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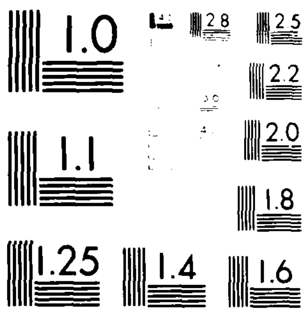

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INSTITUTE FOR PHYSICAL SCIENCE AND TECHNOLOGY

Laboratory for Numerical Analysis

Technical Note BN-1030

University of Maryland
College Park

COMPOSITES WITH A PERIODIC STRUCTURE, MATHEMATICAL ANALYSIS AND NUMERICAL TREATMENT

I. Babuška

R. C. Morgan

October 1984

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COMPOSITES WITH A PERIODIC STRUCTURE MATHEMATICAL ANALYSIS AND NUMERICAL TREATMENT

by

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ABSTRACT

This paper introduces a systematic approach for the derivation of models that describe the behavior of composites with a periodic structure. A technique for analyzing the accuracy of the models is addressed. Although the theory has been developed for the general, n-dimensional setting, the main ideas in this paper are presented for the 1-dimensional case only, for reasons of simplicity. The effectivity of the approach is illustrated with numerical examples. Also, the approach has the potential of being used to adaptively select the best homogenization model.

1. INTRODUCTION

The mathematical analysis of the behavior of composites that have a periodic structure involves the solution of a partial differential equation that has highly oscillatory, periodic coefficients. Although the structure and properties such as existence, uniqueness, and regularity of solutions of this equations are well known, it is impossible to compute the solution in a "standard" way due to the complicated "local" behaviour of the solution. Therefore, various "averaging" techniques that separate the "local" and "global" scales have been devised to develop approximate solutions. These techniques fit under the general category of homogenization, which refers to models of "equivalent", and perhaps fictitious, homogeneous materials that are derived by averaging the properties of the constituent materials of the composite.

Homogenization is widely used in various contexts, and has a long history. One of the first papers ([1]) to address this question is more than 150 years old. Today, there is a large literature dealing with the mathematical and engineering aspects of composite-type materials. For example, [2] and the survey paper [3] address the mathematical aspects of the problem, whereas [4], [5], snd [6] are oriented more towards applications.

Many models of composites are derived with the expectation that the model will have a variety of applications. In general, however, the homogenization should depend on the particular goals of the analysis. A typical situation is discussed in [7] and [8] where it is shown that an analysis of shear waves and longitudinal waves in a periodic medium requires different homogenizations, or models. The relative merits of various homogenizations are discussed in [9].

In this paper, we will discuss the mathematical concepts and the numerical aspects of an homogenization that is appropriate for a particular application and that can be the basis for an adaptive model. For the sake of presenting the ideas clearly, we shall restrict ourselves to a one dimensional problem. The generalization to the n-dimensional case is available in [10], [11], and [12].

2. THE MODEL PROBLEM AND A HOMOGENIZATION CLASS

We will study the solution of the ordinary differential equation

$$(1) \qquad L(u^h) \equiv -\frac{d}{dx}\left(a(\tfrac{x}{h})\frac{du^h}{dx}(x)\right) + b(\tfrac{x}{h})\, u^h(x) = f(x), \quad x \in (-\infty,\infty),$$

where a and b are real, 2π-periodic functions satisfying

$$0 < a_0 \leq a(y) \leq a, \quad \text{and} \quad 0 < b_0 \leq b(y) \leq b,$$

for $-\pi < y \leq \pi$, and h a (small) positive number corresponding to the period of the medium.

In order to discuss properties of u^h, we need the following function spaces:

$$H^k_{per} = \{\text{complex-valued, } 2\pi\text{-periodic functions } \phi \mid$$

$$\|\phi\|^2_{H^k_{per}} \equiv \int_{-\pi}^{\pi} \sum_{j=0}^{k} \left|\frac{d^j\phi}{dy^j}(y)\right|^2 dy < \infty\}, \qquad k = 0,1$$

$$H^k_\nu = \{\text{complex-valued functions } u \text{ defined on } (-\infty,\infty) \mid$$

$$\|u\|^2_{H^k_\nu} \equiv \int_{-\infty}^{\infty} \left(\sum_{j=0}^{k} \left|\frac{d^j u}{dx^j}(x)\right|^2 e^{\nu|x|}\, dx < \infty\right\}, \qquad k = 0,1$$

where ν is a real number. It is shown in [10] that there is a positive number ν_0 (a_0,a,b_0,b) such that for any $0 < \nu < \nu_0$ there exists a unique solution of (1) in $H^1_{-\nu}$ for every $f \in H^0_{-\nu}$.

Next, we introduce the formalism of an homogenization class. In sections 4-5 we discuss several methods of selecting the various elements in the homogenization class. We mention here that this formalism is sufficiently general to include all of the homogenizations that are used in practice. The homogenization of this class consists of (complex-valued) 2π-periodic functions $\{\phi_k: k = 1,\ldots,K\}$ and the triples of constant (complex) coefficient differential operators $\{A_k,B_k,C_k: k = 1,\ldots,K\}$, along with the solution V_k of the equation

$$(2) \qquad A_kV_k = B_k f \qquad \text{for } k = 1,\ldots,K.$$

The function W^h_K, defined by

$$(3) \qquad W^h_K(x) = \sum_{k=1}^{K} \phi_k(\tfrac{x}{h})(C_kV_k)(x)$$

is then used as an approximation of u^h, the solution of (1). The dependence on h of W^h_K is, for the most part, an explicit dependence on h by some of ϕ_k, A_k, B_k, and C_k, and not just on the argument $\frac{x}{h}$. In the succeeding section we will often refer to the differential operators A_k, B_k, and C_k by their respective Fourier symbols $\alpha_k(t)$, $\beta_k(t)$, and $\gamma_k(t)$, which, by our assumptions, are polynomials in t and may depend explicitly on h.

In general, $\{V_k: k = 1,\ldots,K\}$ exhibits the global behavior of the composite, whereas $\{\phi_k: k = 1,\ldots,K\}$ exhibits the local behavior of the composite.

