0 & 0\\ 0 & \sqrt{\frac{\mu}{\rho\omega^2}} & 0\\ 0 & 0 & \sqrt{\frac{\mu}{\rho\omega^2}}\end{pmatrix} \\ &= \rho\omega^2\begin{pmatrix}1/k_p & 0 & 0\\ 0 & 1/k_s & 0\\ 0 & 0 & 1/k_s\end{pmatrix} = \rho\omega^2\frac{\overleftrightarrow{1}}{k}\quad .\end{aligned} \tag{S.60}$$

Since it will play a prominent role below, let us pause to examine the square root of the matrix $\overleftrightarrow{[1/k]}$. Note that $\overleftrightarrow{[1/k]}$ is a diagonal matrix, and as noted above (just above equation (S.49)), for such a diagonal matrix, we can take powers and reciprocals simply by taking powers and reciprocals of the components along the diagonal:

$$\sqrt{\frac{\overleftrightarrow{1}}{k}}=\begin{pmatrix}1/\sqrt{k_p} & 0 & 0\\ 0 & 1/\sqrt{k_s} & 0\\ 0 & 0 & 1/\sqrt{k_s}\end{pmatrix}. \tag{S.61}$$

Going back to equation (S.60) and continuing our calculation, we have

$$\begin{aligned}i\overleftrightarrow{A} &= \rho\omega^2\frac{\overleftrightarrow{1}}{k}+\underbrace{\left[(\lambda+2\mu)\alpha k_p+\lambda\right]}_{\tilde{a}}i\hat{x}\vec{\nabla}_T+\underbrace{\left[\mu\alpha k_s+\mu\right]}_{\tilde{b}}i\vec{\nabla}_T\hat{x}+\mathrm{O}\left(\nabla_T^2\right) \\ &= \rho\omega^2\frac{\overleftrightarrow{1}}{k}+\tilde{a}i\hat{x}\vec{\nabla}_T+\tilde{b}i\vec{\nabla}_T\hat{x}+\mathrm{O}\left(\nabla_T^2\right)\end{aligned}\quad .$$

S.2.2.3 Obtaining $\sqrt{i\vec{\vec{A}}}$ from $i\vec{\vec{A}}$

Next, we will pull out a factor of $\rho\omega^2\overleftrightarrow{[1/k]}$, take the square root and then expand in powers of $\vec{\nabla}_T$. However, this time (unlike above when we pulled out the $\vec{E}$ in equation (S.49)) it matters how we pull out $\overleftrightarrow{[1/k]}$. We will pull out $\overleftrightarrow{[1/k]}$ in as a symmetric a way as possible. Indeed, later in the calculation we will further symmetrize $\sqrt{i\vec{\vec{A}}}$ in order to make it completely symmetric and consequently Hermitian.

Thus, let us pull out $\overleftrightarrow{[1/k]}$ in as symmetric a way as possible:

$$i\vec{\vec{A}} = \rho\omega^2\sqrt{\overleftrightarrow{\frac{1}{k}}}\cdot\sqrt{\overleftrightarrow{\frac{1}{k}}} + \tilde{a}i\hat{x}\vec{\nabla}_T + \tilde{b}i\vec{\nabla}_T\hat{x} + \mathrm{O}\left(\nabla_T^2\right)$$

$$i\vec{\vec{A}} = \rho\omega^2\sqrt{\overleftrightarrow{\frac{1}{k}}}\cdot\sqrt{\overleftrightarrow{\frac{1}{k}}} + \rho\omega^2\overbrace{\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}}^{\mathbf{1}}\cdot\frac{\tilde{a}i}{\rho\omega^2}\hat{x}\vec{\nabla}_T\cdot\overbrace{\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2}}^{\mathbf{1}}$$
$$+\rho\omega^2\overbrace{\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}}^{\mathbf{1}}\cdot\frac{\tilde{b}i}{\rho\omega^2}\vec{\nabla}_T\hat{x}\cdot\overbrace{\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2}}^{\mathbf{1}} + \mathrm{O}\left(\nabla_T^2\right)$$

$$i\vec{\vec{A}} = \rho\omega^2\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2}\cdot\left[\begin{array}{l}\mathbf{1}+\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\frac{\tilde{a}i}{\rho\omega^2}\hat{x}\vec{\nabla}_T\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\\ +\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\frac{\tilde{b}i}{\rho\omega^2}\vec{\nabla}_T\hat{x}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\end{array}\right]\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/2} + \mathrm{O}\left(\nabla_T^2\right).$$

