HETEROGENEOUS SYSTEMS IN *d* DIMENSIONS: LOWER SPECTRUM

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Abstract

The lower part of the spectrum of the Helmholtz equation for a heterogeneous system in a finite region in *d* dimensions, where the solutions to the corresponding homogeneous system are known, can be systematically approximated by means of iterative methods. These methods only require the specification of an arbitrary ansatz and converge to the desired solution, regardless of the strength of the inhomogeneities, provided the ansatz has a finite overlap with it. In this paper, different boundary conditions at the borders of the domain are assumed, and some applications are used to illustrate the methods.

1. Introduction

Consider the properties of heterogeneous systems in one or more dimensions, satisfying the Helmholtz equation

$$(-\Delta_d)\Psi_n(\mathbf{x}) = E_n\Sigma(\mathbf{x})\Psi_n(\mathbf{x}), \tag{1.1}$$

where $\mathbf{x} \equiv (x_1, \ldots, x_d)$, Δ_d is the Laplacian in a region Ω_d in d dimensions, $\Sigma(\mathbf{x}) > 0$ is the density and $\Psi_n(\mathbf{x})$ and E_n are the eigenfunctions and eigenvalues of the equation, respectively. The eigenfunctions of the equation satisfy appropriate conditions on the boundary $\mathbf{x} \in \partial\Omega_d$.

Some heterogeneous systems are naturally present in nature, where the density of the medium has typically random or granular properties, but they can also be artificially created in the laboratory, usually with periodic properties. In particular, the study of composite materials, built of alternating homogeneous layers of materials with different properties, such as density, conductivity, refraction index, etc, is now-a-days gaining importance in different areas of physics and engineering.

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Examples of these systems are numerous, and a full account of the bibliography on the subject is outside the scope of this paper. Some of these problems are: composite membranes [11, 12, 15, 16, 25], periodic multi-layered acoustic waveguides [1], elastic properties in layered media [7, 8, 17, 19, 21, 22], photonic crystals [14] and acoustic waves in strongly heterogeneous porous structures [20], to mention but a few. Both from a physical and a mathematical viewpoint, particularly interesting is the case of periodically layered composite materials, where the typical scale of the microstructure (that is, the period of the layers) is much smaller than the macroscopic scale of the object. The understanding of the macroscopic properties of such systems in terms of their microscopic features is the fundamental goal of the *homogenization method* (see [18] and the references therein).

Here, the current analysis is restricted to the class of problems described by equation (1.1), which is a subset of the general problems listed above, although the basic ideas of the method might be used in more general situations. The goal is to devise a method which allows one to obtain arbitrarily precise approximations to the eigenfunctions and eigenvalues corresponding to the lower part of the spectrum, regardless of the specific details of the problem under consideration, such as the geometrical properties of Ω_d (for $d \neq 2$, the method requires that the solutions to the homogeneous problem are known), the boundary conditions and, even more crucially, the density.

An iterative method is described here, which progressively builds one of the eigenfunctions of equation (1.1) corresponding to the lower states, starting from an almost arbitrary ansatz.

Some of the salient features of this approach are the following:

- the method applies to d-dimensional regions where an orthonormal basis of the Laplacian is known, with the exception of $d = 2$, where this limitation can be circumvented using a conformal mapping which transforms the original simply connected region into a region with a known basis;
- different boundary conditions on $\partial\Omega_d$ can be enforced;
- the convergence of the method is not limited to cases where mild inhomogeneities are present; in other words, the method is truly nonperturbative;
- the rate of convergence can be increased using a judicious choice of the initial ansatz, which can also include variational parameters;
- if the density depends on some perturbative parameter λ, and it reduces to the homogeneous case for $\lambda \to 0$, the iterative method allows one to extract the perturbative expansion for the eigenfunction and eigenvalue of the targeted state to any order with an appropriate number of iterations.

All these aspects are illustrated in this paper, considering examples in one and two dimensions. In particular, the case of a one-dimensional problem with rapidly oscillating density and different boundary conditions (such as Dirichlet, mixed Dirichlet–Neumann, Neumann and periodic) is examined; the *exact* asymptotic

behaviour of the lower eigenvalues of equation (1.1) is analysed when the size of the microstructure goes to zero. For the case of Dirichlet boundary conditions, some results were previously published as a special case [3, 9].