The operators $\{A_k, B_k, C_k: k = 1,\ldots,K\}$ could be easily generalized to pseudo-differential operators, although, for simplicity, we do not consider this case.

3. THE FOURIER TRANSFORMATION

It is shown in [10] that the solution u^h of (1) can be written in the form

$$(4) \qquad u^h(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(t)\phi(\tfrac{x}{h},h,t)e^{itx}\,dt$$

where $\hat{f}$ is the Fourier transformation of f and $y \to \phi(y,h,t)$ is a 2π-periodic complex-valued function that satisfies the differential equation

$$(5) \quad -e^{-ihty}\frac{d}{dy}\left(a(y)\frac{d}{dy}\left(\phi(y,h,t)e^{ihty}\right)\right) + h^2 b(y)\phi(y,h,t) = h^2.$$

The exact meaning of the integral in (4) is given in [10]. Properties of $\phi(y,h,t)$ are studied in detail in [11]. It is shown in [11] that $\phi(y,h,t)$ is analytic in h and t, by which we mean that there is a complex neighborhood of $\mathbb{R}^2$ in $\mathbb{C}^2$ such that about each point in this neighborhood of $\mathbb{R}^2$, the function $(h,t) \to \phi(\cdot,h,t)$ can be expanded in a power series, convergent in H^1_{per}, in which each coefficient is an element of H^1_{per}. In [13], it is shown that $\phi(y,h,t) = O(|t^{-1}|)$ as $|t| \to \infty$. Other representations of u^h, developed in a different context, can be found in [2] and [14].

Now, applying the Fourier transform to (2) and (3) yields

$$(6) \qquad W^h_K(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(t) \sum_{k=1}^{K} \frac{\beta_k(t)}{\alpha_k(t)} \gamma_k(t)\phi_k(\tfrac{x}{h})\, e^{itx}\,dt.$$

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In section 2 we noted that any of ψ_k, α_k, β_k, and γ_k may depend on h. Upon setting

$$Q_K(y,h,t) = \sum_{k=1}^{K} \frac{\beta_k(t)}{\alpha_k(t)} \gamma_k(t)\psi_k(y) \tag{7}$$

it follows from (4) and (6) that

$$u^h(x) - W_K^h(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(t)(\phi(\tfrac{x}{h},h,t) - Q_k(\tfrac{x}{h},h,t))e^{itx}\, dt.$$

Thus, the error that arises from approximating u^h by W_K^h depends on the difference

$$\phi(y,h,t) - Q_K(y,h,t). \tag{8}$$

Consequently, for a given h, we want to find 2π-periodic functions $\{\psi_k: k = 1,\ldots,K\}$ and constant coefficient differential operators $\{A_k, B_k, C_k: k = 1,\ldots,K\}$ so that (8) is small in the sense that

$$\int_{-\pi}^{\pi} \int_{-\infty}^{\infty} |\phi(y,h,t) - Q_K(y,t)|^2 |g(t)|^2\, dt\, dy \tag{9}$$

is small, where either $g = \hat{f}$ or, considering a class of functions f, $g(t) = (1+t^2)^{-n}$, for example. In particular, the quality of a given homogenization and the range of its application are determined by (9).

4. THE FIRST HOMOGENIZATION: EXPANDING IN POWERS OF h

As we pointed out in section 3, $\phi(\cdot,h,t)$ is an analytic function of h and t. Consequently, we can write

(10) $$\phi(\cdot,h,t) = \phi_0(\cdot,t) + \phi_1(\cdot,t)h + \phi_2(\cdot,t)h^2 + \cdots .$$

The functions $\{\phi_j(\cdot,t): j = 0,1,\ldots\}$ can be determined by expanding (5) in powers of h and substituting (10). Solving for the first few $\phi_j(\cdot,t)$ yields

(11) $$\begin{cases} \phi_0(y,t) = g_0(t) = \dfrac{1}{At^2+B} \\[2ex] \phi_1(y,t) = it\, g_0(t)\chi_1(y) \\[2ex] \phi_2(y,t) = (it)^2 g_0(t)\chi_{2,2}(y) + g_0(t)\chi_{2,0}(y) + g \text{ [illegible] }_2(it) \end{cases}$$

where

(12) $$A = \frac{1}{2\pi}\int_{-\pi}^{\pi} (a(y) + a(y)\frac{d\chi_1}{dy}(y))dy$$

$$B = \frac{1}{2\pi}\int_{-\pi}^{\pi} b(y)dy;$$

$p_2(it)$ is a fourth degree, even polynomial in it that has real coefficients; and χ_1, $\chi_{2,0}$, $\chi_{2,2}$ are real-valued functions in H^1_{per} satisfying

$$-\frac{d}{dy}(a(y)\frac{d\chi_1}{dy}(y)) = \frac{da}{dy}(y),$$

$$-\frac{d}{dy}(a(y)\frac{d\chi_{2,0}}{dy}(y)) = -b(y),$$

$$-\frac{d}{dt}(a(y)\frac{d\chi_{2,2}}{dy}(y)) = -a(y)(1 + \frac{d\chi_1}{dy}(y)) + \frac{d}{dy}(a(y)\chi_1(y)),$$

on $(-\pi,\pi)$ and

$$\int_{-\pi}^{\pi} \chi_1(y)dy = \int_{-\pi}^{\pi} \chi_{2,0}(y)dy = \int_{-\pi}^{\pi} \chi_{2,2}(y)dy = 0.$$

Substituting (10) and (11) into (4), we can suggest the following homogenization in terms of the homogenization class that we introduced in section 2, because the variables y and t can be separated in each $\phi_j(y,t)$ and because $\phi_j(y,t)$ is a rational function of t.

$$\psi_1 = 1, \quad \psi_2 = \chi_1, \quad \psi_3 = \chi_{2,0}, \quad \psi_4 = \chi_{2,2}, \quad \text{and} \quad \psi_5 = 1.$$

The Fourier symbols of the differential operators are

$$\begin{array}{lll}
\alpha_1(t) = At^2 + B, & \beta_1(t) = 1, & \gamma_1(t) = 1, \\
\alpha_2(t) = At^2 + B, & \beta_2(t) = 1, & \gamma_2(t) = hit, \\
\alpha_3(t) = At^2 + B, & \beta_3(t) = 1, & \gamma_3(t) = h^2, \\
\alpha_4(t) = At^2 + B, & \beta_4(t) = 1, & \gamma_4(t) = h^2(it)^2, \\
\alpha_5(T) = (At^2 + B)^2, & \beta_5(t) = 1, & \gamma_5(t) = h^2.
\end{array}$$

This homogenization is accurate when f is smooth and h is small. Also, only the Fourier symbols $\gamma_k(t)$ for $k > 2$ depend explicitly on h.

