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A MULTIRESOLUTION APPROACH TO HOMOGENIZATION AND EFFECTIVE MODAL ANALYSIS OF COMPLEX BOUNDARY VALUE PROBLEMS*

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Abstract. We apply multiresolution techniques to study the effective properties of boundary value problems. Conditions under which boundary values are preserved in the effective ("homogenized") formulation are developed and discussed. Relations between the eigenfunctions and eigenvalues of the generic formulation and those of the effective formulation are explored and their dependence on the micro-scale is studied. Applications to the construction of effective Green functions in a complex lamination are discussed. The analytic results are demonstrated via numerical computations.

Key words. multiresolution, wavelets, homogenization, smoothing, boundary value problems, effective properties, wave propagation

AMS subject classifications. 35B27, 78M40, 74Q10, 34B24, 34C29, 42C99

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1. Introduction.

Sturm–Liouville equations and eigenfunctions/eigenvalues problems are some of the most fundamental tools in mathematical physics, with applications to statics (electromagnetics or mechanics), the theory of wave propagation, sound and vibration, quantum mechanics, and more. The eigenvalues of a statical or dynamical problem and the associated eigenfunctions (or modes) convey indispensable information about the physics of the problem and constitute a solid basis for a plethora of analytical and computational techniques—for brevity termed here *modal analysis*—such as modes expansion, characteristic Green function procedure (resolvent), and alternative wavefield representations, to name a few.

The efficacy of modal analysis, however, critically depends on one's ability to predict the specific mode shapes and the associated eigenvalues. Let $\mathbf{L}(q,\lambda)$ be a linear operator of the Sturm–Liouville type, with $q(x)$ representing the system heterogeneity and λ a parameter. A boundary value problem can be expressed formally by the equation

$$\mathbf{L}(q,\lambda_n)u_n = 0, \qquad x \in D, \tag{1.1}$$

augmented by auxiliary boundary conditions. Exact analytic expressions for the mode shapes $u_n(x)$ and eigenvalues λ_n are available only for (the extremely simple) physical configurations that are faithfully modeled by constant coefficients differential equations ($q = \text{const.}$) or by differential equations with nonconstant coefficients ($q = q(x)$) that can be mapped to an appropriate *canonical* structure [1]. Then, $\pi|\lambda_n|^{-1/2}$ provides a reasonably accurate estimate of the length-scale on which the corresponding

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eigenfunction (or mode) varies. This estimate can be used to develop asymptotic solutions for cases in which the equation coefficients vary slowly compared to the variation in the mode shapes. A celebrated example is the WKB approach to modal analysis (see [1]). Let ℓ be the smallest length-scale associated with the medium variability $q(x)$. Then, the WKB asymptotic solution holds for modes satisfying

$$\pi^{-1} |\lambda_n|^{1/2} \ell \gg 1. \tag{1.2}$$

A rough estimate of the lowest eigenvalue is given by $|\lambda_1| = (\pi/L)^2$, where L denotes the size of the physical domain on which the problem is defined. Since $|\lambda_n|$ increases monotonically with n, condition (1.2) can always be satisfied for sufficiently large n. Unfortunately, however, it is often the set of lowest eigenvalues and modes that conveys most of the information of interest. Traditional asymptotic methods thus fail to predict the useful information for problems where the system heterogeneity length-scale is much smaller than the size of the domain on which the problem is defined. There we have

$$\pi^{-1} |\lambda_n|^{1/2} \ell \ll 1 \qquad \forall n \leq N, \tag{1.3}$$

where N is, say, 10 or larger. In the mode set satisfying (1.3), $\pi |\lambda_n|^{-1/2}$ is only one of the length-scales on which the nth mode is described, and certainly not the smallest. Each mode also contains length-scales $\ell/2^m$ with m nonnegative integers.

The purpose of the present study is to investigate the relationships between the small scale structure of a system heterogeneity (a structure described on the length-scale $\ell \ll L$) and the eigenvalues and modes of the corresponding Sturm–Liouville problem. In particular, we shall use multiresolution theory and wavelets to derive a new boundary value formulation governing the large scale features of the modes in the set (1.3). By large scale features of a given mode $u_n(x)$ we mean the mode component $u_n^s(x)$ that is described on the length-scale given by $\pi |\lambda_n|^{-1/2}$. To accomplish such a formulation, three fundamental issues are addressed. The first concerns the *existence of an effective measure in the context of boundary value problems.* That is, the existence of $q^{(\text{eff})}(x)$, described on the length-scale L, such that the large scale component of the mode solutions of (1.1) satisfies exactly the same formulation, with q replaced by its effective measure,

$$\mathbf{L}(q^{(\text{eff})}(x), \lambda_n^*) u_n^s = 0, \qquad x \in D, \tag{1.4}$$

and augmented by the *appropriate* boundary conditions. Recall, however, that the boundary conditions accompanying (1.1) apply to the *complete* mode description $u_n(x)$ and *not* to its large scale component $u_n^s(x)$. Thus, part and parcel of the first issue is the second one: *What are the appropriate boundary conditions for the large scale formulation?* In particular, in what cases do the generic boundary conditions written for the complete formulation (1.1) apply to the large scale formulation (1.4) as well? It will be shown that Neumann, Dirichlet, and a certain type of impedance boundary condition can be transferred to the effective, macro-scale formulation without change. The third issue relates to the set of eigenvalues λ_n^*. The large scale formulation (1.4) is tuned to govern the large scale component $u_n^s(x)$ of the modes $u_n(x)$ in (1.1). At first glance, this implies a clear and explicit relation between the two sets of modes. The relation between the two sets of eigenvalues λ_n and λ_n^*, however, remains implicit. We ask: *What is this relation?* In particular, how does it

depend on the micro-scale? It will be shown that a *spectral equivalence* can be established: λ_n^* is a good approximation to λ_n as the micro-scale becomes sufficiently small.

Finally, a note of interpretation is in order. In attempting to homogenize eigenfunction solutions, one should exercise special care interpreting the resulting "effective eigenfunctions." It arises from the difficulty, in the prehomogenized problem, to distinguish between those rapid variations of a high-order mode, *which are due to the mode order*, from those rapid variations which are due to the intricate structure of the coefficients. Let us explain. It is recognized that homogenization and effective properties imply a smoothing. In our formulation, the scale for accomplishing the smoothing is specified and finite. The scales on which the higher-order modes vary must always decrease with increasing mode order, to the point of vanishing as the mode order becomes infinite. This is true even for an equation with constant coefficients. It is clear, then, that the smoothing of all modes that are of higher order than the one identified by a prescribed, finite smoothing-scale, must obtain the trivial result of zero. Thus, if one accepts an homogenization of the boundary value problem in the usual sense, the associated effective problem can contain no modes with a modal order greater than some N. Interpreting this conclusion either physically or mathematically would seem to be problematic. The key to circumventing what seems to be problematic lies in redefining, or reshaping, our understanding of the meaning of "homogenization" in the context of eigenfunction problems. Thus, if l is the smoothing-scale and L is the outer dimension of the problem, defined $N = L/l$, one can require of the homogenized formulation that (a) its first N modes are identical to the large scale component of the first N modes of the prehomogenized formulation, and (b) the corresponding eigenvalues are identical, at least for certain types of boundary conditions and in some asymptotic sense. There is no physical, mathematical, or engineering sense in looking to the higher modes: one cannot distinguish uniquely between the variations of a mode that are due to its high order and the variations due to the coefficients' complexity.

We shall use multiresolution decomposition, in conjunction with the methodology used in [2, 3, 4, 5, 6, 7], to address the issues articulated above and to develop a formulation governing large scale, locally averaged versions of the modes. We note that multiresolution analysis and wavelets have been used recently by Brewster and Beylkin in [8] for numerical homogenization, i.e., for generating an equation with slowly varying coefficients whose solution has the same large scale behavior as that of the original equation. The basic ideas are similar to those developed in [2, 3]. The work in [8] is devoted mainly to a sophisticated "decimation" process in which an efficient numerical algorithm for estimating the large scale response component is developed. It does not address directly the questions articulated above. Using the multiresolution approach, the works in [4, 6] reconstruct the classical result of homogenization of the equation $(Qu')' = f$, in the context of acoustic scattering. While the classical formulations apply only as a weak asymptotic limit [9] and require the existence of a gap in the heterogeneity scales, the multiresolution formulation can in principle be applied to any multiscale heterogeneity, and the existence of a scale gap is required only for the derivation of closed form analytic expressions for the effective properties. Using the multiresolution approach, the classical result was rederived later by Gilbert [10], together with a correction term. In [11], Beylkin and Coult used the algorithm developed in [8] to investigate the numerical homogenization of boundary value problems. Their work, however, does not provide analytic expression

for the effective properties and does not address the issue of the appropriate boundary conditions for the homogenized problem.

We note that our multiresolution approach resembles in form multigrid or multilevel numerical methods [12, 13, 14, 15]. In both cases the formulation involves the combination of at least two grids having different resolution levels, and a Schur complement structure is used to connect between various levels. Multigrid methods were used to solve elliptic boundary value problems [13, 14, 15]. However, in multigrid techniques one generally uses computations done on a coarse grid, to accelerate convergence and obliterate errors in computations done on the finer grid. In the actual multigrid method implementation schemes, one iterates back and forth ("cycles") between the coarse and fine grids until convergence on the *fine* grid is reached. A number of iteration procedures and convergence theorems were developed in this regard [14]. While in multigrid approach the *fine* grid computation is the ultimate goal, the homogenization approach goes in a counter direction. Here one wishes to "fold" the effect of the fine scales onto a large scale grid, and the goal is to get an accurate description of the solution macro-scale component. The aforementioned folding is done with a Schur complement. Furthermore, the homogenization approach developed here eventually leads to closed form expressions for the macro-scale (effective) problem representation.

The structure of the paper is as follows. In section 2 we briefly summarize multiresolution decomposition (MRD) theory. Section 3 provides the main derivations and results concerning multiresolution homogenization of boundary value problems. In section 4 we discuss application to propagation in complex layered media. Numerical examples are provided in section 5 and concluding remarks in section 6.

2. Multiresolution and smoothing. We shall use the theory of MRD and wavelets [16] to develop a formulation governing the large scale response. Basically, the procedure is identical to that discussed in [2, 3, 4, 5, 6]. Let $\{V_j\}_{j\in\mathbb{Z}}$ be a nested sequence of linear spaces that constitutes an MRD of $L_2(R)$ ($\mathbb{Z}$ is the set of all integers). Further, let $\phi(x)$ and $\psi(x)$ be the corresponding scaling function and wavelet, respectively. The function $\phi_{jn}(x)$ is defined via $\phi(x)$ as $\phi_{jn}(x) = 2^{j/2}\phi(2^j x - n)$, and a similar definition holds for $\psi_{mn}(x)$. Then, $\{\phi_{jn}\}_{n\in\mathbb{Z}}$ is an orthogonal basis of V_j, and $\{\psi_{jn}\}_{n\in\mathbb{Z}}$ is an orthogonal basis of O_j, the orthogonal complement of V_j in V_{j+1}. An approximation of a function $f(x)$ at a resolution k can be written as the sum of two mutually orthogonal functions, namely, a smooth (f^s) component and a detail (f^d) component. We have

$$f(x) \simeq f^s(x) + f^d(x), \tag{2.1}$$

where

$$f^s(x) = \mathbf{P}_j f(x) = \sum_n s_n \phi_{jn}(x), \qquad s_n = \langle f, \phi_{jn}\rangle, \tag{2.1a}$$

$$f^d(x) = \mathbf{D}_j^k f(x) = \sum_{m=j}^{k-1}\sum_n d_{mn}\psi_{mn}(x), \qquad d_{mn} = \langle f, \psi_{mn}\rangle. \tag{2.1b}$$

The asymptotic equality in (2.1) becomes exact in the limit $k \to \infty$. Here, $\langle\cdot,\cdot\rangle$ denotes the inner product of $L_2(R)$, and $j < k$ is some reference resolution—a judicious choice of which depends on the physics of the problem. The scaling functions

