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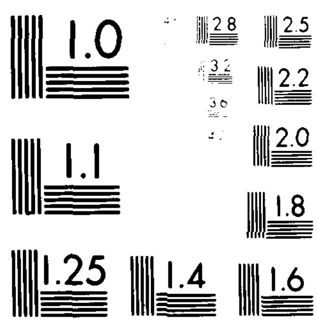

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MRC Technical Summary Report #2263

ON THE SCHROEDINGER CONNECTION

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R. E. Meyer and J. F. Painter

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

August 1981

(Received June 18, 1981)

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National Science Foundation
Washington, DC 20550

UNIVERSITY OF WISCONSIN-MADISON
MATHEMATICS RESEARCH CENTER

ON THE SCHROEDINGER CONNECTION

R. E. Meyer and J. F. Painter*

Technical Summary Report #2263
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ABSTRACT

A new and more direct approach to the connection of wave amplitudes across turning points and singular points of physical Schroedinger equations is summarized. It interprets the connection formulae as an asymptotic expression of the branch structure of the singular point. It also extends turning-point theory to almost the whole class of singular points of physical wave- or oscillator-equations by a new approach to irregular singular points of ordinary differential equations. This reveals an unexpected and striking two-variable structure of the solutions even close to a singular point.

AMS (MOS) Subject Classifications: 34E20, 41A60, 30E15.

Key Words: oscillator modulation, wave modulation, WKB-connection, turning point, irregular singular point.

Work Unit Number 2 - Physical Mathematics

*Lawrence Livermore Laboratory, Livermore, California 94550.

Sponsored by the United States Army under Contract No. DAAG29-80-C-0041. The work was supported partially by the National Science Foundation under Grant No. MCS 8001960 and by the Wisconsin Alumni Research Foundation.

SIGNIFICANCE AND EXPLANATION

This work concerns the modulation of waves or oscillating systems, which pervade all the science and engineering disciplines. Modulation occurs when waves travel through an inhomogeneous material in which the local propagation velocity differs from place to place, as it normally does, both in nature and in technical devices. The resulting change to the waves is mostly gradual, but occasionally drastic, as at a shadow-boundary, where oscillation turns into decay and quiescence over just a few wavelengths. When this phenomenon can be analyzed via an ordinary differential equation, such a boundary is called a turning point.

At first, only the simplest turning points representing the most typical shadow boundaries were studied. But then some phenomena, such as wave reflection and scattering cross-sections, especially for the Schroedinger equation of Quantum Mechanics, came to be traced to hidden turning and singular points that become visible only when real distance (or time) is embedded in its complex plane. When the material properties vary in a general manner, (which can often be observed only incompletely) such hidden transition points can have arbitrarily complex structure. The following work extends the basic mathematical formulae for connecting wave amplitudes across a transition point to a larger class of variations in the material properties than had been accessible up to now, and it achieves it by a simpler and more direct procedure. It is hoped, of course, that this will contribute to technical improvements in wave modulation and scattering calculations and will make problems accessible that had been intractable before.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

ON THE SCHROEDINGER CONNECTION

R. E. Meyer and J. F. Painter*

A more direct approach to the connection of wave-amplitudes across general turning points and singular points of wave- and oscillator equations has been found. It emphasizes and extends the view [1, p. 481] that the connection formulae are an asymptotic expresssion of the branch structure of the singular point. It also extends present turning-point theory via new results on very irregular points of differential equations

(1) $$\varepsilon^2 d^2w/dz^2 + p(z)w(z) = 0$$

with constant ε that are physical Schroedinger equations in the sense that the concept of wavelength (or period) can be defined.

A natural (Liouville-Green) variable x measured in units of local wavelength is then also definable. Limit points of singular points of $p(z)$ will be excluded, as will singular points artificially introduced to represent radiation conditions. Any turning- or singular point of $p(z)$ must then correspond to a definite x, and with both chosen as origin,

(2) $$x = \frac{i}{\varepsilon} \int_0^z [p(t)]^{1/2} dt$$

must exist, at least as a multivalued function, on a neighborhood of zero.

For a clear theory, this hypothesis should be rephrased in terms of the natural variable: an analytic branch $r(x)$ of $p^{1/4}$ is defined on a Riemann surface element D about $x = 0$ which includes $-\pi < \arg x < 2\pi$ (i.e.,

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three Stokes sectors, in turning-point terminology) so that $idz/dx = \varepsilon/r^2$ is integrable at $x = 0$.