Setting $K = 1$ (i.e., using ψ_1, $\alpha_1(t)$, $\beta_1(t)$, and $\gamma_1(t)$ only) yields the classical homogenization that is studied e.g. in [2], [15], but is derived there by different means. The asymptotic rate at which W_K^h approximates u^h as $h \to 0$ is studied in [2] and [15] for $K = 1,2$.

We will now illustrate some of these ideas with an example. Let

$$a(y) = \begin{cases} 1, & -\pi < y < -\frac{\pi}{2} \\ 10, & -\frac{\pi}{2} < y < \frac{\pi}{2} \\ 1, & \frac{\pi}{2} < y < \pi \end{cases} \tag{13}$$

and

$$b(y) = 1. \tag{14}$$

Figures 1a,b,c, and 2a,b,c contain graphs of $\mathrm{Re}\,\phi(y,h,t)$ and $\mathrm{Im}\,\phi(y,h,t)$ as a function of $t > 0$ $[\phi(y,h,t) = \overline{\phi(y,h,-t)},\ \phi(y,h,t) = \overline{\phi(-y,h,t)}\ ]$ for various values of y and h. We see that $\phi(y,h,t)$ does not depend on y very much when h is small and when t is not very large.

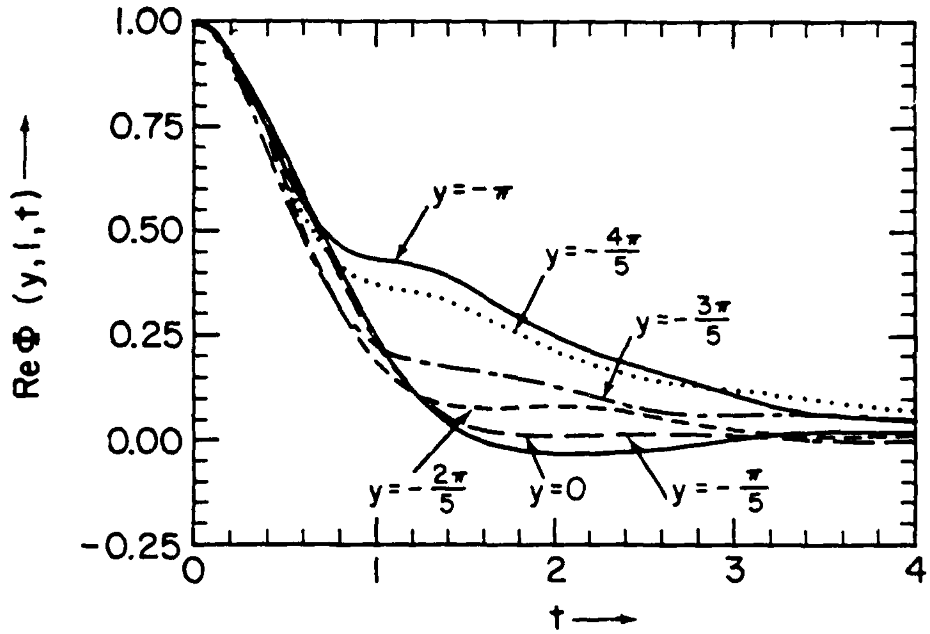

Figure 1a: $h = 1$.

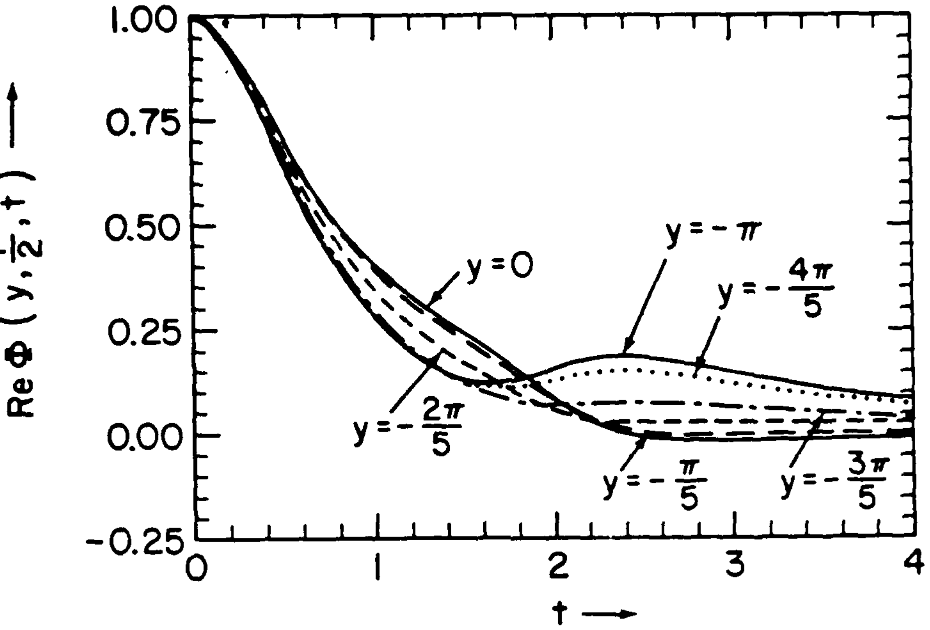

Figure. 1b: $h = 1/2$.