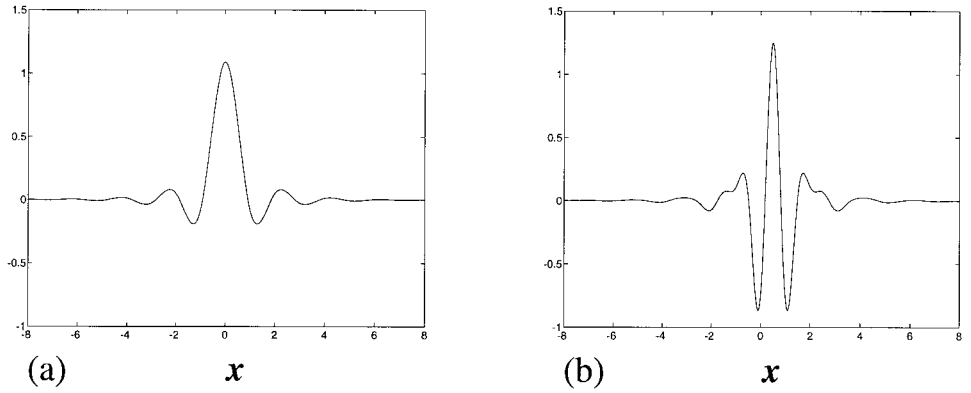

FIG. 2.1. *The cubic spline Battle–Lemarie multiresolution system.* (a) *The scaling function* $\phi(x)$. (b) *The wavelet* $\psi(x)$.

and wavelets satisfy the orthonormality relations $\langle \phi_{jn}, \phi_{jn'} \rangle = \delta_{nn'}$, $\langle \psi_{mn}, \psi_{m'n'} \rangle = \delta_{mm'}\delta_{nn'}$, and $\langle \phi_{jn'}, \psi_{mn} \rangle = 0 \ \forall j \leq m$. Thus, $\mathbf{P}_j$ and $\mathbf{D}_j^k$ in (2.1a)–(2.1b) are projection operators satisfying $\mathbf{D}_j^k \mathbf{P}_{j'} = \mathbf{P}_{j'} \mathbf{D}_j^k = 0 \forall j \geq j'$. ϕ and ψ are either of compact support or fast decreasing and are centered more or less about the origin. They can be interpreted, respectively, as defining a local low-pass filter and a local band-pass filter. Examples are shown in Figure 2.1. From the dilation translation relations articulated above, it follows that the terms ψ_{mn} in (2.1b) are situated, respectively, around the points

$$x_{mn} = n2^{-m}. \tag{2.2}$$

The functions $u^s(x)$ and $u^d(x)$ in (2.1) can be interpreted as a locally smoothed, or averaged, description of $u(x)$ on the length-scale 2^{-j}, and a signal describing the finer details covering length-scales ranging from $2^{-(j+1)}$ to 2^{-k}, respectively. Here and henceforth we refer to the number 2^{-m} and the index m as a length-scale and the resolution associated with it, respectively.

2.1. Local irregularity and wavelets. Wavelet coefficients in the presence of an irregularity play an important role in the present study. The issue has been studied in the general framework of the Hölder regularity condition and Hölder spaces [16, 17]. For the purposes of the present work, however, we shall sacrifice generality and cite a simplified version of a known result. We have the following theorem (see, for example, [16]).

THEOREM 2.1. *Let* $\phi(x), \psi(x)$ *be the scaling function and the wavelet associated with an MRD of* $L_2(R)$, *and* $\phi(x), \psi(x) \in C^N$ *(the space of* N*times continuously differentiable functions). If* $f(x) \in C^M$ *and* $M < N$, *then*

$$|\langle \psi_{mn}, f \rangle| \leq c2^{-m(M+3/2)}, \tag{2.3a}$$

$$|\langle \phi_{mn}, f \rangle| \leq c2^{-m/2}, \tag{2.3b}$$

where c *is an* $O(1)$ *constant.*

A proof can be found, for example, in [16]. This result will be used in section 3.3 to derive upper bounds for the norms of the various operators involved in the expression of the effective properties operator.

3. Effective properties and the basic boundary value problem.

3.1. Basic equations and problem definition. We start with the standard second-order boundary value problem

$$\frac{d}{dx}\left(Q(x)\frac{d}{dx}\,u(x)\right)+\lambda u(x)=s(x),\qquad 0\le x\le 1, \tag{3.1}$$

submitted to the homogeneous boundary conditions,

$$\alpha_{1,2}u(x)+\beta_{1,2}\frac{d}{dx}\,u(x)=0\quad\text{at}\quad x=0,1, \tag{3.1a}$$

where the indices $1,2$ correspond to $x=0,1$, respectively. The parameters α_i,β_i $(i=1,2)$ are determined by the type of physical boundary. Equation (3.1a) can be viewed as a *local impedance boundary condition.* $s(x)$ is an arbitrary source term. We assume throughout that $Q(x)$ is strictly positive and rewrite it as

$$Q(x)=1+q(x); \tag{3.1b}$$

thus $q(x)$ represents the system heterogeneity. We say that $q(x)$ possesses a complex structure. By that we mean the scale for observing the variations in $q(x)$ is much smaller than the dimensions of the domain on which the boundary value problem is defined. The latter is chosen to be a unity (see (3.1)); thus the former, i.e., the scale on which $q(x)$ varies, is $1/50$ or smaller. We are interested in $u^s(x)$—the smooth component of the solution $u(x)$ of (3.1). It is the component of $u(x)$ that varies on length-scales of the order of the physical domain on which the problem is defined, say $1/10$ and above. Thus, we define $u^s(x)$ via (2.1)–(2.1a), with $j=3$ or 4. One obvious way to obtain $u^s(x)$ is to solve for the complete solution $u(x)$ and then to operate with $\mathbf{P}_j$. In addition to being tedious and far from elegant, this route obscures the relations between the small scale structure and the large scale response. Thus, our goal is to develop a new boundary value problem with (possibly) "simpler" heterogeneity function $q^{(\mathrm{eff})}(x)$ (i.e., a heterogeneity that varies on scales of the order of 1), whose solutions (eigenfunctions) are identical to the large scale component of those of (3.1). The new heterogeneity function is termed the *effective measure* of $q(x)$.

With these results, and with the results reported in our previous studies [2, 3, 4, 5, 6], one can generalize the homogenization procedure reported here to cases where the problem consists of two heterogeneity functions, $Q(x)$ and $M(x)$,

$$\frac{d}{dx}\left(Q(x)\frac{d}{dx}\,u(x)\right)+\lambda M(x)u(x)=s(x),\qquad 0\le x\le 1, \tag{3.2}$$

subject to the same boundary conditions as in (3.1a). This generalization provides the effective properties of Q and M in the same meaning articulated above. This study is reported in [18, 19, 20].

3.2. Integral equation formulation. A boundary value problem written as a second-order differential equation as in (3.1) requires an *explicit* specification of the associated boundary conditions at two distinct points (see (3.1a)). This fact clearly constitutes a fundamental difficulty in developing the new formulation for $u^s(x)$, since the generic boundary conditions in (3.1a) are written for the complete solution $u(x)$ and *not* for its smooth component $u^s(x)$. Thus, the incorporation of explicit, local boundary conditions requires a passage from values of $u(x)$ at isolated

points to values of $u^s(x)$ at isolated points. By virtue of (2.1a), this passage cannot be uniquely described.

One may address the articulated difficulty by rewriting the boundary value problem in terms of a second kind of Fredholm integral equation. It is well known that the latter incorporates boundary conditions inherently and implicitly. By that we mean *the boundary conditions are incorporated in the structure of the integral kernel* and are not specified explicitly "at a point." Thus, the incorporation of boundary conditions in such integral equation formulations requires a mapping of functions. The latter, in general, does not seem to suffer from the ill posedness articulated above. As we shall see, this indeed is the case, although some exceptions may occur. Furthermore, the effective properties of a Fredholm integral equation formulation can be directly analyzed and studied by the multiresolution and smoothing procedure developed in [2, 3, 4, 5, 6]. Thus, we devote the present subsection to deriving from (3.1)–(3.1b) a new formulation:

$$v(x) = f(x) + \mathbf{L}v, \tag{3.3}$$

where $\mathbf{L}$ is the integral operator

$$\mathbf{L}v = \int_0^1 k(x,y)q(y)v(y)\,dy. \tag{3.3a}$$

Here $f(x)$ is a known forcing term that can be interpreted as the system response in the absence of the heterogeneity, $q(x)$ is the heterogeneity function, and $k(x,y)$ is a known kernel. For convenience in later use, the operator $\mathbf{L}$ can be written as a background operator $\mathbf{L}_b$ operating on the multiplication of $q(x)$ and $v(x)$:

$$\mathbf{L}v = \mathbf{L}_b(qv), \qquad \mathbf{L}_b f = \int_0^1 k(x,y)f(y)\,dy. \tag{3.3b}$$

A first step toward a Fredholm integral equation formulation would be to define the background problem—a problem presented by (3.1)–(3.1a) with $Q(x) = 1$ ($q(x) = 0$). The associated Green function $G^b(x,y)$ satisfies

$$\left(\frac{d^2}{dx^2} + \lambda\right) G^b(x,y) = -\delta(x-y), \tag{3.4}$$

subjected to the same boundary conditions as in (3.1a). There is a well-established procedure for computing $G^b(x,y)$ analytically [1]. Let $\eta_1(x)$ and $\eta_2(x)$ be two independent functions satisfying

$$\eta_i''(x) + \lambda\eta_i(x) = 0, \qquad i = 1, 2, \tag{3.5a}$$

$$\alpha_1\eta_1(0) + \beta_1\eta_1'(0) = 0 \qquad \text{(boundary condition at } x = 0), \tag{3.5b}$$

$$\alpha_2\eta_2(1) + \beta_2\eta_2'(1) = 0 \qquad \text{(boundary condition at } x = 1), \tag{3.5c}$$

$$\eta_1\eta_2' - \eta_1'\eta_2 = 1 \qquad \text{(normalization)}. \tag{3.5d}$$

A prime denotes a derivative with respect to the argument. Thus, $\eta_1(x)$ and $\eta_2(x)$ are solutions of the *unforced* background problem (by (3.5a)) satisfying the boundary conditions of the original problem at $x = 0$ and $x = 1$, respectively (by (3.5b)–(3.5c)), and the Wronskian normalization condition (by (3.5d)). Then, $G^b(x,y)$ is given by

$$G^b(x,y) = \begin{cases} -\eta_1(x)\eta_2(y), & x \le y, \\ -\eta_1(y)\eta_2(x), & x > y. \end{cases} \tag{3.6}$$

The following properties of $G^b(x,y)$ are straightforward to derive (the subscript x denotes a partial derivative with respect to x):

$$G^b_x(x,y) = \begin{cases} -\eta_1'(x)\eta_2(y), & x < y, \\ -\eta_1(y)\eta_2'(x), & x > y, \end{cases} \quad \lim_{\epsilon\to 0} G^b_x(x,y)\Big|_{x=y-\epsilon}^{x=y+\epsilon} = -1 \tag{3.7}$$

and

$$G^b_{xy}(x,y) \equiv \frac{\partial^2}{\partial x\,\partial y} G^b(x,y) = \delta(x-y) + \overline{G}(x,y), \tag{3.8}$$

where $\overline{G}(x,y)$ is given by

$$\overline{G}(x,y) = \begin{cases} -\eta_1'(x)\eta_2'(y), & x \le y, \\ -\eta_1'(y)\eta_2'(x), & x > y. \end{cases} \tag{3.8a}$$

Note that $\overline{G}(x,y)$ is *continuous* at $x = y$. The last results will be useful in subsequent derivations.

Integral equation formulation can be obtained by rewriting (3.1) with the heterogeneity term $(qu')'$, moving it to the right-hand side, and presenting the solution as a convolution of G^b with the extended source term $s(x) - (qu')'$. The result is

$$u(x) = u_0(x) + \int_0^1 G^b(x,y)\,[q(y)u'(y)]'\,dy, \tag{3.9}$$

where $u_0(x)$ is the background system response to $s(x)$,

$$u_0(x) = -\int_0^1 G^b(x,y)s(y)\,dy. \tag{3.9a}$$

Equation (3.9) is integrodifferential. It can be transformed into an integral equation of the second kind by the following steps. We define $v(x)$,

$$v(x) = u'(x). \tag{3.10}$$

Taking the derivative of (3.9) with respect to x and integrating by parts we get an equation written for $v(x)$,

$$v(x) = v_0(x) + G^b_x(x,y)q(y)v(y)\Big|_{y=0}^{y=1} - \int_0^1 G^b_{xy}(x,y)q(y)v(y)\,dy, \tag{3.11}$$

where

$$v_0(x) = -\int_0^1 G^b_x(x,y)s(y)\,dy. \tag{3.11a}$$

The last result possesses the form of a second kind Fredholm integral equation written for $v(x)$, except for the second term on the right-hand side which still requires a specification of the unknown at the boundary points. As we show in the next subsections, this term can be omitted or replaced by an operation on $v(x)$.