The paper is organized as follows: in Section 2, the proposed method is described and related theorems are proven, which apply both to the case where the spectrum of the problem does not contain a zero mode and to the case where a zero mode is present; Section 3 illustrates a few applications of the method in one and two dimensions. The paper concludes with a discussion on some possible extensions of the present work in Section 4.

2. The method

In this section, different approaches are described, which can be used to obtain approximations to the normal modes of the Helmholtz equation for a d-dimensional region with a variable density. The techniques that are used do not require that the inhomogeneities are small, and that the convergence towards the targeted state is always granted. The choice of a suitable ansatz containing variational parameters may increase the convergence.

Consider a region of space in d dimensions, Ω_d, and a density $\Sigma(\mathbf{x}) > 0$ which varies over Ω_d; let $\Xi^{(0)}(\mathbf{x})$ be an arbitrary function defined on Ω_d, which has an overlap with the lowest mode of the Helmholtz equation (1.1), $\Psi_n(\mathbf{x})$, where n is the set of numbers which specify an eigenfunction.

We assume that the spectrum of equation (1.1) does not contain a zero mode (a mode with vanishing eigenvalue) and, therefore, its eigenfunctions obey specific boundary conditions on $\partial\Omega_d$; in one dimension, for instance, only Dirichlet boundary conditions at both ends, or mixed Dirichlet and Neumann boundary conditions at each end are allowed.

Let $G(\mathbf{x}; \mathbf{y})$ be the Green's function of the homogeneous problem on Ω_d, obeying the same boundary conditions as Ψ. We call $\Psi_0(x_1, \ldots, x_d)$ the eigenfunction of the fundamental mode.

Under these assumptions, we have the following theorem.

THEOREM 2.1 (Spectrum without zero mode). *For $p \to \infty$, the sequence of functions*

$$\Xi^{(p)}(\mathbf{x}) = \sqrt{\Sigma(\mathbf{x})} \int_{\Omega_d} G(\mathbf{x}; \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} \Xi^{(p-1)}(\mathbf{y}) \, d^d y \qquad (2.1)$$

converges to the lowest mode of equation (1.1), *having an overlap with $\Xi^{(0)}$. In particular, if $\Xi^{(0)}$ has an overlap with the fundamental mode of equation* (1.1), *then*

$$\Psi_0(\mathbf{x}) = \lim_{p \to \infty} \frac{\Xi^{(p)}(\mathbf{x})}{\sqrt{\Sigma(\mathbf{x})}}.$$

PROOF. The proof is simple: we may cast equation (1.1) in the form

$$\frac{1}{\sqrt{\Sigma(\mathbf{x})}}(-\Delta_d)\frac{1}{\sqrt{\Sigma(\mathbf{x})}}\Phi_n(\mathbf{x}) = E_n\Phi_n(\mathbf{x}), \qquad (2.2)$$

where $\Psi_n(\mathbf{x}) = \Phi_n(\mathbf{x})/\sqrt{\Sigma(\mathbf{x})}$. Notice that equations (1.1) and (2.2) are isospectral, and let

$$\hat{O} \equiv \frac{1}{\sqrt{\Sigma(\mathbf{x})}}(-\Delta_d)\frac{1}{\sqrt{\Sigma(\mathbf{x})}}$$

be the operator appearing on the left-hand side of equation (2.2). The spectrum of $\hat{O}$ is bounded from below and contains only positive eigenvalues; the ansatz $\Xi^{(0)}(x_1, \ldots, x_d)$ can be decomposed in the basis of the eigenfunctions of equation (2.2)

$$\Xi^{(0)}(\mathbf{x}) = \sum_n c_n \Phi_n(\mathbf{x}).$$

Equation (2.1) may be written as

$$\Xi^{(p)} = \hat{O}^{-1}\Xi^{(p-1)}, \tag{2.3}$$

where

$$\hat{O}^{-1} \equiv \sqrt{\Sigma(\mathbf{x})}(-\Delta_d)^{-1}\sqrt{\Sigma(\mathbf{x})}$$

is the inverse operator (that is, $\hat{O}\hat{O}^{-1} = \hat{O}^{-1}\hat{O} = \mathbf{1}$).