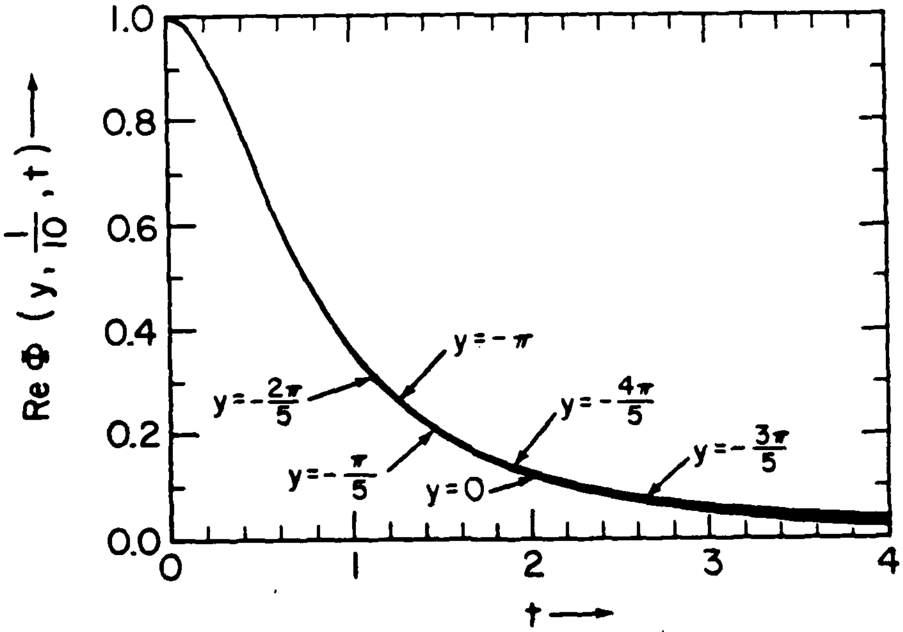

Figure 1c: $h = 1/10$.

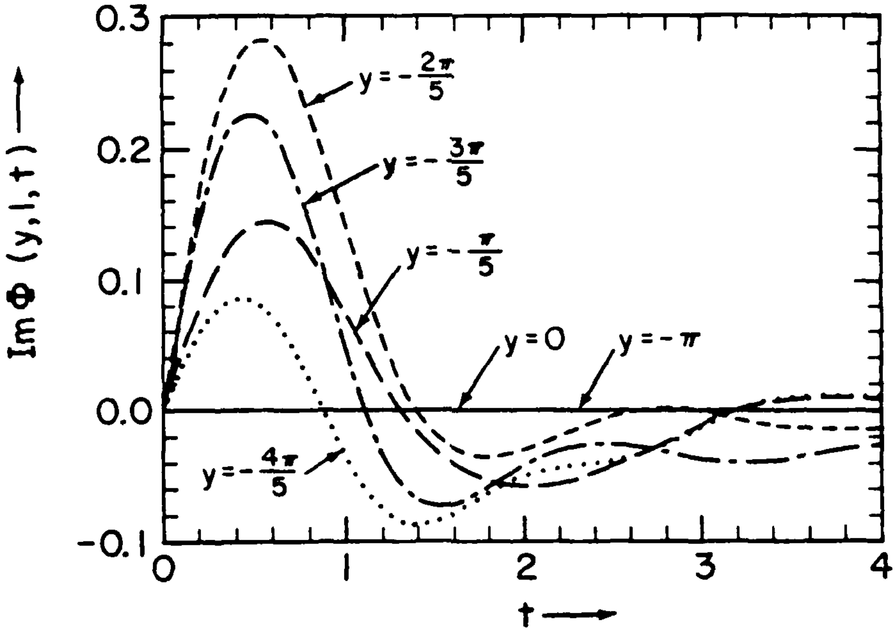

Figure 2a: h = 1

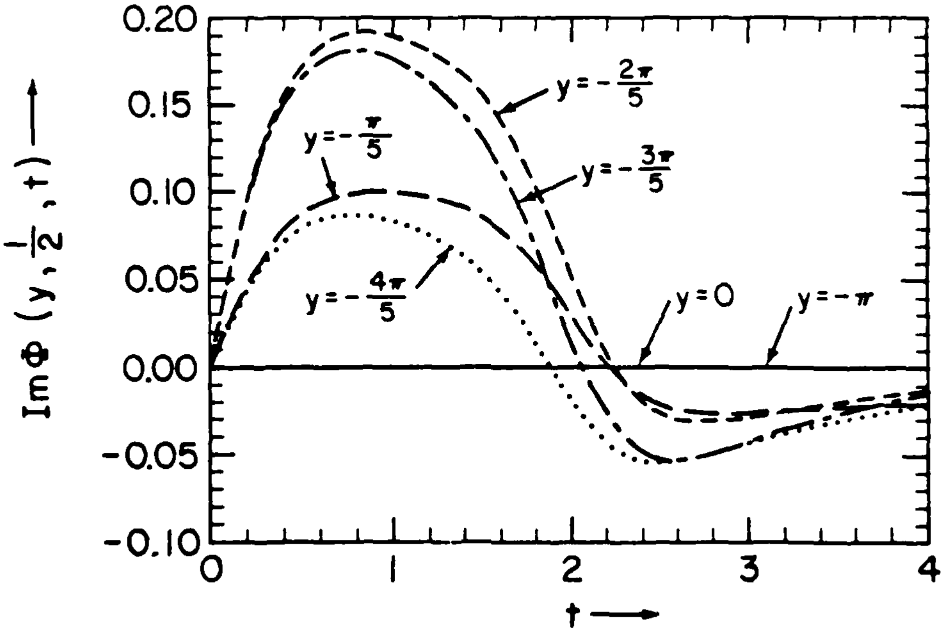

Figure 2b: h = 1/2 .