3.2.1. Homogeneous Neumann or Dirichlet boundary conditions. For a homogeneous Neumann boundary condition ("hard boundary"), we have $u'(x) = v(x) = 0$ at the boundary ($\alpha = 0$ in (3.1a)). For a homogeneous Dirichlet condition ("soft boundary"), we have $u(x) = 0$ at the boundary ($\beta = 0$ in (3.1a)). Then, from (3.5b)–(3.5c), $\eta_i(x) = 0$ at the boundary, and it follows from (3.7) that $G_x^b(x, y) = 0$ for $y = 0$ or $y = 1$. Thus, for both Neumann and Dirichlet boundary conditions, the second term on the right-hand side of (3.11) vanishes, and we are left with the desired form (3.3)–(3.3b), where

$$f(x) = v_0(x), \tag{3.12a}$$

$$k(x, y) = -G_{xy}^b(x, y). \tag{3.12b}$$

Note that this result is obtained also for the mixed case, with a Dirichlet condition at one boundary point and a Neumann condition at the second.

3.2.2. General impedance boundary condition. For a general impedance boundary condition, $\alpha_i \neq 0$ and $\beta_i \neq 0$ in (3.1a). Then, the second term on the right-hand side of (3.11) cannot, in general, be omitted *unless* one sets $q(x) = 0$ at the boundaries, in which case the equation reduces again to (3.3)–(3.3b) with (3.12a)–(3.12b). If $q \neq 0$ at the boundaries, however, one may try to *replace* $v(0)$ and $v(1)$ by operations on $v(x)$. Toward this end, we substitute (3.8) and (3.1b) into (3.11),

$$v(x)Q(x) = v_0(x) + G_x^b(x, y)q(y)v(y)\big|_{y=0}^{y=1} - \int_0^1 \overline{G}(x, y)q(y)v(y)\, dy \tag{3.13}$$

and take the limit as $x \to 0$ and as $x \to 1$. The resulting equations can be viewed as a linear set written for the unknowns $v(0)$ and $v(1)$. In a matrix form it is written as

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} v(0) \\ v(1) \end{pmatrix} = \begin{pmatrix} v_0(0) - \mathbf{L}_0 v \\ v_0(1) - \mathbf{L}_1 v \end{pmatrix}, \tag{3.14}$$

where the a_{ij} are known numbers

$$a_{11} = Q(0) + G_x^b(0^+, 0)\, q(0), \tag{3.14a}$$

$$a_{12} = -G_x^b(0, 1)\, q(1), \tag{3.14b}$$

$$a_{21} = G_x^b(1, 0)\, q(0), \tag{3.14c}$$

$$a_{22} = Q(1) - G_x^b(1^-, 1)\, q(1), \tag{3.14d}$$

and $\mathbf{L}_0, \mathbf{L}_1$ are the *functionals*,

$$\mathbf{L}_i v = \int_0^1 \overline{G}(i, y)q(y)v(y)\, dy, \qquad i = 0, 1. \tag{3.14e}$$

Since $G_x^b(x, y)$ is discontinuous at $x = y$, $G_x^b(0^+, 0)$ and $G_x^b(1^-, 1)$ are to be taken as the limits

$$G_x^b(0^+, 0) = \lim_{x>0,\, x\to 0} G_x^b(x, 0), \tag{3.15a}$$

$$G_x^b(1^-, 1) = \lim_{x<1,\, x\to 1} G_x^b(x, 1), \tag{3.15b}$$

evaluated, respectively, via the expressions for $x > y$ and $x < y$ in (3.7).

Equation (3.14) can be solved for $v(0)$ and $v(1)$ in terms of $\mathbf{L}_{0,1}v$, *provided the determinant*

$$\Delta = a_{11}a_{22} - a_{12}a_{21} \tag{3.16}$$

does not vanish. These solutions can then be substituted back into (3.13). The result is again the desired formulation (3.3)–(3.3b), where the source term $f(x)$ and the operator kernel $k(x,y)$ are given by

$$\begin{aligned} f(x) = v_0(x) &+ \frac{q(0)}{\Delta}\left[a_{12}v_0(1) - a_{22}v_0(0)\right] G_x^b(x,0) \\ &+ \frac{q(1)}{\Delta}\left[a_{11}v_0(1) - a_{21}v_0(0)\right] G_x^b(x,1), \end{aligned} \tag{3.17a}$$

$$\begin{aligned} k(x,y) &= -G_{xy}^b(x,y) - \frac{q(0)}{\Delta}\left[a_{12}\overline{G}(1,y) - a_{22}\overline{G}(0,y)\right] G_x^b(x,0) \\ &\quad - \frac{q(1)}{\Delta}\left[a_{11}\overline{G}(1,y) - a_{21}\overline{G}(0,y)\right] G_x^b(x,1) \\ &= -G_{xy}^b(x,y) - g_0(x,y) - g_1(x,y). \end{aligned} \tag{3.17b}$$

Thus, as long as the determinant in (3.16) does not vanish one can derive the Fredholm integral equation formulation. $f(x)$ and $k(x,y)$ of the more general boundary condition are given by those of the homogeneous Neumann or Dirichlet conditions (see (3.12a)–(3.12b)) with added terms $g_0(x,y)$, $g_1(x,y)$ that are proportional to $q(x)$ at the boundaries. These added terms vanish when $q(x)$ vanishes at the boundaries, or when the impedance conditions reduce to the Neumann or Dirichlet conditions. We emphasize that the added terms are continuously differentiable to any order and vary on the length-scale of unity; they are described on the large scale only.

3.3. The formulation governing large scale response. We have shown that the boundary value problem (3.1)–(3.1a) can be written as the Fredholm integral equation formulation in (3.3)–(3.3b), where the specific form of the forcing term and the operator kernel depends on the boundary conditions. The procedure proposed in [2, 3, 4, 5, 6] can now be applied to derive a formulation written directly on the large scale response $v^s(x)$, defined as

$$v^s(x) = \mathbf{P}_j v(x), \tag{3.18}$$

where j corresponds to the reference or smoothing-scale 2^{-j}. By applying $\mathbf{P}_j$ and $\mathbf{D}_j^k$ to both sides of (3.3), expressing $v(x)$ as the sum of $v^s(x)$ and $v^d(x)$ as in (2.1), and then casting the resulting equations in a matrix form, we get

$$\begin{pmatrix} \mathbf{I} - \mathbf{\Phi} & -\mathbf{C} \\ -\bar{\mathbf{C}} & \mathbf{I} - \mathbf{\Psi} \end{pmatrix} \begin{pmatrix} \vec{s} \\ \vec{d} \end{pmatrix} = \begin{pmatrix} \vec{s_0} \\ \vec{d_0} \end{pmatrix}, \tag{3.19}$$

where the coefficients of $v^s(x)$—which apply to the scaling functions summation—are collected in the vector $\vec{s}$, and the coefficients of $v^d(x)$—which apply to the wavelet summation—are collected in $\vec{d}$. Thus, $\vec{s}$ and $\vec{d}$ are unknown vectors representing the large scale response and the remaining fine details of the response, respectively. The same interpretation applies for the known scaling functions and wavelets coefficients

vectors $\vec{s_0}$ and $\vec{d_0}$. $\mathbf{I}$ is the identity matrix and $\mathbf{\Phi}, \mathbf{C}, \bar{\mathbf{C}},$ and $\mathbf{\Psi}$ are matrix operators with elements

$$\Phi_{n',n} = \langle \mathbf{L}\phi_{jn}, \phi_{jn'} \rangle = \langle q\phi_{jn}, \mathbf{L}_b^* \phi_{jn'} \rangle, \tag{3.20a}$$

$$C_{n',mn} = \langle \mathbf{L}\psi_{mn}, \phi_{jn'} \rangle = \langle q\psi_{mn}, \mathbf{L}_b^* \phi_{jn'} \rangle, \tag{3.20b}$$

$$\bar{C}_{m'n',n} = \langle \mathbf{L}\phi_{jn}, \psi_{m'n'} \rangle = \langle q\phi_{jn}, \mathbf{L}_b^* \psi_{m'n'} \rangle, \tag{3.20c}$$

$$\Psi_{m'n',mn} = \langle \mathbf{L}\psi_{mn}, \psi_{m'n'} \rangle = \langle q\psi_{mn}, \mathbf{L}_b^* \psi_{m'n'} \rangle. \tag{3.20d}$$

Here $\mathbf{L}_b^*$ is the adjoint of $\mathbf{L}_b$. The set in (3.19) provides the starting point for a multiresolution study of the scattering problem. From the lower half of (3.19) the response detail component $\vec{d}$ can be expressed in terms of the response large scale component $\vec{s}$. When the result is substituted into the upper half of (3.19) we get a formulation governing $\vec{s}$:

$$\left[\mathbf{I} - \mathbf{\Phi} - \mathbf{C}\left(\mathbf{I} - \mathbf{\Psi}\right)^{-1} \bar{\mathbf{C}}\right] \vec{s} = \vec{s_0}. \tag{3.21}$$

We have assumed here that $v_0(x)$ is described on large scales only; thus $\left\|f^d(x)\right\| \ll \|f^s(x)\|$ (see the discussion after (3.17b)) and the small scale forcing vector $\vec{d_0}$ has been neglected.

The formulation in (3.21) governing the large scale response was termed in [2, 3, 4, 5, 6] the *formulation smooth*. It has been shown that he operator $\mathbf{\Phi}$ is nothing but a matrix representation of the operator $\mathbf{L}$ with $q(x)$ replaced by its smooth component $q^s(x)$ (or large scale component). The latter is given by a relation similar to (2.1a): $q^s(x) = \mathbf{P}_j q(x)$. The elements of $\mathbf{\Phi}$ can be computed by (3.20a) with $q(x)$ replaced by $q^s(x)$. The information on the small scale heterogeneity $q^d(x)$ appears only in $\mathbf{C}\left(\mathbf{I} - \mathbf{\Psi}\right)^{-1} \bar{\mathbf{C}}$; recall the interpretation of ϕ_{jn} and ψ_{mn} as low-pass and band-pass filters. Thus, the operator $\mathbf{C}\left(\mathbf{I} - \mathbf{\Psi}\right)^{-1} \bar{\mathbf{C}}$ is the *effective material operator* (EMO). It describes how the small scale heterogeneity $q^d(x)$ affects the large scale response. A general measure of the potential degree of this effect is the EMO norm. If $\left\|\mathbf{C}\left(\mathbf{I} - \mathbf{\Psi}\right)^{-1} \bar{\mathbf{C}}\right\| \ll \|\mathbf{\Phi}\|$, then the small scale heterogeneity has practically no effect on the large scale response. If these norms are comparable, then a small scale heterogeneity can have a significant effect on the large scale response. An estimate of the EMO norm can be derived by using the bounds in section 2.1. It is recognized that the integral kernel $k(x, y)$ is closely related to the background problem Green function $G^b(x, y)$. The latter is irregular at $x = y$. Similarly, one may expect that the heterogeneity function $q(x)$ possesses an irregular behavior of some order. These properties are used in the following theorem.

THEOREM 3.1. *Let $k(x, y)$ be the integral operator kernel. Let $k(\cdot, y) \in C^p$, $q(\cdot) \in C^{p'}$, and $\phi(x), \psi(x) \in C^N$ with $N > \max(p, p')$. Then*

$$\|\mathbf{\Psi}\|^2 \leq cN_0^2 \frac{2^{-2j(p'+p+2)}}{\left[1 - 2^{-2(p+1)}\right]\left[1 - 2^{-2(p'+1)}\right]}, \tag{3.22a}$$

$$\left\|\bar{\mathbf{C}}\right\|^2 \leq cN_0^2 \frac{2^{-2j(p+1)}}{1 - 2^{-2(p+1)}}, \tag{3.22b}$$

$$\|\mathbf{C}\|^2 \leq cN_0^2 \frac{2^{-2j(p'+1)}}{1 - 2^{-2(p'+1)}}, \tag{3.22c}$$

where $c = O(1)$ and N_0 is the number of resolution 0 grid points covering the domain of interest.