In the natural variable, with $w(z) = y(x)$, (1) takes the form

(3) $$y'' + 2r^{-1}r'y' = y, \quad r'/r = (\varepsilon/2ip)d(p^{1/2})/dz \quad ,$$

and wave modulation is therefore controlled by r'/r; since $p = p(z)$, also εx depends only on z, by (2), and xr'/r depends only on εx, by (3). Turning points and singular points of (1) are all singular points of (3), and when they do not lie on the real axes of z or x, physics places no further, general restriction on their nastiness. For the results here reported, the following, secondary hypothesis has been found sufficient: a limit of xr'/r can be identified,

$$xr'/r \to \gamma \in \mathbb{C} \quad \text{as} \quad \varepsilon x \to 0 \quad ,$$

uniformly in the Riemann surface element Δ of εx in which xr'/r has been defined. Equivalently,

$$p^{1/4} = r(x) = x^{\gamma}\rho(\varepsilon x)$$

with a function $\rho(\xi)$ analytic on Δ and <u>"mild"</u> in the sense

(4) $$(\xi/\rho)d\rho/d\xi = \phi(\xi) \to 0 \quad \text{as} \quad \xi \to 0, \text{ uniformly in } \Delta \quad .$$

As a consequence, ρ varies less than any nonzero real power,

$$\forall \nu > 0, \ |\xi^{\nu}\rho^{\pm 1}| \to 0 \quad \text{as} \quad \xi \to 0 \quad ,$$

and γ represents the "nearest power" of x in $r(x) = p^{1/4}$ The primary integrability hypothesis implies $\text{Re}\ \gamma < 1/2$.

The class of singular points thus defined includes all turning points of second-order equations in the literature [2], it extends even the class of [3]. Note the arbitrary multivaluedness of $r(x)$ and $p(z)$. The definition of (1) is purely <u>local</u>, described by

$$z^{-1} \int_0^z [p(t)/p(z)]^{1/2} dt \to 1 - 2\gamma \in \mathbb{C} \quad \text{as} \quad z \to 0 \quad .$$

For $\varepsilon = 0$, also $\phi(\varepsilon x) = 0$ in (4), and the singular point is regular; the irregularity function ϕ therefore discloses a diffeomorphism between irregular and regular points. The superfluous constant ε in (1) reveals itself as an homotopy parameter indicating an avenue of approach to large classes of irregular points.

The branch structure of a regular point can be characterized by Frobenius' fundamental system [1, p. 149] $f_s(x)$, $x^{1-2\gamma}f_m(x)$ with (usually) entire f_s, f_m (and $f_s(0) = f_m(0) = 1$). Irregular points have a similar f.s. $y_s(x)$, $y_m(x)$ with distinct branch points [4]:

Theorem 1. If $|\varepsilon x|$ is not too large, (3) has a solution $y_m(x) = z(x)\hat{y}(x)$ analytic on D with

$$z(x) = x^{1-2\gamma}\zeta(\varepsilon x), \qquad \hat{y}(x) = 1 + \sum_{1}^{\infty} \alpha_n(\varepsilon x)(x/2)^{2n}$$

with mild (in the sense of (4)), but generally multivalued ζ and α_n; the α_n have bounds giving the series infinite convergence radius.

Theorem 2. For non-integer $\frac{1}{2} - \text{Re}\,\gamma$ and small enough $|\varepsilon x|$, (3) has a solution

$$y_s(x) = 1 + \sum_{1}^{\infty} \beta_n(\varepsilon x)(x/2)^{2n}$$

analytic on D with mild and bounded, but generally multivalued, β_n; and the convergence radius is again unbounded.

Observe the two-variable structure in terms of x and εx and that the local definition of (1) supports a solution representation of global nature in x, even if local in εx, - - a mathematical key to wave modulation and asymptotic connection. As $\varepsilon x \to 0$, $y_s(x)$ and $\hat{y}(x)$ approach evenness, which suggests a characterization [4] of the departure of y_s, $\hat{y}$ from the entirety of their counterparts f_s, f_m (which are even for (3)):

Theorem 3. For x and $xe^{-\pi i}$ in D and not too large $|\varepsilon x|$,

$$|\hat{y}(x)-\hat{y}(xe^{-\pi i})| \le \delta_m(|\varepsilon x|)\Gamma(m)|x/2|^{2-m}I_m(|x|)$$

and $\delta_m(|\varepsilon x|) \to 0$ as $|\varepsilon x| \to 0$. For non-integer $\frac{1}{2} - \mathrm{Re}\,\gamma$ and small enough $|\varepsilon x|$, also

$$|y_s(x)-y_s(xe^{-\pi i})| \le \delta_s(|\varepsilon x|)C(\gamma)|x/2|^{2-s}I_s(|x|)$$

and $\delta_s(|\varepsilon x|) \to 0$ as $|\varepsilon x| \to 0$.

Here $m = 3/2 - \mathrm{Re}\,\gamma - \mathrm{lub}|\phi(\varepsilon x) + (\varepsilon x/\zeta)d\zeta/d(\varepsilon x)| > 0$, $s = \frac{1}{2} + \mathrm{Re}\,\gamma - \mathrm{lub}|\phi(\varepsilon x)|$ and I denotes the modified Bessel function. As $|\varepsilon x| \to 0$, y_s and $\hat{y}$ therefore tend to even functions of x uniformly on compacts; for fixed $|\varepsilon x|$, their oddness can grow at most exponentially with $|x|$.

Integer values of $\frac{1}{2} - \mathrm{Re}\,\gamma$ Correspond to the Frobenius exceptions where f_s has a logarithmic branch point [1, p. 150], and y_s can then be characterized by a limit process [4], but loses the symmetry bound of Theorem 3.