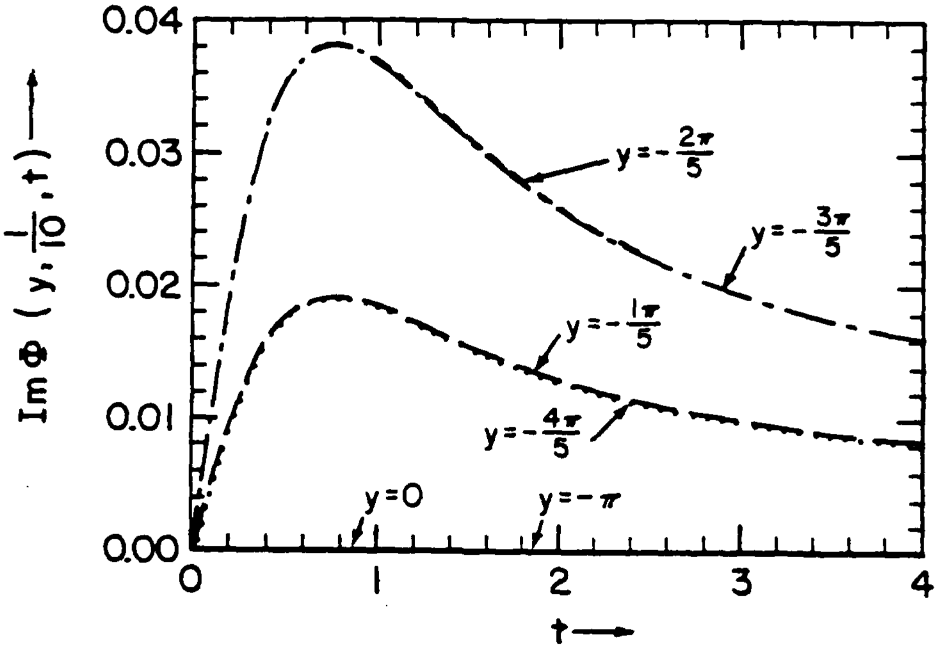

Figure 2c: $h = 1/10$.

For $h = 1, \frac{1}{2}$, figures 3a and 3b compare $\mathrm{Re}\ \phi(-.8\pi,h,t)$ with $\mathrm{Re}\ Q_K(-.8\pi,h,t)$ when ϕ_0 $(K = 1)$ and when $\phi_0(\cdot,t) + \phi_1(\cdot,t)h + \phi_2(\cdot,t)h^2$ $(K = 3)$ are retained in (10) (recall that $\mathrm{Re}\ \phi_1 = 0$). If $h = 1$, it is clear that it is best to use just one term in (10). However, if $h = \frac{1}{2}$, then adding the third term $\phi_2(\cdot,t)h^2$, will improve the approximation if $|t|$ is not too large; this leads to increased accuracy when f is sufficiently smooth. A similar situation occurs when comparing $\mathrm{Im}\ \phi$ with $\mathrm{Im}\ Q_K$; see figures 4a,b. As h decreases to 0 we see two effects. First, if f is sufficiently smooth, it will be advantageous to include more terms in (10). Second, a given truncation of the series in (10) will provide a good approximation of $\phi(\cdot,h,t)$ for larger and larger values of $|t|$; i.e., the smoothness restrictions on f can be relaxed as $h \to 0$.

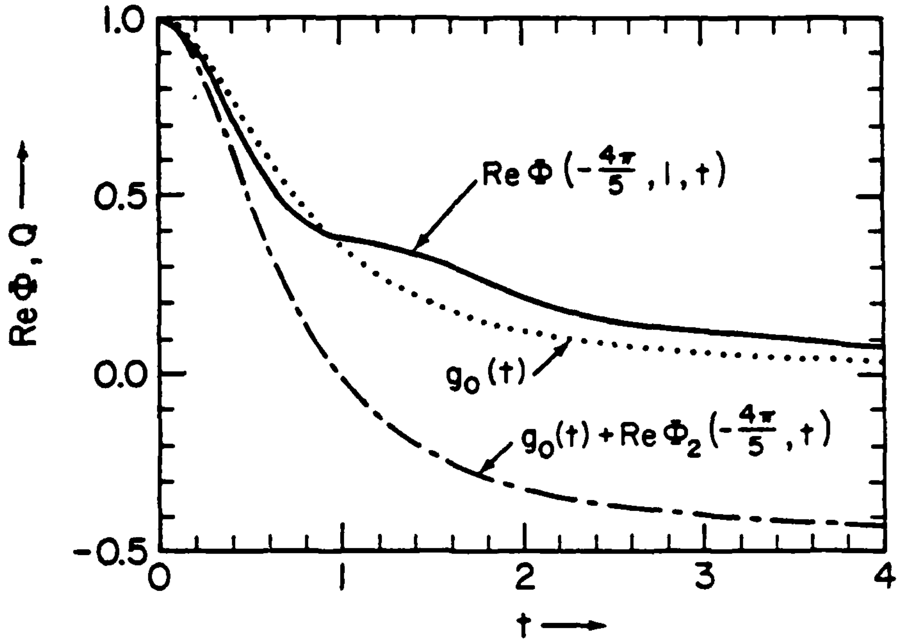

Figure 3a: h = 1.

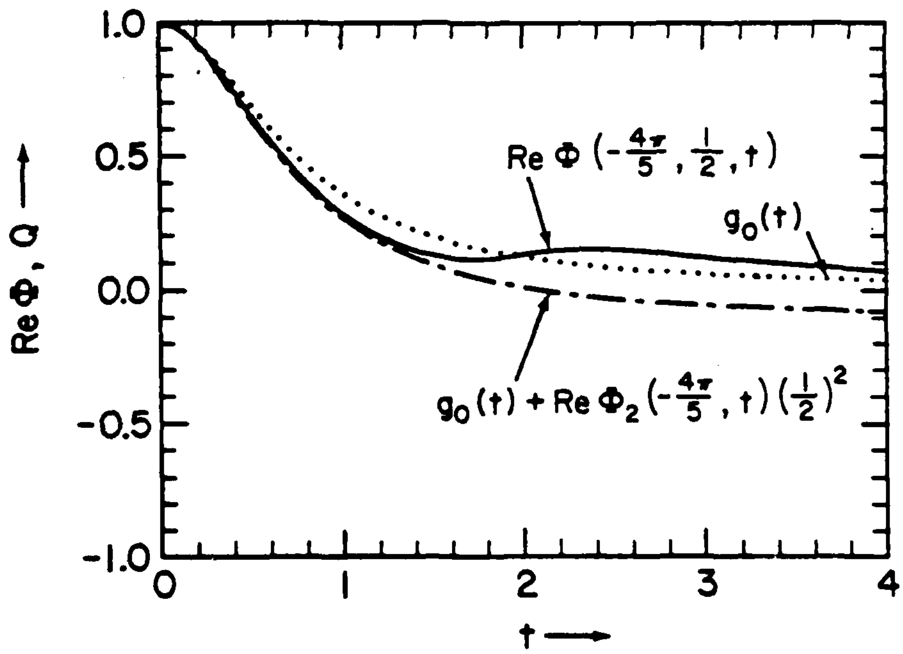

Figure 3b: h = ½ .