Proof. We start with the operator $\mathbf{\Psi}$. The corresponding matrix elements are given in (3.20d). From Theorem 2.1 we have $|\mathbf{L}_b^* \psi_{m'n'}(x)| \leq c2^{-m'(p+3/2)}$, and with basic spectral techniques it is straightforward to show that $\mathbf{L}_b^* \psi_{m'n'} \in C^{p+N+1}$. Substituting back into the expression for $\Psi_{m'n',mn}$ and applying Theorem 2.1 again we get $|\Psi_{m'n',mn}| \leq c2^{-m'(p+3/2)-m(p'+3/2)}$. With the matrix norm induced by the Euclidean vector norm we now have

$$\begin{aligned}
\|\mathbf{\Psi}\|^2 &\leq \sum_{mnm'n'} |\Psi_{m'n',mn}|^2 \leq c \sum_{m,m'=j}^{\infty} \sum_{\substack{n(m) \\ n'(m')}} 2^{-m'(2p+3)-m(2p'+3)} \\
&= cN_0^2 \sum_{m,m'=j}^{\infty} 2^{-2m'(p+1)-2m(p'+1)} \qquad (n(m) = N_0 2^m) \\
&= cN_0^2 \frac{2^{-2j(p'+p+2)}}{\left[1-2^{-2(p+1)}\right]\left[1-2^{-2(p'+1)}\right]}\,, \qquad (3.23)
\end{aligned}$$

which is the result in (3.22a). Similar considerations lead to (3.22b)–(3.22c). ∎

We have assumed here that the multiresolution system is "more regular" than the integral kernel and the heterogeneity. If $k(x,y)$ or $q(x)$, or both, are smooth to the extent that this assumption does not apply, the bounds for the inner products in Theorem 2.1 would be smaller. In such cases the operator norm bounds can be shown to be smaller than those given in (3.22a)–(3.22c).

3.4. Effective measures in formulations with mildly singular kernels. As predicted already in [2, 3, 4, 5, 6] the results stated in Theorem 3.1 suggest that the EMO norm is dominated by the kernel singularity. For highly singular kernels the EMO affects the large scale response significantly. For continuous kernels, even for mildly singular ones, its effect is negligible and we find that $\vec{s}$ is governed by

$$(\mathbf{I} - \mathbf{\Phi})\, \vec{s} = \vec{s}_0. \qquad (3.24)$$

Thus, by reversing the steps leading from the integral equation formulation (3.3)–(3.3b) to (3.21) we find that for such kernels the large scale response v^s is governed by exactly the same formulation, with $q(x)$ replaced by its smooth component $q^s(x)$—recall that $q^s(x)$ is the only measure of $q(x)$ that affects $\mathbf{\Phi}$. The formulation for $v^s(x)$ then takes on the form

$$v^s(x) = f(x) + \mathbf{L}_b(q^s v^s). \qquad (3.25)$$

This means that the effective measure of $q(x)$ is simply $q^s(x)$. Since in these cases $\|\mathbf{\Psi}\| \ll 1$ and $\|\bar{\mathbf{C}}\| \ll 1$ we get from the lower half of (3.19) that $\|\vec{d}\| \ll \|\vec{s}\|$ or

$$\left\|v^d\right\| \ll \|v^s\|\,. \qquad (3.25a)$$

3.5. The effective heterogeneity. In the problem treated in the present work it is clear that the kernel is highly singular. It is described by a smooth function *and* a Dirac δ distribution. The immediate consequence of this fact is that microscale heterogeneity can have a significant effect on the large scale response. This has been demonstrated already in [3, 4, 5, 6] analytically and numerically for open (free boundary) problems, and the boundary value problem discussed here exhibits the same behavior. Thus, here $q^{(\text{eff})}(x) \neq q^s(x)$. However, one can still derive a simple

analytic expression for the effective measure of $q(x)$ by following the steps derived first in [4]. Note that in all cases discussed here, the only singular component of $k(x,y)$ is $\delta(x-y)$. The rest is continuous. By performing the integration over $\delta(x-y)$ in closed form and moving the result to the left-hand side we obtain

$$v(x)Q(x) = f(x) + \mathbf{\Gamma}_b(qv), \tag{3.26}$$

where $Q(x) = 1 + q(x)$, $f(x)$ is given in (3.12a) or (3.17a), and $\mathbf{\Gamma}_b$ is an integral operator of the same structure as $\mathbf{L}_b$ in (3.3b) with the kernel $\Gamma(x,y)$,

(3.26a)
$$\Gamma(x,y) = \begin{cases} -\overline{G}(x,y), & \text{Neumann or Dirichlet b.c.} \\ -\overline{G}(x,y) - g_0(x,y) - g_1(x,y), & \text{Impedance b.c.} \end{cases}$$

Let us define the new variable $T(x)$ via the local constitutive relation

$$T(x) = v(x)Q(x). \tag{3.27}$$

From (3.26) the formulation governing $T(x)$ is

$$T(x) = f(x) + \mathbf{\Gamma}_b\left(\frac{q}{Q}T\right), \tag{3.28}$$

which is now a second kind Fredholm integral equation formulation for $T(x)$, with a continuous kernel $\Gamma(x,y)$. The effective measure of the heterogeneity relevant for $T(x)$ is nothing but $\mathbf{P}_j\,(q/Q) = (q/Q)^s$ (see the discussion in subsection 3.4). In other words, the formulation governing $T^s(x)$ is

$$T^s(x) = f(x) + \mathbf{\Gamma}_b\left[\left(\frac{q}{Q}\right)^s T^s\right] \tag{3.29a}$$

and

$$\left\|T^d\right\| \ll \left\|T^s\right\|. \tag{3.29b}$$

By rewriting (3.27) for $v^s(x)$ in terms of $T(x)$ and using (3.29b), we find

$$v^s(x) = T^s(x)\left(\frac{1}{Q(x)}\right)^s \qquad \Longrightarrow T^s(x) = \left[\left(\frac{1}{Q(x)}\right)^s\right]^{-1} v^s(x). \tag{3.30}$$

Substituting the last expression back into (3.29a) we find a formulation governing $v^s(x)$ only:

$$v^s(x)Q^{(\mathrm{eff})}(x) = f(x) + \mathbf{\Gamma}_b\left(q^{(\mathrm{eff})}v^s\right), \tag{3.31}$$

where

$$Q^{(\mathrm{eff})}(x) = \left[\left(\frac{1}{Q(x)}\right)^s\right]^{-1}, \qquad q^{(\mathrm{eff})}(x) = Q^{(\mathrm{eff})}(x) - 1. \tag{3.32}$$

This last formulation—governing the large scale response—is identical to the generic formulation that governs the complete response (3.26), except that the heterogeneity $q(x)$ has been replaced by its *effective measure* $q^{(\mathrm{eff})}(x)$, the expression of which

is given in (3.32). Note that the kernel $\Gamma(x,y)$ in the formulation governing $v^s(x)$ is identical in form to the kernel in the formulation for the complete response $v(x)$. However, the forcing term $f(x)$ in the new formulation (3.31), as well as the kernel itself, still contains expressions depending on the numbers $Q(0), Q(1)$. This fact cannot be overemphasized. While the structure of the equation is preserved, the specific prescriptions for both the forcing term $f(x)$ and the kernel $k(x,y)$, are not; the effective formulation cannot be obtained by a mere replacement $q \to q^{(\text{eff})}$. On the other hand, there are three specific scenarios for which the aforementioned dependencies on $Q(0), Q(1)$ cancel. These are (see subsection 3.2 and (3.17a)–(3.17b)) (i) Neumann boundary conditions, (ii) Dirichlet boundary conditions, (iii) natural impedance boundary conditions: (3.1a) with $\beta_1 = Q(0)$, $\beta_2 = Q(1)$. Under these boundary conditions the prescriptions are preserved, and the effective formulation in its entirety (including the algebraic expressions for $f(x), k(x,y)$) is given by the replacement $q \to q^{(\text{eff})}$. Thus, for these boundary conditions one can reverse the steps leading from (3.1)–(3.1a) to (3.26) and obtain the effective boundary value problem

$$\frac{d}{dx}\left(Q^{(\text{eff})}(x)\frac{d}{dx}\,u^s(x)\right) + \lambda u^s(x) = s(x), \qquad 0 \le x \le 1, \tag{3.33}$$

where $Q^{(\text{eff})}(x)$ is given in (3.32) and is subject to the following homogeneous boundary conditions: (i) Effective Neumann boundary conditions: $v^s = u^{s\prime} = 0$, if the generic boundary conditions were of the Neumann type. (ii) Effective Dirichlet boundary conditions: $u^s = 0$, if the generic boundary conditions were of the Dirichlet type. (iii) Effective natural impedance boundary conditions: $\alpha_{1,2}u^s(x) + Q^{(\text{eff})}(x)v^s(x) = 0$ at $x = 0, 1$, if the generic boundary conditions were of the natural impedance type.

Finally, we note that from (3.27) and (3.30) we can identify a rule for smoothing the product Qv,

$$(Qv)^s = Q^{(\text{eff})}(x)\, v^s(x), \tag{3.34}$$

which will be found useful later.

3.6. The eigenfunctions and eigenvalues. The analysis leading to the effective formulation in (3.33) was based on the assumption that λ is not a critical value of the operators involved. That is, we have implicitly assumed, for example, that (3.19) possesses a unique solution. This assumption fails when λ is an eigenvalue of the problem. In this subsection we wish to study how the eigenvalues and eigenfunctions of the complete formulation in (3.1) relate to those of the effective formulation in (3.33). We start with the following simple theorem.

THEOREM 3.2. *Let $\{f_n^\epsilon\}$ be an orthonormal basis in a Hilbert space H that depends on the parameter ϵ. Let $\{g_n\}$ be an orthonormal sequence in H. The following hold:*

1. *If $\forall\, m \neq n$, $\langle f_n^\epsilon, g_m\rangle \to 0$ as $\epsilon \to 0$, then $f_n^\epsilon \to g_n$ as $\epsilon \to 0$ $\forall\, n$.*
2. *If $\forall\, m \neq n$, $\langle f_n^\epsilon, g_m\rangle = 0$, then $f_n^\epsilon = g_n$ $\forall\, n$.*

Proof. Expand g_m by the set $\{f_n^\epsilon\}$,

$$g_m = \sum_i a_i^m(\epsilon) f_i^\epsilon, \qquad a_i^m(\epsilon) = \langle g_m, f_i^\epsilon\rangle. \tag{3.35}$$

Moving the mth term to the left and using orthogonality of the f_n^ϵ, we get

$$\|g_m - a_m^m(\epsilon) f_m^\epsilon\|^2 = \sum_{n\neq m} |\langle g_m, f_n^\epsilon\rangle|^2. \tag{3.36}$$

Since $\{f_n^\epsilon\}$ is a basis for any ϵ, the sequence (in n) $\{a_n^m(\epsilon)\}$ is square summable. Also, by hypothesis, for any given pair $(m \neq n)$ we have $\langle g_m, f_n^\epsilon \rangle \to 0$ as $\epsilon \to 0$. Therefore the sum on the right-hand side of (3.36) above must vanish with ϵ. In other words,

$$\|g_m - a_m^m(\epsilon) f_m^\epsilon\| \to 0 \quad \text{as} \quad \epsilon \to 0; \tag{3.37}$$

that proves 1 above. The identity in 2 follows immediately. □

Let $u_n(x)$, λ_n be the nth eigenfunction and eigenvalue associated with the complete formulation in (3.1). Let $u_n^*(x)$, λ_n^* be those associated with the effective formulation in (3.33). The pairs u_n, λ_n and u_m^*, λ_m^* satisfy the equations

$$(Q\, v_n)' + \lambda_n u_n = 0, \tag{3.38a}$$

$$(Q^{(\text{eff})}\, v_m^*)' + \lambda_m^* u_m^* = 0, \tag{3.38b}$$

where a prime denotes a derivative with respect to the argument, $v = u'$. u_n and u_m^* satisfy the same boundary conditions (see (3.1a) and the discussion after (3.33)). Since both equations are real and self-adjoint, the eigenfunctions and eigenvalues are real in both cases. We shall assume throughout that

$$\lambda_n \neq \lambda_m^* \qquad \forall m \neq n. \tag{3.38c}$$

Since $Q^{(\text{eff})}$ is a slowly varying large scale heterogeneity, the first N eigenfunctions of (3.38b) satisfy (see section 3.6.1)

$$u_n^* \in V_j \qquad \forall n \leq N = 2^j, \tag{3.39a}$$

$$v_n^* \in V_j \qquad \forall n \leq N = 2^j. \tag{3.39b}$$

We shall restrict our discussion to these first N eigenfunctions. Note also that for these first N modes the relation in (3.29b) is valid (because the results of section 3.4 and (3.25a) in particular still hold in the context of the formulation for T in (3.29a)), so the smoothing rule (3.34) still holds:

$$\mathbf{P}_j\,(Qv_n) \equiv (Qv_n)^s = Q^{(\text{eff})} v_n^s. \tag{3.40}$$

Furthermore, if $\bar{V}_j$ is a linear subspace of V_j consisting of all functions in V_j that satisfy the same boundary conditions as u_n^*, then the set $\{u_n^*\}_{n=1,\ldots,N}$ is an orthonormal basis of $\bar{V}_j$.