Now, we can take the square root:

$$\sqrt{i\vec{\vec{A}}} = \sqrt{\rho\omega^2}\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/4}\cdot\left[\begin{array}{l}\mathbf{1}+\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\frac{\tilde{a}i}{\rho\omega^2}\hat{x}\vec{\nabla}_T\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\\ +\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\cdot\frac{\tilde{b}i}{\rho\omega^2}\vec{\nabla}_T\hat{x}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{-1/2}\end{array}\right]^{1/2}\cdot\left(\overleftrightarrow{\frac{1}{k}}\right)^{1/4} + \mathrm{O}\left(\nabla_T^2\right),$$

and expand

$$\sqrt{i\overleftrightarrow{A}} = \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/4} \cdot \left[\begin{array}{l} \mathbf{1} + \frac{1}{2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/2} \cdot \frac{\tilde{a}i}{\rho\omega^2}\hat{x}\vec{\nabla}_T \cdot \left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/2} \\ + \frac{1}{2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/2} \cdot \frac{\tilde{b}i}{\rho\omega^2}\vec{\nabla}_T\hat{x} \cdot \left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/2} \end{array}\right] \cdot \left(\frac{\overleftrightarrow{1}}{k}\right)^{1/4} + \mathrm{O}\left(\nabla_T^2\right).$$

Thus,

$$\sqrt{i\overleftrightarrow{A}} = \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2} + \frac{1}{2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/4} \cdot \frac{\tilde{a}i}{\sqrt{\rho\omega^2}}\hat{x}\vec{\nabla}_T \cdot \left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/4} + \frac{1}{2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/4} \cdot \frac{\tilde{b}i}{\sqrt{\rho\omega^2}}\vec{\nabla}_T\hat{x} \cdot \left(\frac{\overleftrightarrow{1}}{k}\right)^{-1/4} + \mathrm{O}\left(\nabla_T^2\right).$$

Now, recall that $\left[\overleftrightarrow{1/k}\right]^{-1/4}$ is a diagonal matrix, and so it is easy to take the reciprocal. The result is $\left[\overleftrightarrow{1/k}\right]^{-1/4} = \vec{k}^{1/4} = k_p^{1/4}\hat{x}\hat{x} + k_s^{1/4}\left(\hat{y}\hat{y} + \hat{z}\hat{z}\right)$. Thus, we have

$$\sqrt{i\overleftrightarrow{A}} = \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2} + \frac{1}{2}\frac{\tilde{a}i}{\sqrt{\rho\omega^2}}\underbrace{\vec{k}^{1/4}\cdot\hat{x}}_{k_p^{1/4}\hat{x}}\underbrace{\vec{\nabla}_T\cdot\vec{k}^{1/4}}_{\vec{\nabla}_T k_s^{1/4}} + \frac{1}{2}\frac{\tilde{b}i}{\sqrt{\rho\omega^2}}\underbrace{\vec{k}^{1/4}\cdot\vec{\nabla}_T}_{\vec{\nabla}_T k_s^{1/4}}\underbrace{\hat{x}\cdot\vec{k}^{1/4}}_{k_p^{1/4}\hat{x}} + \mathrm{O}\left(\nabla_T^2\right)$$

$$= \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2} + \frac{1}{2}\frac{k_p^{1/4}k_s^{1/4}}{\sqrt{\rho\omega^2}}i\left[\tilde{a}\hat{x}\vec{\nabla}_T + \tilde{b}\vec{\nabla}_T\hat{x}\right] + \mathrm{O}\left(\nabla_T^2\right).$$

Now we symmetrize $\sqrt{i\overleftrightarrow{A}}$ (formally, this would involve splitting operators, integrating by parts and rearranging terms):

$$\hat{x}\vec{\nabla}_T \to \frac{1}{2}\left(\hat{x}\vec{\nabla}_T + \vec{\nabla}_T\hat{x}\right) \quad ; \quad \vec{\nabla}_T\hat{x} \to \frac{1}{2}\left(\hat{x}\vec{\nabla}_T + \vec{\nabla}_T\hat{x}\right),$$

and

$$\sqrt{i\overleftrightarrow{A}} = \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2} + \frac{1}{2}\frac{k_p^{1/4}k_s^{1/4}}{\sqrt{\rho\omega^2}}i\left(\frac{\tilde{a}+\tilde{b}}{2}\right)\left[\hat{x}\vec{\nabla}_T + \vec{\nabla}_T\hat{x}\right] + \mathrm{O}\left(\nabla_T^2\right)$$

$$= \sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2} + \frac{\sqrt{\rho\omega^2}}{2}\frac{\left(k_p k_s\right)^{1/4}}{2}i\left(\frac{\tilde{a}+\tilde{b}}{\rho\omega^2}\right)\left[\hat{x}\vec{\nabla}_T + \vec{\nabla}_T\hat{x}\right] + \mathrm{O}\left(\nabla_T^2\right). \quad \text{(S.62)}$$