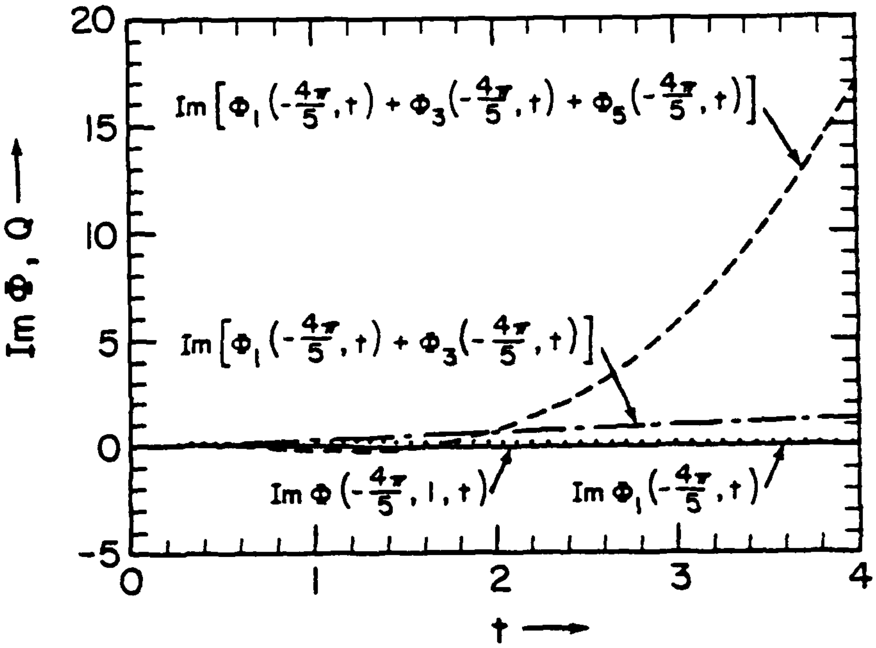

Figure 4a: h = 1.

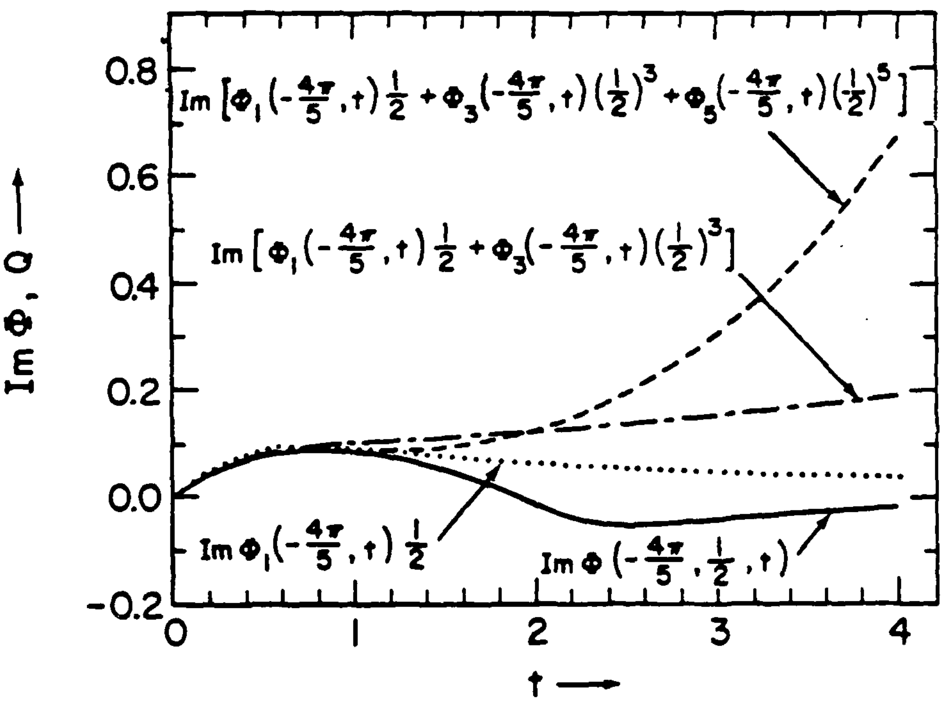

Figure 4b: h = $\frac{1}{2}$.

5. THE SECOND HOMOGENIZATION: EXPANSION IN POWERS OF t

In section 4, we expanded $\phi(\cdot,h,t)$ in powers of h. Because $\phi(\cdot,h,t)$ is also analytic in t we can write

$$\phi(\cdot,h,t) = \phi_0(\cdot,h) + it\,\phi_1(\cdot,h) + (it)^2\phi_2(\cdot,h) + \cdots \tag{15}$$

or

$$\frac{1}{\phi(\cdot,h,t)} = \phi_0^*(\cdot,h) + it\,\phi_1^*(\cdot,h) + (it)^2\phi_2^*(\cdot,h) + \cdots\ . \tag{16}$$

Substituting (15) or (16) into (4) will specify the functions ψ_k and the differential operators A_k, B_k, and C_k that should be used. Note that in this case, the functions ψ_k will depend on h, whereas the differential operators can be chosen independently of h.

The approximation based on (16) is preferable to the one based on (15) because $\phi(\cdot,h,t) \sim O(|t|^{-1})$ as $|t| \to \infty$. With a and b given by (13) and (14) in section 4, figures 5a,b compare $\mathrm{Re}\,\phi(-.8\pi,h,t)$ with $\mathrm{Re}\,Q_K(-.8\pi,h,t)$ for $h = 1$ and $h = 1/2$, using an increasing number of terms in (16). Figures 6a,b compare $\mathrm{Im}\,\phi(-.8\pi,h,t)$ and $\mathrm{Im}\,Q_K(-.8\pi,h,t)$.