We now perform an inner product of (3.38a) and (3.38b) with u_m^* and u_n, respectively, and subtract the second from the first. The result is

$$\langle u_m^*, (Qv_n)' \rangle - \langle u_n, (Q^{(\text{eff})} v_m^*)' \rangle + \langle u_n, u_m^* \rangle\, (\lambda_n - \lambda_m^*) = 0, \tag{3.41}$$

where we have used the realness of the quantities involved. Integration by parts gives

$$u_m^* Q v_n \,\big|_0^1 - u_n Q^{(\text{eff})} v_m^* \big|_0^1 + \langle v_n, Q^{(\text{eff})} v_m^* \rangle - \langle v_m^*, Q v_n \rangle + \langle u_n^s, u_m^* \rangle (\lambda_n - \lambda_m^*) = 0 \tag{3.42}$$

and we have used the identity $\langle u_n, u_m^* \rangle = \langle u_n^s, u_m^* \rangle$. From (3.39a)–(3.39b) it follows that $v_m^* = \mathbf{P}_j v_m^*$. Thus,

$$\begin{aligned} \langle v_m^*, Q v_n \rangle &= \langle \mathbf{P}_j v_m^*, Q v_n \rangle \\ &= \langle v_m^*, \mathbf{P}_j (Q v_n) \rangle \qquad (\mathbf{P}_j \text{ is self-adjoint}) \\ &= \langle v_m^*, Q^{(\text{eff})} v_n^s \rangle \qquad (\text{by (3.40)}). \end{aligned} \tag{3.43}$$

With this last result and by realness of the Q's and v's the first and second inner products in (3.42) can be written as

$$\langle v_n, Q^{(\mathrm{eff})} v_m^* \rangle - \langle v_m^*, Q v_n \rangle = \langle v_n, Q^{(\mathrm{eff})} v_m^* \rangle - \langle v_n^s, Q^{(\mathrm{eff})} v_m^* \rangle = \langle v_n^d, Q^{(\mathrm{eff})} v_m^* \rangle, \tag{3.44}$$

where v_n^d is the detail (micro-scale) component of v_n. Substituting back to (3.42) we find

$$\langle u_n^s, u_m^* \rangle \, (\lambda_n - \lambda_m^*) = [u_n Q^{(\mathrm{eff})} v_m^* - u_m^* Q v_n]_0^1 - \langle v_n^d, Q^{(\mathrm{eff})} v_m^* \rangle. \tag{3.45}$$

Let ℓ be the micro-scale (the length-scale on which v_n^d varies) and L_m^* be the length scale on which the mode v_m^* varies. Since the effective formulation consists of large scale coefficients only, it follows that L_m^* is determined only by the mode order, and is given, roughly, by $1/m$. Now define

$$\epsilon(\ell) = \ell / L_m^*. \tag{3.46}$$

It is clear that the rightmost term in (3.45) above vanishes as the parameter ϵ goes to zero. This fact is used next to establish a spectral equivalence between the effective and complete boundary value problems.

Homogeneous Neumann or Dirichlet boundary conditions. In this case the first term in the right-hand side of (3.45) vanishes. Then

$$\langle u_n^s, u_m^* \rangle = -\langle v_n^d, Q^{(\mathrm{eff})} v_m^* \rangle \to 0 \quad \text{as} \quad \epsilon \to 0 \quad \forall n \neq m, \tag{3.47a}$$

$$\langle u_n^s, u_n^* \rangle \, (\lambda_n - \lambda_n^*) = -\langle v_n^d, Q^{(\mathrm{eff})} v_n^* \rangle \to 0 \quad \text{as} \quad \epsilon \to 0. \tag{3.47b}$$

Then, by (3.47a) and Theorem 3.2 we get

$$u_n^s \to u_n^* \quad \text{as} \quad \ell / L_n^* \to 0 \tag{3.48a}$$

and with this last result (3.47b) gives

$$\lambda_n \to \lambda_n^* \quad \text{as } \ell / L_n^* \to 0. \tag{3.48b}$$

Hence, a "spectral equivalence" is established: if the micro-scale is sufficiently small, the effective eigenvalue λ_n^* is a good approximation to the true eigenvalue λ_n, and the effective mode u_n^* is a good approximation of the nth mode macro-scale component, u_n^s. We shall demonstrate these results numerically in section 5.

Impedance boundary conditions. Here, the first term on the right-hand side of (3.45) does not vanish. The consequences are that, in general, $u_n^s \neq u_n^*$ and $\lambda_n \neq \lambda_n^*$. Note, however, that for any fixed x, $u_n'(x)$ increases with n. Thus, when associated with the eigenfunctions, impedance boundary conditions converge to Neumann boundary conditions in the limit of large n. This implies that for impedance boundary conditions and for a sufficiently small ϵ, we get, as n increases,

$$u_n^* \longrightarrow u_n^s, \tag{3.49a}$$

$$\lambda_n^* \longrightarrow \lambda_n. \tag{3.49b}$$

We shall demonstrate this convergence in section 5.

Natural impedance boundary conditions. Let us consider the following boundary conditions:

$$Q(x)v(x) + \alpha_{1,2}u(x) = 0 \quad \text{at} \quad x = 0, 1 \tag{3.50a}$$

for the complete formulation and

$$Q^{(\text{eff})}(x)v^*(x) + \alpha_{1,2}u^*(x) = 0 \quad \text{at} \quad x = 0, 1 \tag{3.50b}$$

for the effective formulation. With these boundary conditions, $Qv_n = -\alpha_{1,2}u_n$ and $Q^{(\text{eff})}v_m^* = -\alpha_{1,2}u_m^*$ at the boundaries. Under these conditions the first term on the right-hand side of (3.45) vanishes and (3.48a)–(3.48b) hold again. This result is of particular importance, as the impedance boundary condition given in (3.50a) is used in many physical problems (see, for example, section 3.2 in [1]). The fact that the identities in (3.48a)–(3.48b) hold when the impedance boundary condition of (3.50b) is applied to the effective formulation means that the effective measure of Q is also the relevant one for establishing the effective modes in the impedance case.

3.6.1. Comment. Since the problem is of finite support and $u_n^s(x)$ is defined by (2.1a), it is clear that $u_n^s(x)$ possesses a finite number of degrees of freedom: 2^j. Thus, the effective modal problem in (3.38b) cannot be taken "too far"; the large scale modal solutions and the corresponding eigenvalues $u_n^*(x)$, λ_n^* make sense only as long as the associated macro-scale 2^{-j} is large compare to the micro-scale *and* for $n \leq 2^j$. This is consistent with the requirement $\epsilon \to 0$ in (3.48a)–(3.48b), and only under this condition is a spectral equivalence established. Another way of looking at it is the following. For smooth heterogeneity the length-scale on which $u_n(x)$ varies is $\lambda_n^{-1/2}$. Since $\lim_{n\to\infty} \lambda_n^*$ is unbounded, we find that $u_n^*(x)$ varies on infinitely small scales when n becomes sufficiently large. This contradicts the definition of large scale response. The key lies in the understanding of (3.33) and (3.38b) as formulations defined over a finite dimensional linear space—the dimension is 2^j. This comment is nothing but the mathematical expression of the interpretation issue discussed in the introduction.

4. The effective Green function of a complex waveguide. The Green function associated with an electromagnetic or acoustic wave propagation in a complex, planarly layered medium can be modeled by a wave equation of the form

$$\begin{aligned} &\left[\frac{\partial}{\partial x} Q(x) \frac{\partial}{\partial x} + \frac{\partial^2}{\partial z^2} + \Omega^2 \right] G\,(x, z\,; x', z') \\ &\qquad = -\delta(x - x')\delta(z - z'), \qquad 0 \leq x \leq 1, \end{aligned} \tag{4.1}$$

subject to the same boundary conditions as given in (3.1a). An outgoing wave radiation condition is assumed at $|z| \to \infty$. Here x and z are the cross range and range directions, respectively.

By performing a Fourier transformation of (4.1) in the z direction we find an equation of the same structure as (3.1),

$$\left[\frac{d}{dx} Q(x) \frac{d}{dx} + \left(\Omega^2 - \zeta^2\right) \right] \tilde{G}(x, \zeta\,; x', z') = -\delta(x - x')e^{-i\zeta z'}, \qquad 0 \leq x \leq 1. \tag{4.2}$$

Here G and $\tilde{G}$ are related via the Fourier transform pair

$$\tilde{G}(x,\zeta\,;x',z') = \int_{-\infty}^{\infty} G(x,z\,;x',z')\,e^{-i\zeta z}\,dz, \tag{4.3a}$$

$$G(x,z\,;x',z') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{G}(x,\zeta\,;x',z')\,e^{i\zeta z}\,d\zeta. \tag{4.3b}$$

The one-dimensional Green function $\tilde{G}$ can be expressed by the modal summation [1]

$$\tilde{G}(x,\zeta\,;x',z') = -\sum_n \frac{u_n(x)u_n(x')}{\lambda-\lambda_n}e^{-i\zeta z'}, \tag{4.4}$$

where

$$\lambda = \Omega^2 - \zeta^2, \tag{4.4a}$$

and where $u_n(x)$ and λ_n are the eigenfunctions and eigenvalues in (3.38a)—the transverse modal formulation associated with (4.1). When (4.3b)–(4.4a) are used in conjunction with the residue theorem we get the modal representation of $G(x,z\,;x',z')$,

$$G(x,z\,;x',z') = \frac{i}{2}\sum_n \frac{u_n(x)u_n(x')}{\zeta_n}e^{i\zeta_n|z-z'|}, \tag{4.5}$$

where

$$\zeta_n = \sqrt{\Omega^2-\lambda_n}, \qquad \mathrm{Re}\zeta_n \geq 0, \quad \mathrm{Im}\zeta_n \geq 0. \tag{4.5a}$$

Equation (4.5) conveys a modal representation for the *complete* Green function of the *complete* problem. Since $Q(x)$ is assumed to vary on the micro-scale the question of a reduced, or smoothed, Green function arises. One obvious answer can be to smooth (4.5),

$$\begin{aligned} G^s(x,z\,;x',z') &= \mathbf{P}_j G(x,z\,;x',z') \qquad (\mathbf{P}_j \text{ operates on the } x\text{-dependence}) \\ &= \frac{i}{2}\sum_{n=1}^{N} \frac{u_n^s(x)u_n(x')}{\zeta_n}e^{i\zeta_n|z-z'|}, \end{aligned} \tag{4.6}$$

where N is chosen according to the smoothing length-scale 2^j. Clearly, there is a conceptual problem with (4.6): reciprocity is lost ($G(r,r') \neq G(r',r)$). Furthermore, the x' dependence is still described on the micro-scale and a knowledge of the *complete* modes is needed to correctly obtain it.