Next we evaluate $\left(\tilde{a}+\tilde{b}\right)/\left(\rho\omega^2\right)$:

$$\frac{\tilde{a}+\tilde{b}}{\rho\omega^2}=\underbrace{\overbrace{\frac{\lambda+2\mu}{\rho\omega^2}}^{1/k_p^2}\alpha k_p+\overbrace{\frac{\lambda+2\mu}{\rho\omega^2}}^{1/k_p^2}-\overbrace{\frac{\mu}{\rho\omega^2}}^{1/k_s^2}}_{\tilde{a}/\rho\omega^2}+\underbrace{\overbrace{\frac{\mu}{\rho\omega^2}}^{1/k_s^2}\alpha k_s+\overbrace{\frac{\mu}{\rho\omega^2}}^{1/k_s^2}}_{\tilde{b}/\rho\omega^2}$$

$$=\frac{1}{k_p^2}\alpha k_p+\frac{1}{k_p^2}-\frac{1}{k_s^2}+\frac{\alpha k_s}{k_s^2}=\alpha\left(\frac{1}{k_p}+\frac{1}{k_s}\right)+\frac{1}{k_p^2}-\frac{1}{k_s^2}\quad .$$

Now, recall equation (S.59)

$$\alpha\equiv\frac{1}{2}\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)k_p\quad\text{or}\quad\frac{1}{k_p^2}-\frac{1}{k_s^2}=\frac{2\alpha}{k_p},$$

so

$$\frac{\tilde{a}+\tilde{b}}{\rho\omega^2}=\alpha\left(\frac{1}{k_p}+\frac{1}{k_s}+\frac{2}{k_p}\right)=\alpha\left(\frac{3}{k_p}+\frac{1}{k_s}\right),$$

and substituting the definition of α equation (S.59)

$$\frac{\tilde{a}+\tilde{b}}{\rho\omega^2}=\frac{1}{2}\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)\left(3+\frac{k_p}{k_s}\right).\qquad\text{(S.63)}$$

This quantity is positive: with $k_p^2=\rho\omega^2/(\lambda+2\mu)$, $k_s^2=\rho\omega^2/\mu$ and $\lambda>-2\mu/3$ (see reference [156]), we have $k_p^2<k_s^2$, $1/k_p^2>1/k_s^2$ and so $\left(\tilde{a}+\tilde{b}\right)/\left(\rho\omega^2\right)>0$.

Substituting (S.63) into (S.62), we have

$$\sqrt{i\overleftrightarrow{A}}=\sqrt{\rho\omega^2}\left(\frac{\overleftrightarrow{1}}{k}\right)^{1/2}+\frac{\sqrt{\rho\omega^2}}{8}\left(k_pk_s\right)^{1/4}\left(\frac{1}{k_p^2}-\frac{1}{k_s^2}\right)\left(3+\frac{k_p}{k_s}\right)i\left[\hat{x}\vec{\nabla}_T+\vec{\nabla}_T\hat{x}\right]+\mathrm{O}\left(\nabla_T^2\right).\qquad\text{(S.64)}$$

From (S.57), with the usual choice $a=1/\left(\omega\rho_0c_0^s\right)$, we have

$$\vec{\chi}=\sqrt{\frac{1}{\omega\rho_0c_0^s}}\sqrt{i\overleftrightarrow{A}}\cdot\vec{u}\,.\qquad\text{(S.65)}$$

If we set $\overleftrightarrow{D}\equiv\sqrt{i\overleftrightarrow{A}}$, equation (S.65) with definitions (S.64) and (S.61) match the result given in Section 7.2 (i.e., the transformation given by equation (7.15) with definitions (7.16) and (7.17)).

S.2.2.4 The minimal connection

Equation (S.65) (with (S.64) and (S.61)) should probably already be considered to be the minimal endpoint correction. To be specific, even in the minimal correction, we should probably include 1st order in $\vec{\nabla}_T$. In the endpoint transformations for the acoustic and electromagnetic fields, the lowest order in $\vec{\nabla}_T$ was 2nd order, and then it made sense to consider the 0th order in $\vec{\nabla}_T$ to be the minimal correction.

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