Comparing figures 3a,b with 5a,b and figures 4a,b with 6a,b, we see that the quality of both of these homogenizations is about the same, possibly with some preference for the homogenization based on (16).

In [12], the homogenizations that are described in sections 4 and 5 here, are analyzed in detail in the n-dimensional case. There, estimates of $\phi(\cdot,h,t) - Q_K(\cdot,h,t)$ in various norms; e.g., H^o_{per} and H^1_{per}, are given.

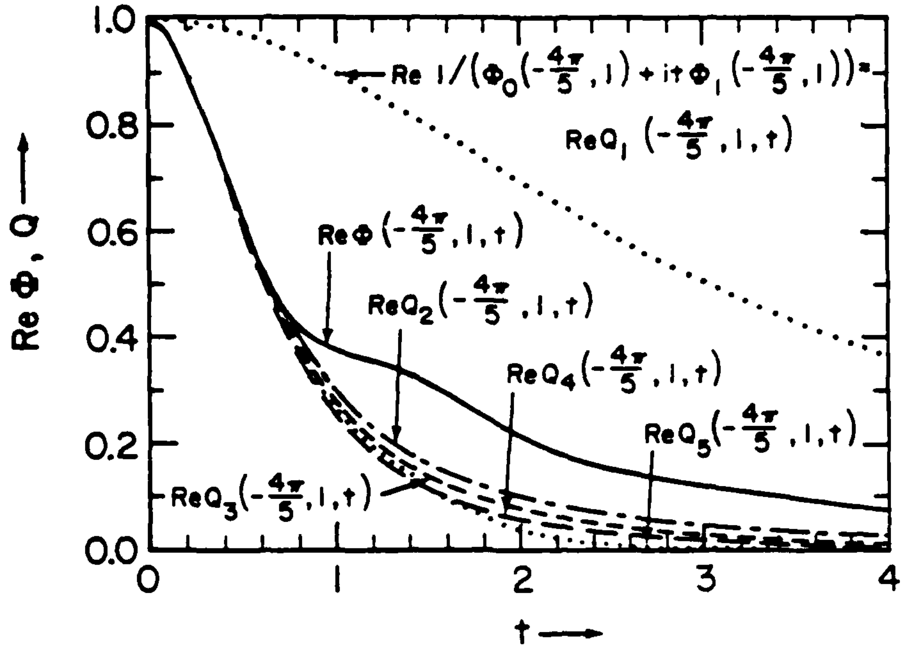

Figure 5a: h = 1 .

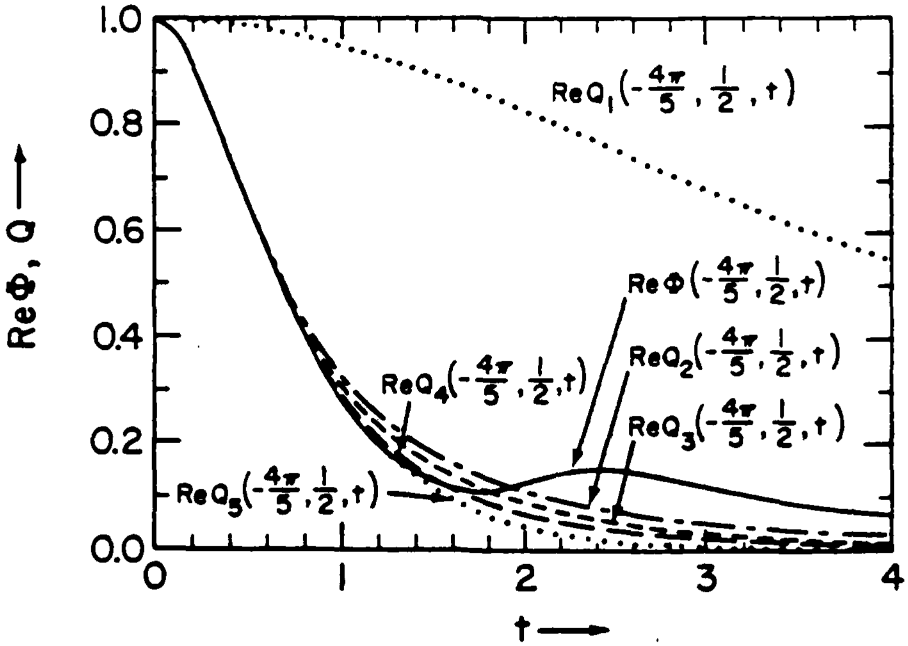

Figure 5b: h = ½ .

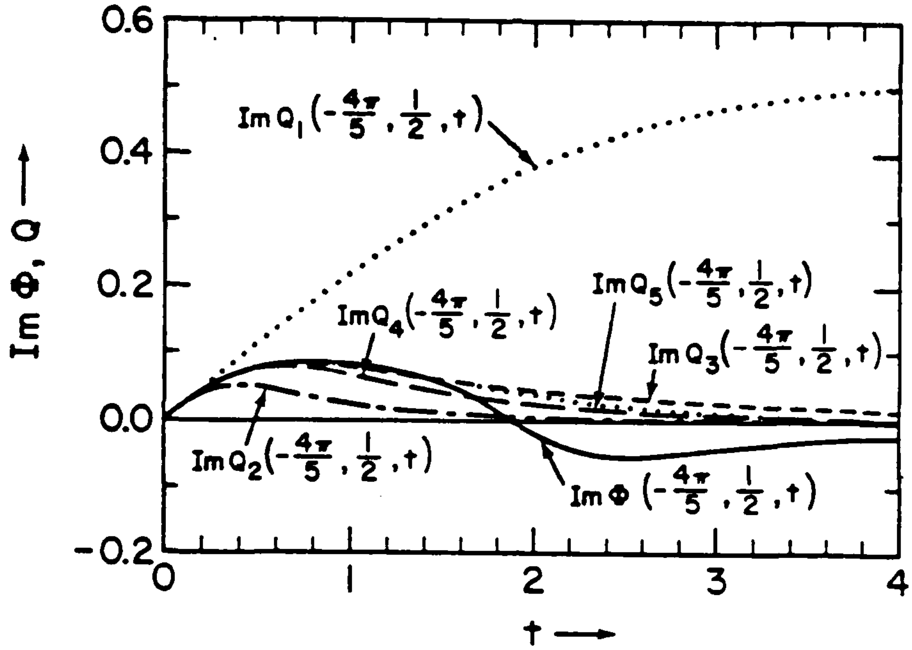

Figure 6a: h = 1.