To address the issue systematically one must first derive an *effective* boundary value problem that can be identified as the transverse modal formulation associated with (4.1). To preserve reciprocity, the former should be self-adjoint. Under the conditions for which $\lambda_n = \lambda_n^*$ (see the end of section 3.6), we identify (3.38b) or (3.33) as the appropriate effective boundary value problem and repeat the steps in (4.4)–(4.5a). The result is the *effective* Green function

$$G^{(\mathrm{eff})}(x,z\,;x',z') = \frac{i}{2}\sum_{n=1}^{N} \frac{u_n^s(x)u_n^s(x')}{\zeta_n}e^{i\zeta_n|z-z'|} \tag{4.7}$$

which possesses the correct form. Here again summation must be restricted to the first few modes (see section 3.6.1). Note that $G^{(\mathrm{eff})}$ can be expressed also as

$$G^{(\mathrm{eff})}(x,z\,;x',z') = \mathbf{P}_j\mathbf{P'}_j G(x,z\,;x',z'), \tag{4.8}$$

where $\mathbf{P}_j$ and $\mathbf{P'}_j$ act on the x and x' dependencies, respectively.

5. Numerical example. In this section we demonstrate the results presented in section 3.6. We start by checking the spectral equivalence relation described by (3.48a)–(3.48b) for a fixed but small micro-scale. The quality of the spectral equivalence as a function of the micro-scale will be examined afterwards. Thus, we start by choosing two functions, namely, $Q_1(x)$ and $Q_2(x)$, as two test cases for synthesizing the complex heterogeneity:

$$\text{(5.1a)} \qquad \text{case 1:} \quad Q(x) = Q_1(x) = 1 + a\cos(100\pi x);$$

$$\text{(5.1b)} \qquad \text{case 2:} \quad Q(x) = Q_2(x) = 1 + a\sin(\pi x)\sin(100\pi x).$$

The characteristic length-scale of the inner structure is, roughly, 1/100 in both cases. The factor a determines the microstructure magnitude—the latter vanishes when $a = 0$. $q(x)$ vanishes at the boundaries in case 2, but not in case 1. Since the smoothing operator $\mathbf{P}_j$ practically performs local spatial integration over intervals of length larger than the micro-scale (say 1/16), a good approximation of $Q^{(\text{eff})}(x)$ can be derived analytically using standard tables of integrals. The effective measures are given by

$$\text{(5.2a)} \qquad \text{case 1:} \quad Q^{(\text{eff})}(x) = Q_1^{(\text{eff})}(x) = \sqrt{1-a^2};$$

$$\text{(5.2b)} \qquad \text{case 2:} \quad Q^{(\text{eff})}(x) = Q_2^{(\text{eff})}(x) = \sqrt{1-a^2\sin^2(\pi x)}.$$

The functions $Q_{1,2}(x)$ are shown in Figure 5.1 together with the respective effective measures $Q_{1,2}^{(\text{eff})}(x)$, for $a = 0.5$.

Let us demonstrate the relations between u_n, λ_n and u_n^*, λ_n^* numerically, for the above case of a fixed and small micro-scale. We start with case 1 and Dirichlet boundary conditions. Figure 5.2(a) compares u_n to u_n^* for $n = 1$ and $n = 10$. For this set of parameters, $\epsilon = \ell/L_n^* \ll 1$, so (3.48a)–(3.48b) predict an approximate spectral equivalence. The microstructure magnitude is $a = 0.9$. As predicted in section 3.6, $(u_n)^s = u_n^*$; see (3.48a). Figure 5.2(b) compares $\sqrt{\lambda_n}/\pi$ to $\sqrt{\lambda_n^*}/\pi$ vs. a for the first 10 modes. The equality predicted in (3.48b) is evident. Note that for $a = 0$ (no microstructure) we find $\sqrt{\lambda_n} = \sqrt{\lambda_n^*} = n\pi$, and the lines "bend down" as the microstructure magnitude increases. These phenomena demonstrate that microstructure heterogeneity can have a profound effect on the eigenvalues. As the figure shows, however, this effect can be introduced into the boundary value problem by using the effective (smooth) measure $Q^{(\text{eff})}$ instead of the complex Q. Indeed, the relation predicted by (3.48b) for small $\ell/L_n^* : \lambda_n = \lambda_n^*$, is evident for the entire range of a. Figure 5.3 shows the same, but for case 2 with Dirichlet boundary conditions. Figures 5.4 and 5.5 show the same, for cases 1 and 2, respectively, but with Neumann boundary conditions. All the results are consistent with the relation predicted by (3.48a)–(3.48b) and also demonstrate that microstructure heterogeneity can have a profound effect on the eigenvalues.

Figure 5.6 compares the eigenfunctions u_n to u_n^* for case 1 with symmetric impedance boundary conditions $\alpha_1 = \beta_1 = \alpha_2 = \beta_2 = 1$. Three modes are depicted: $n = 1, 3,$ and 10. The first corresponds to a negative eigenvalue. The results are in agreement with (3.49a). Similar behavior was observed for the corresponding eigenvalues. Figure 5.7 shows the modes and eigenvalues of case 1 with the natural impedance boundary conditions. The results are in good agreement with what is anticipated in (3.48a)–(3.48b).

We turn now to check the spectral equivalence as a function of the micro-scale.

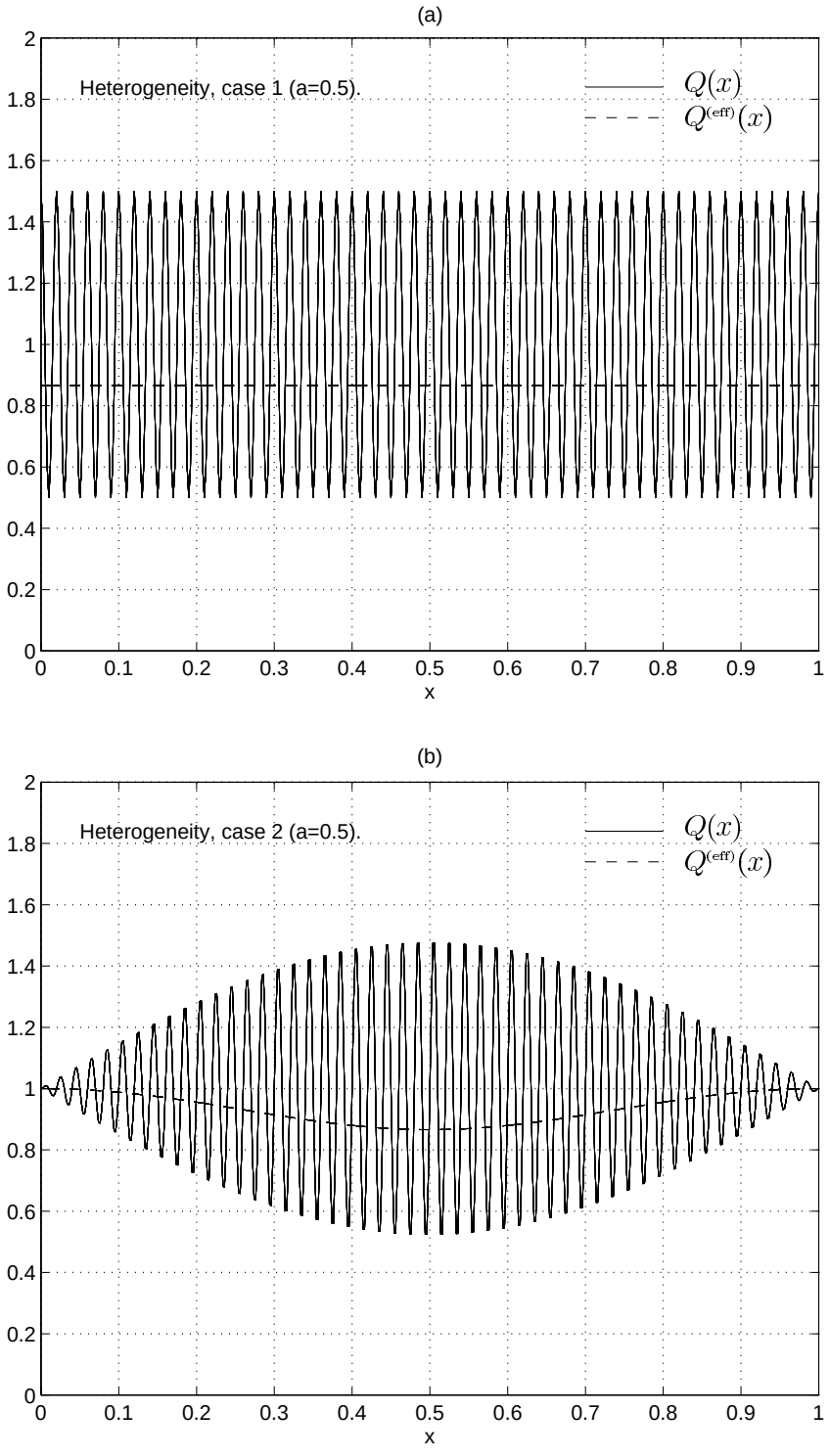

FIG. 5.1. *Examples of $Q(x)$ (solid line) and its effective measure $Q^{(\mathrm{eff})}(x)$ (dashed line) for $a = 0.5$.* (a) *case* 1 (*equations* (5.1a) *and* (5.2a)). (b) *case* 2 (*equations* (5.1b) *and* (5.2b)).

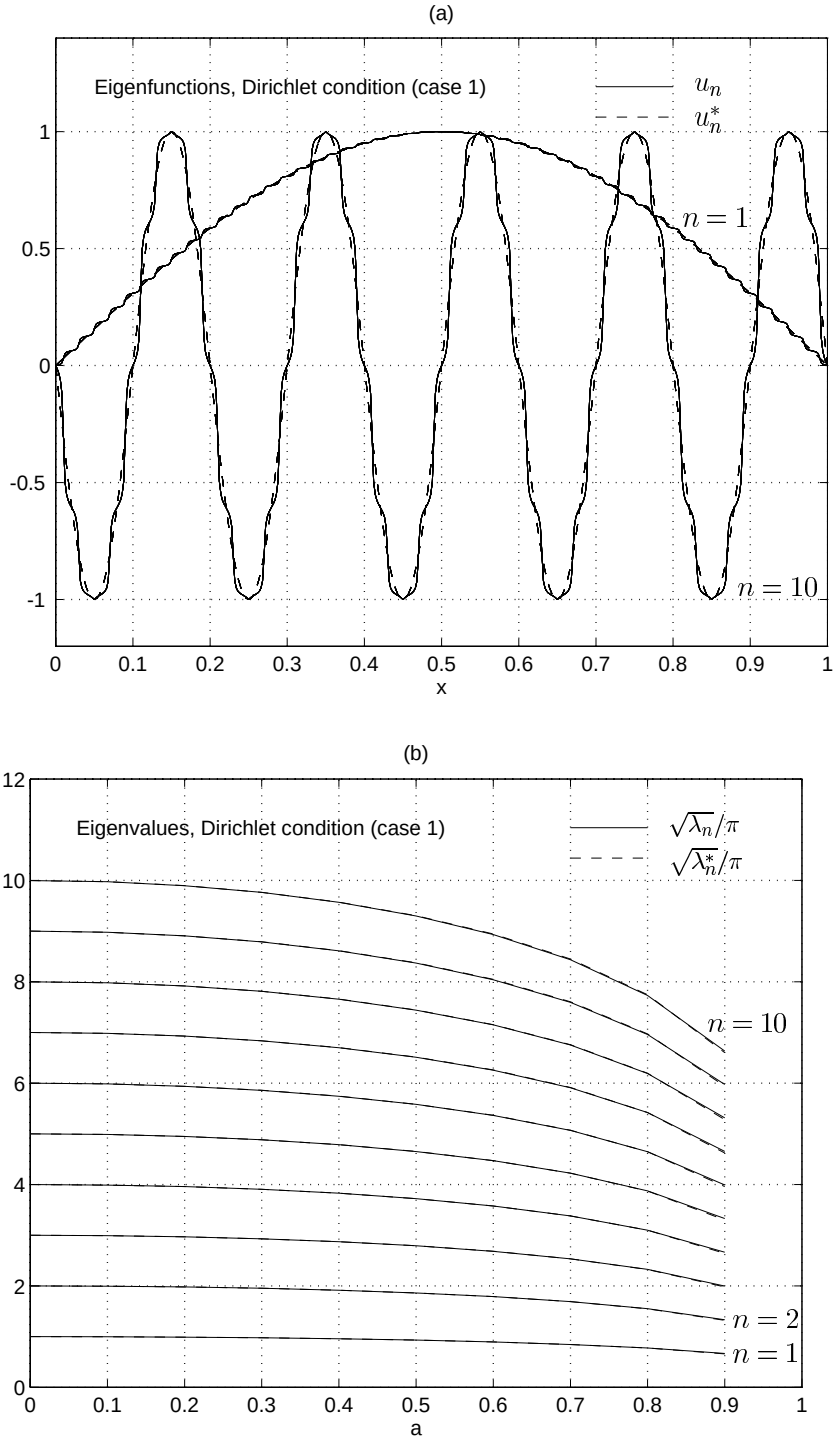

FIG. 5.2. *Eigenfunctions and eigenvalues of the complete problem* (3.38a) *and the effective problem* (3.38b)*, for case* 1 *with Dirichlet boundary conditions.* $Q(x)$ *and* $Q^{(\mathrm{eff})}(x)$ *are shown in Figure* 5.1(a). (a) $u_n(x)$ *(solid line) and* $u_n^*(x)$ *(dashed line) for* $n = 1, 10$. (b) $\sqrt{\lambda_n}/\pi$ *(solid line) and* $\sqrt{\lambda_n^*}/\pi$ *(dashed line) vs. a for the first* 10 *modes.*