Far from a singular point, the solutions of genuine Schroedinger equations are wave-like. More precisely, $r(x)y(x) = W(x)$ satisfies $W'' = (1 + r''/r)W$ with $r''/r = x^{-2}[\gamma(\gamma-1) + \phi(2\gamma-1+\phi+\varepsilon x\phi'/\phi)] \in L(P)$ on paths $P \subset D$ bounded from $x = 0$ so that [1, p.222] a "WKB" solution pair

$$W_+(x) = a(x)e^x, \qquad W_-(x) = b(x)e^{-x}$$

exists with a, b analytic on D and bounded for large $|x|$ (provided $|\varepsilon x|$ is slightly restricted so that ϕ and $\xi\phi'$ are bounded). The decay of $|r''/r|$ at large $|x|$ also assures [1, p. 223,224] limits of a, b as $|x| \to \infty$ with $(\arg x)/\pi$ an integer, which are <u>wave-amplitudes</u> of (1).

Any solution must be a linear combination of W_+, W_-, i.e.,

$$r(x)y_m(x) = \tilde{a}_m(x)e^x + \tilde{b}_m(x)e^{-x} \quad , \tag{5}$$

and similarly with subscript s, with similarly bounded $\tilde{a}_m,\ldots,\tilde{b}_s$, some of which must be multivalued like ry_m. Connecting wave-amplitudes of (1) therefore means [1, p. 481] answering questions like

$\tilde{a}_m(\infty \exp 2\pi i) - \tilde{a}_m(\infty) = ?$

However, $\tilde{\alpha}_m, \ldots$ are normalized via y_m, y_s, which introduces an ε-dependence, and since $|x|$ is bounded on D for fixed $\varepsilon \neq 0$, the connection question can be asked only in the limit $\varepsilon \to 0$. Scrutiny of the normalization [5] shows that

$$\tilde{a}_m/(\rho\zeta) = a_m, \quad \tilde{b}_m/(\rho\zeta) = b_m, \quad \tilde{a}_s/\rho = a_s, \quad \tilde{b}_s/\rho = b_s \quad ,$$

rather than $\tilde{a}_m, \ldots$ are certain to have limits as $\varepsilon \to 0$ and $|x| \to \infty$. Directly meaningful connection questions should therefore be phrased like

$a_m(\infty \exp 2\pi i) - a_m(\infty) = ?$

Now, if $\exp(-\pi i) = j$ and x and jx are in D, then (5) at x and jx implies the further identity

$$\begin{aligned}[\hat{y}(x) - \hat{y}(jx)]x^{1-\gamma}e^{-|x|} &= [a_m(x) - j^{\gamma-1}b_m(jx)]e^{x-|x|} \\ &\quad + [b_m(x) - j^{\gamma}\ a_m(jx)]e^{-x-|x|}\end{aligned} \tag{6}$$

on D. Remarkably, Theorem 3 permits us to let $|x| \to \infty$ while $|\varepsilon x| \to 0$ so that the lefthand side of (6) still tends to zero! E.g., $|x| = |\log \delta_m(|\varepsilon x|)|$ serves. The choices $\arg x = 0, \pi, 2\pi$ then imply the connection answers

$$\begin{pmatrix} a_m(\infty) \\ b_m(\infty/j) \\ a_m(\infty/j^2) \end{pmatrix} = j^{\gamma-1} \begin{pmatrix} b_m(j\infty) \\ a_m(\infty) \\ b_m(\infty/j) \end{pmatrix}$$

whence also

$$\begin{aligned} a_m(\infty e^{2\pi i}) - a_m(\infty) &= 2i\sin(\gamma\pi)\, b_m(\infty e^{\pi i}) \quad , \\ b_m(\infty e^{\pi i}) - b_m(\infty e^{-\pi i}) &= 2i\sin(\gamma\pi)\, a_m(\infty) \quad . \end{aligned} \tag{7}$$

For y_s, (6) holds with y_s, s and γ in the respective places of $\hat{y}$, m and $1-\gamma$, and if $\frac{1}{2} - \mathrm{Re}\,\gamma$ is not an integer, Theorem 3 leads to (7) also with subscript s. Hence, (7) holds for any solution $y(x) = w(z)$ of (1), with interpretation appropriate to the normalization. (The proof [5] excludes integer $\frac{1}{2} - \mathrm{Re}\,\gamma$, but see [3].)

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ICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
ER 2263	2. GOVT ACCESSION NO. AD-A110	3. RECIPIENT'S CATALOG NUMBER 471
title) oedinger Connection		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period
		6. PERFORMING ORG. REPORT NUMBER
: and J. F. Painter		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041 MCS 8001960
ORGANIZATION NAME AND ADDRESS :s Research Center, University of Street Wisconsin Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 2 - Physical Mathematics
IG OFFICE NAME AND ADDRESS (see Item 18 below)		12. REPORT DATE August 1981
		13. NUMBER OF PAGES 7
AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

ON STATEMENT (of this Report)

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ON STATEMENT (of the abstract entered in Block 20, if different from Report)

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