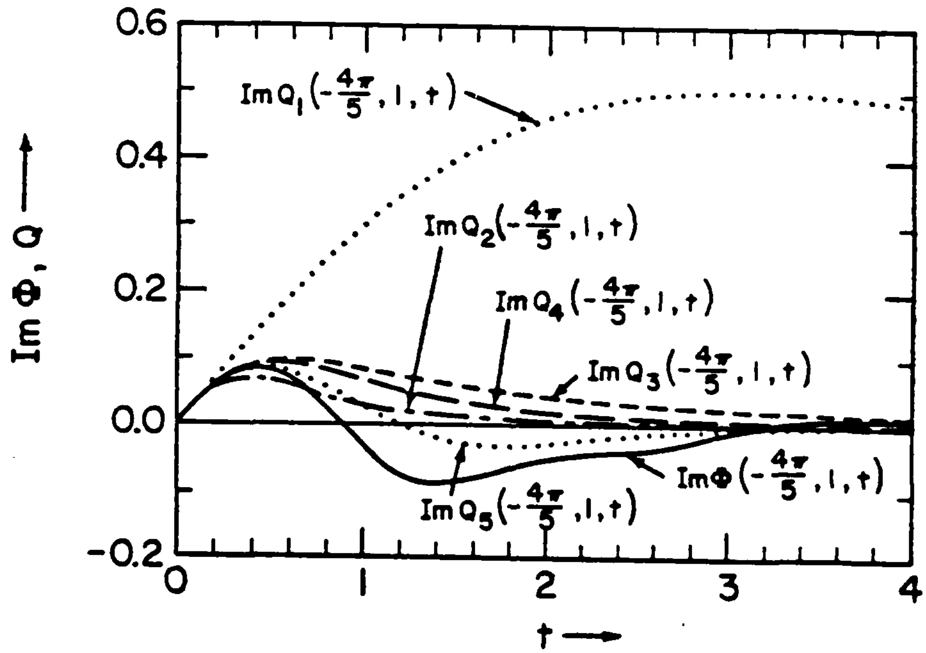

Figure 6b: h = 1/2.

6. OTHER HOMOGENIZATIONS

Obviously, our approach gives rise to many other homogenizations. Each one is motivated, more or less, by the desire to minimize (9). Here, we mention some obvious choices.

1) Since $\phi(\cdot,h,t)$ is a 2π-periodic function, we write

$$\phi(y,h,t) = \sum_{k=-\infty}^{\infty} c_k(h,t)e^{iky}. \tag{17}$$

Approximating $c_k(h,t)$ by the rational function $\frac{\beta_k(t)}{\alpha_k(t)}$, and using only K terms in (17) yields an homogenization that is in the homogenization class described in section 2.

2) Instead of using the functions e^{iky} as a basis, construct a basis by applying the Gram-Schmidt orthonormalization process to the functions $\{\phi(\cdot,h,t_k): k = 1,\ldots\}$, where t_k is chosen, perhaps adaptively, in an appropriate manner. Substituting this orthonormal basis for $\{e^{iky}: k = 0,\pm 1,\ldots\}$ in (17), we can proceed as we did there.

3) For "each" $y \in (-\pi,\pi)$, approximate $\phi(y,h,t)$ by a rational function $\frac{\beta_y(t)}{\alpha_y(t)}$, and solve $A_yW_y = B_yf$. Then

$$u^h(x) = W_y(x) \quad \text{for} \quad y = \frac{x}{h} \pmod{2\pi} \quad \text{and} \quad x \in \mathbf{R}.$$

7. BOUNDED DOMAIN

Let $\Omega_+ = \{x | x > 0\}$ and $\Omega_- = \{x | x < 0\}$, and let the differential operator L be defined as in (1). Suppose that (1) were defined on Ω_+ with the boundary condition $u(0) = 0$. Then a solution can be developed in the following manner. Extend the function f into Ω_-; select an ("outside") function f_0, whose support is small, close to the origin, and contained in Ω_-; and solve the equation

$$L(u^h) = f + cf_0 \quad \text{on} \quad \mathbb{R}^1,$$

where c is chosen so that $u^h(0) = 0$. Note the choice of c and f_0 do not affect the value of $L(u^h)$ on Ω_+ since $f_0 = 0$ there. In two or more dimensions the technique is similar.

This is the technique that is used, for example, in the theory of elliptic equations, where the "outside" functions are Dirac functions and the error on the boundary is minimized. This method appears to be effective for solving harmonic or biharmonic equations, especially when the position of the Dirac functions are comuputed during the minimization procedure. See e.g. [16] and [17]. For problems in two or more dimensions, this technique needs to be experimented with because the solution exhibits a boundary layer (see [18]).

8. NUMERICAL ASPECTS

The procedure we have outlined in this paper for deriving approximations of u^h through approximations of $\phi(\cdot,h,t)$, has certain advatantages from the numerical point of view. A (single) finite element program can be used to solve for $\phi(\cdot,h,t)$ as defined by (5) (also in two dimensions), where h and t are input parameters. Because (5) is defined on one "cell" only, it is possible to solve for $\phi(\cdot,h,t)$ with a high degree of accuracy by using a sufficient number of elements. The derivatives of $\phi(\cdot,h,t)$, with respect to h and t, can then be computed by numerical differentiation. This avoids the need for deriving the analytic expansions by hand, which is virtually impossible to do for higher orders. The graphs in this paper are based on results that were computed by this method.

The rational functions that were introduced in this paper can be computed in a standard way. The functions α_k, β_k, and γ_k can then be derived from these rational functions, and used to construct the differential operators A_k, B_k, and C_k of section 2. Solving for V_k in equation (2) can be done by either of the finite element or finite difference methods. Furthermore, it would still be possible to solve (2) if A_k and B_k were pseudo-differential operators.

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