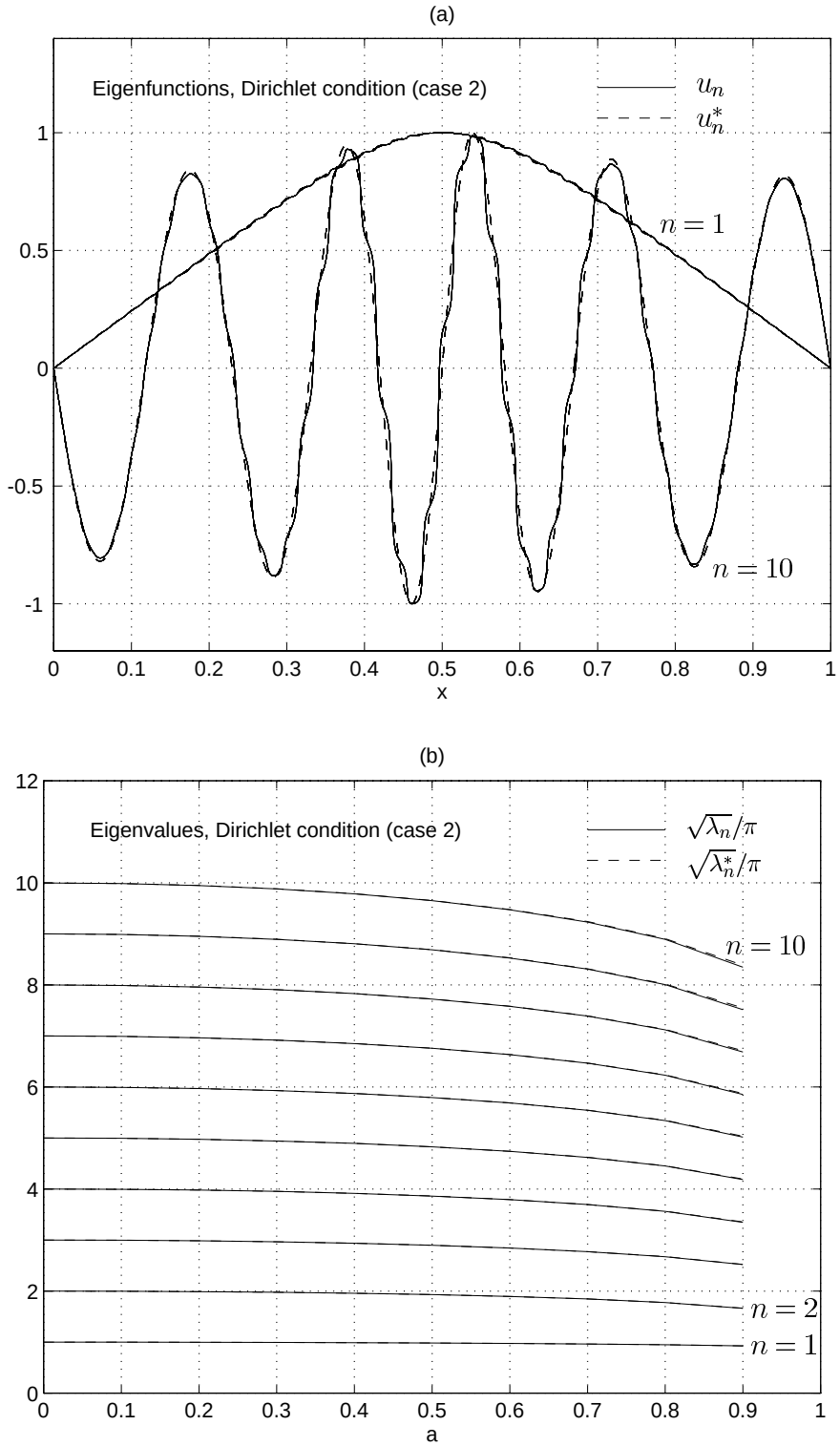

FIG. 5.3. *The same as Figure* 5.2*, but for case* 2 *with Dirichlet boundary conditions.*

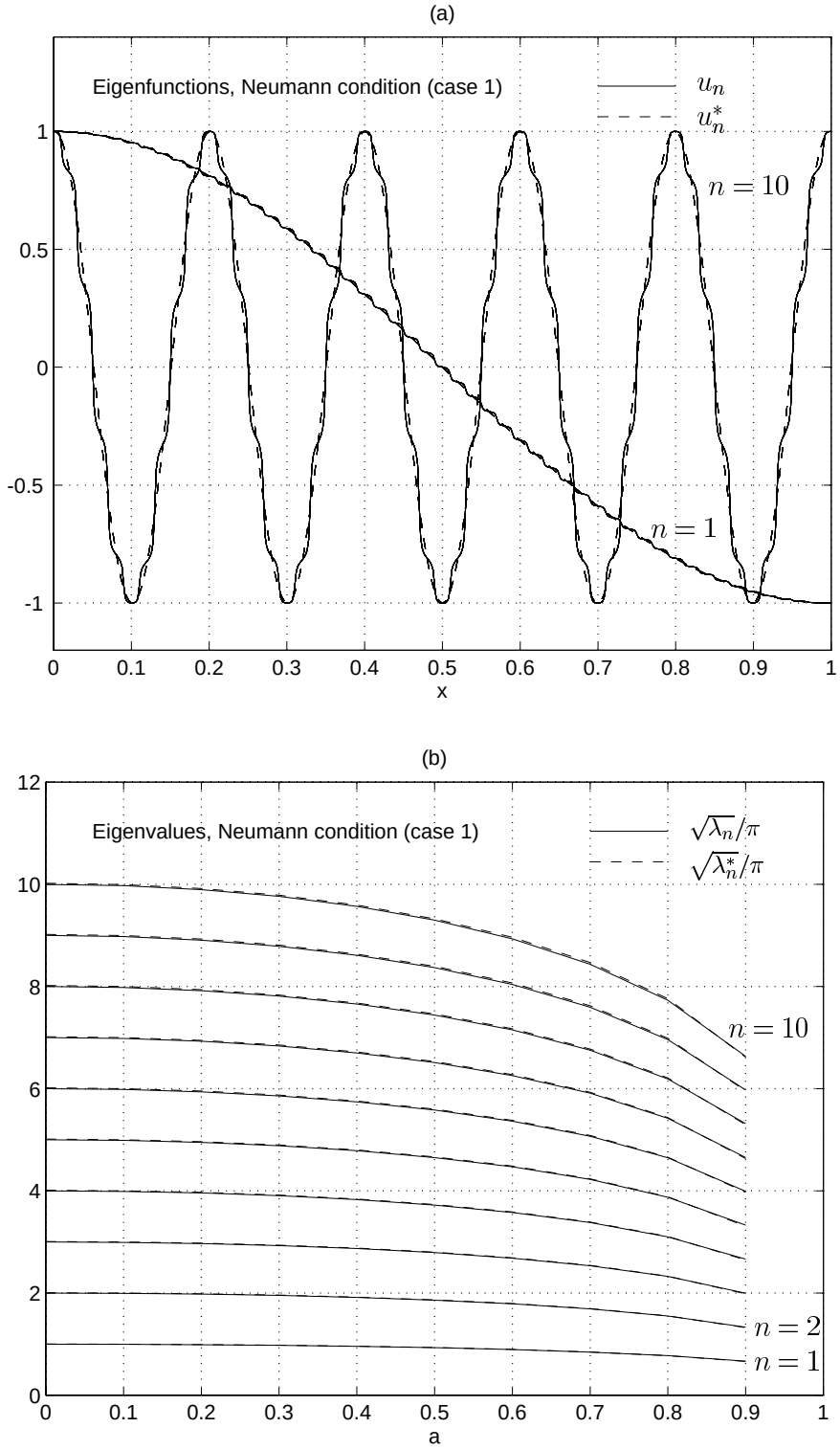

FIG. 5.4. *The same as Figure* 5.2*, but for case* 1 *with Neumann boundary conditions.*

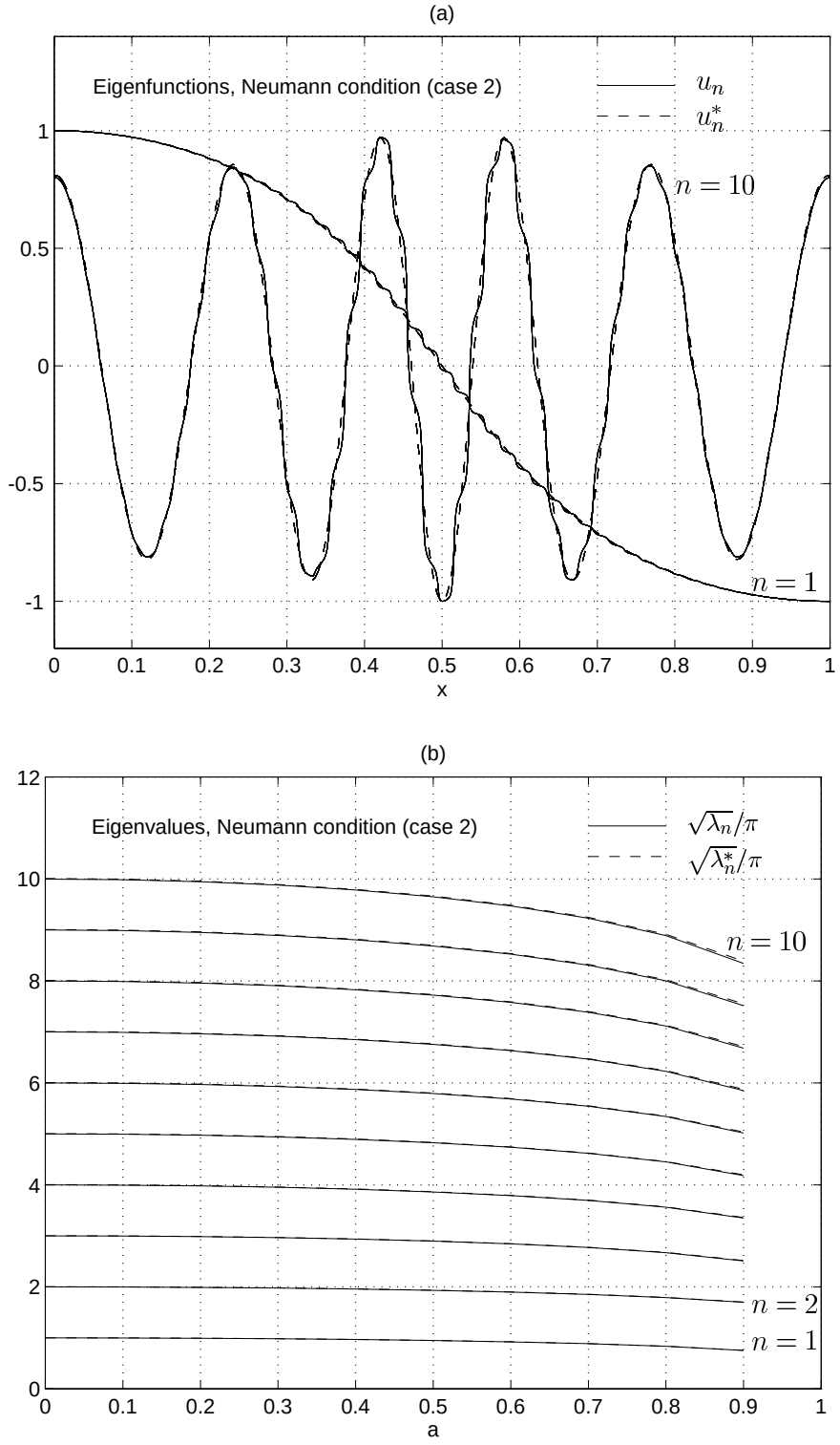

FIG. 5.5. *The same as Figure* 5.2*, but for case* 2 *with Neumann boundary conditions.*

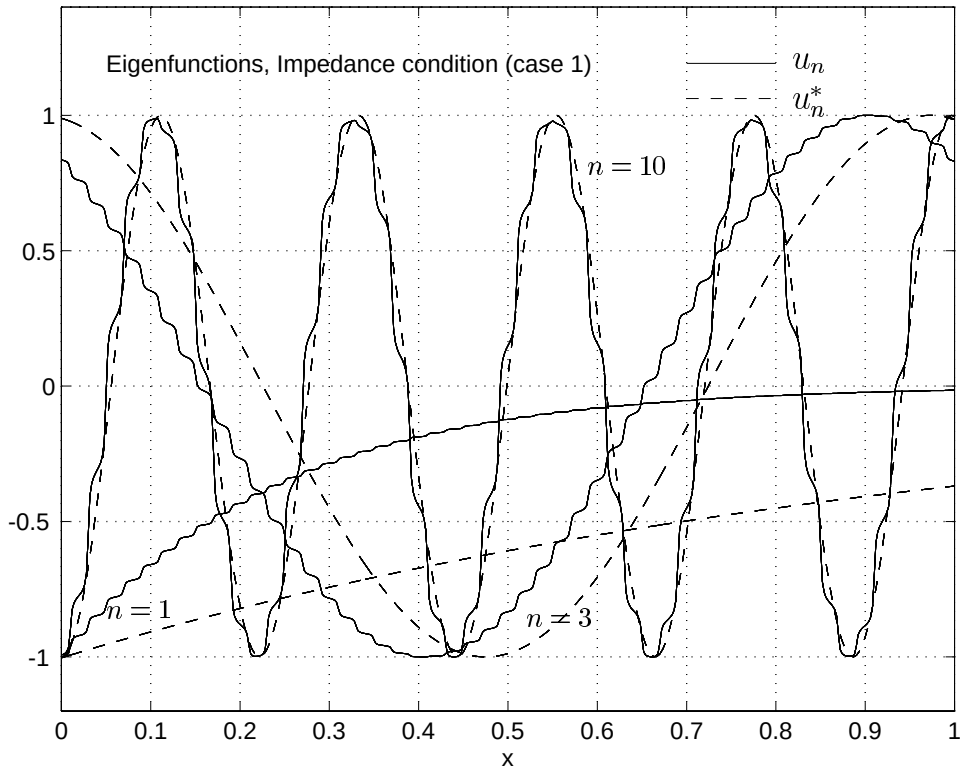

FIG. 5.6. *The same as Figure* 5.2(a)*, but for case* 1 *with impedance boundary conditions. Shown are the first, third, and tenth eigenfunctions.*

Toward this end, we choose

$$Q(x) = 1 + 0.5\cos(\kappa\pi x) \tag{5.3}$$

with Dirichlet boundary conditions, and compare λ_n^* to λ_n for a set of κ values. The associated length-scale is given, roughly, by $1/\kappa$. Figure 5.8 shows the relative difference

$$\left|\frac{\lambda_n^* - \lambda_n}{\lambda_n}\right| \tag{5.4}$$

as a function of the mode order n, for $\kappa = 20$ to $\kappa = 100$ in steps of 10. It is seen that the relative difference is kept below 1% for $n \leq \kappa/4$. Similar results were obtained for the modes.

6. Conclusions. The effective properties of a complex boundary value problem were studied. We have developed a new formulation with a slowly varying coefficient $Q^{(\text{eff})}(x)$, whose solution is identical to the large scale component of the solution to the generic boundary value problem. A key issue in such a study is the appropriate representation of the boundary conditions; since the latter are written as values of the *complete* solution at two isolated points, they cannot be directly applied to the large scale formulation, as the latter is written on the large scale solution component only. We have addressed this difficulty by rewriting the boundary value problem

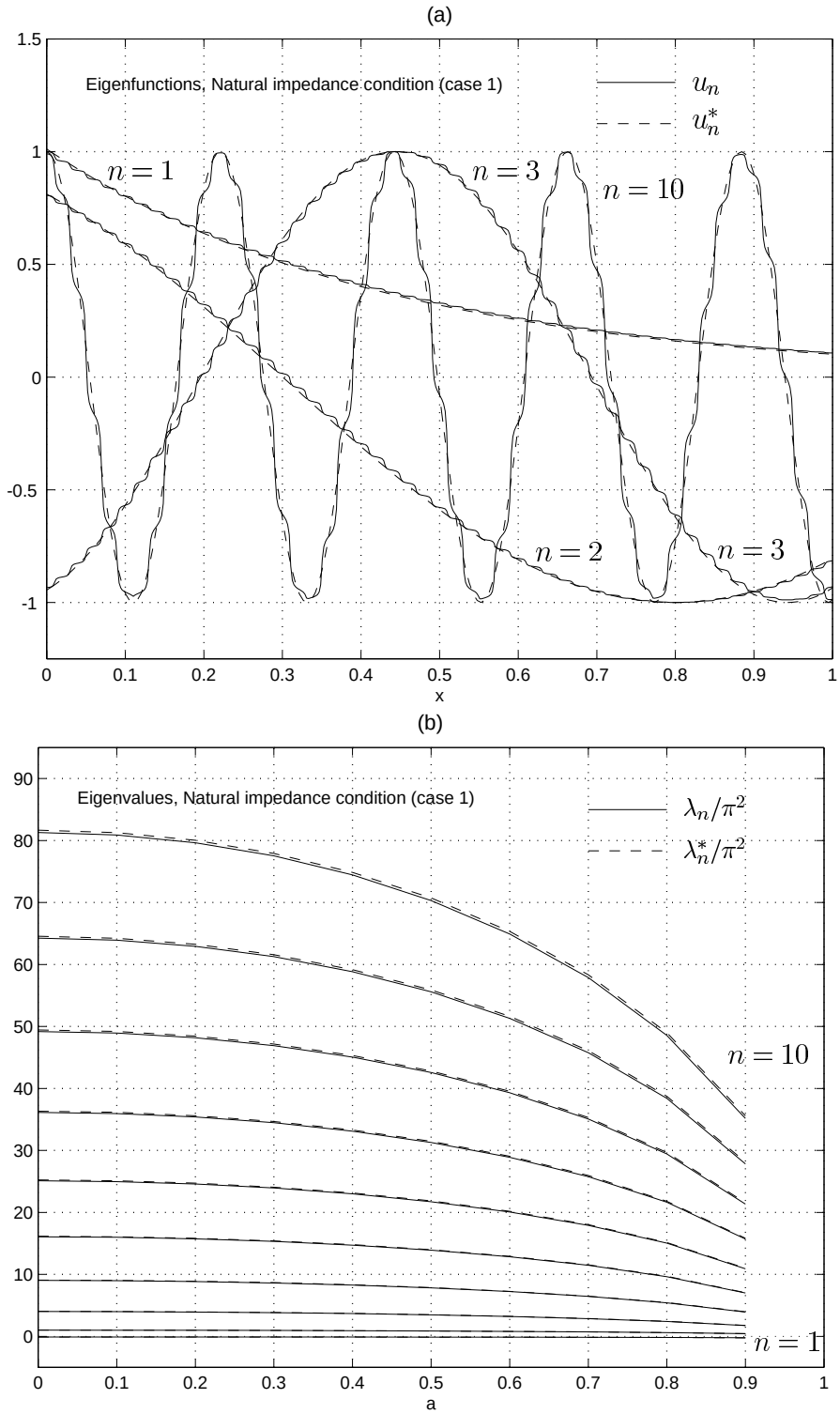

FIG. 5.7. *The same as Figure* 5.2*, but for case* 1 *with the natural impedance boundary conditions.*

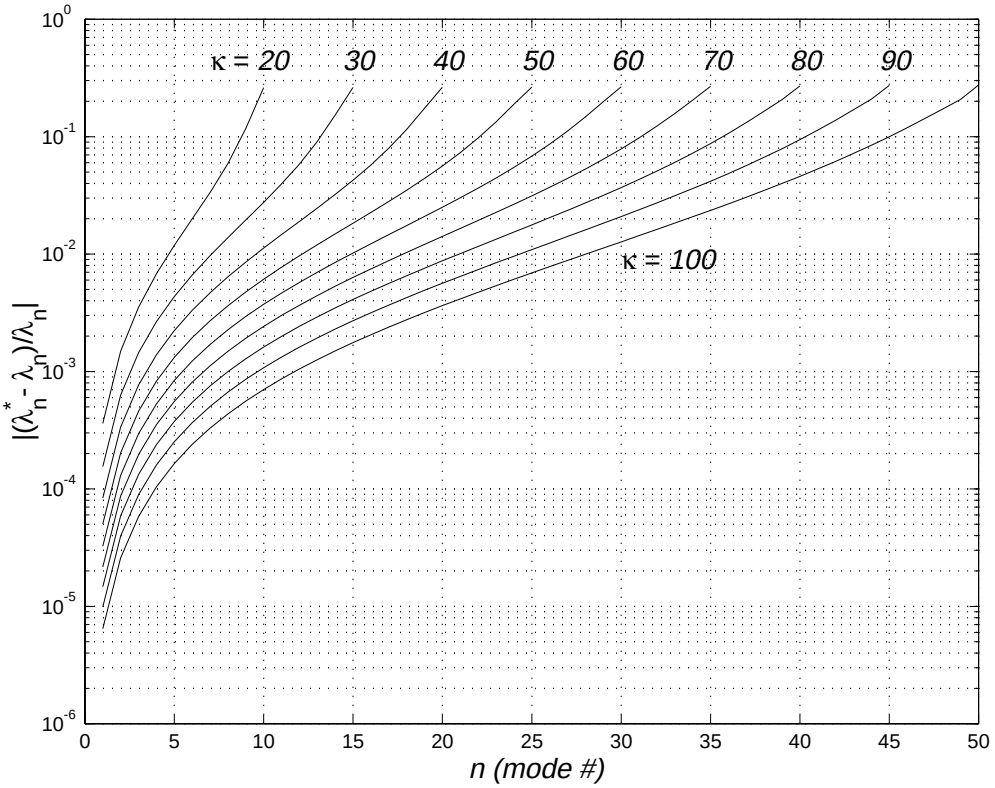

FIG. 5.8. *A comparison of λ_n^* to λ_n, as a function of n, for a set of micro-scales $\ell = 1/\kappa$.*

as a second kind Fredholm integral equation formulation. The latter is known to incorporate boundary conditions inherently and in a "natural way." Such an integral equation formulation can be straightforwardly achieved for homogeneous Neumann or Dirichlet conditions, or when the heterogeneity $q(x)$ vanishes at the boundaries. Its derivation in the more general case of impedance boundary conditions *and* $q(x)$ that does not vanish at the boundaries is not always possible. In these cases the formulation can be derived only when the determinant Δ in (3.16) does not vanish. Cases in which $\Delta = 0$ are more subtle and will be addressed elsewhere.

We have derived an effective measure $Q^{(\mathrm{eff})}(x)$ for the case of $\Delta \neq 0$. Then, the effective boundary value problem possesses the same form as the generic one, with $Q(x)$ replaced by $Q^{(\mathrm{eff})}(x)$ and with the same boundary conditions (as the integral kernel structure is preserved). In these cases we have studied the relation between the eigenfunctions and eigenvalues of the generic problem (u_n, λ_n), and these of the effective problem (u_n^*, λ_n^*). It has been shown that for homogeneous Neumann or Dirichlet conditions, or for the natural impedance boundary conditions, (u_n^*, λ_n^*) constitute a good approximation to (u_n^s, λ_n) in the limit of small micro-scale.

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