The spectrum of $\hat{O}^{-1}$ is positive and bounded both from below and from above; therefore, after p repeated applications of equation (2.3),

$$\Xi^{(p)}(\mathbf{x}) = \sum_n \frac{c_n}{E_n^p}\Phi_n(\mathbf{x}).$$

When $p \to \infty$, only the term with the lowest eigenvalue of $\hat{O}$ with nonvanishing coefficient c_n survives; this completes the proof of the theorem. $\qquad\square$

We need to separately discuss the case of a spectrum containing a zero mode (in one dimension, this case corresponds to Neumann or periodic boundary conditions). We assume that the spectrum of equation (1.1) contains a zero mode. Consider a d-dimensional region of space, Ω_d, and a density $\Sigma(x_1, \ldots, x_d) > 0$ which varies over Ω_d, and let $\Xi^{(0)}(x_1, \ldots, x_d)$ be an arbitrary function defined on Ω_d, which has an overlap with the lowest mode of the Helmholtz equation (1.1) with positive eigenvalue.

Let $G^{(0)}(x_1, \ldots, x_d; y_1, \ldots, y_d)$ be the *regularized* Green's function of the homogeneous problem on Ω_d, obeying the same boundary conditions as Ψ. The function $\Psi_0(x_1, \ldots, x_d)$ is called the eigenfunction of the zero mode, corresponding to the vanishing eigenvalue, and $\Psi_1(x_1, \ldots, x_d)$ the eigenfunction of the mode with smallest positive eigenvalue.

THEOREM 2.2 (Spectrum containing a zero mode). *For $p \to \infty$, the sequence of functions*

$$\tilde{\Xi}^{(p)}(\mathbf{x}) = \sqrt{\Sigma(\mathbf{x})}\int_{\Omega_d} G^{(0)}(\mathbf{x};\mathbf{y})\sqrt{\Sigma(\mathbf{y})}\Xi^{(p-1)}(\mathbf{y})\,d^dy, \tag{2.4}$$

$$\Xi^{(p)}(\mathbf{x}) = \tilde{\Xi}^{(p)}(\mathbf{x}) - \sqrt{\Sigma(\mathbf{x})}\frac{\int_{\Omega_d}\sqrt{\Sigma(\mathbf{y})}\tilde{\Xi}^{(p)}(\mathbf{y})\,d^dy}{\int_{\Omega_d}\Sigma(\mathbf{y})\,d^dy} \tag{2.5}$$

converges to the lowest mode of equation (1.1) *with positive eigenvalue having an overlap with* $\Xi^{(0)}$. *In particular, if* $\Xi^{(0)}$ *has an overlap with the mode with the smallest positive eigenvalue, then*

$$\Psi_1(\mathbf{x}) = \lim_{p \to \infty} \frac{\Xi^{(p)}(\mathbf{x})}{\sqrt{\Sigma(\mathbf{x})}}.$$

PROOF. First, we note that the explicit form of the eigenfunction of the zero mode is known, namely,

$$\Psi_0(\mathbf{x}) = 1/\sqrt{V_\Omega},$$

where V_Ω is the volume of Ω_d; this implies that

$$\Phi_0(\mathbf{x}) = \sqrt{\frac{\Sigma(\mathbf{x})}{V_\Omega}}.$$

As discussed by the current author in an earlier paper [6], it is convenient to define the modified operator

$$\hat{O}_\gamma \equiv \frac{1}{\sqrt{\Sigma(\mathbf{x})}}(-\Delta + \gamma)\frac{1}{\sqrt{\Sigma(\mathbf{x})}},$$

where $\gamma \to 0^+$; similarly, equation (1.1) can be modified as

$$(-\Delta + \gamma)\Psi_n(\mathbf{x}) = E_n\Sigma(\mathbf{x})\Psi_n(\mathbf{x}).$$

Thus, the presence of a zero mode is avoided when $\gamma > 0$.

The Green's function is now

$$G_\gamma(\mathbf{x}, \mathbf{y}) = \frac{1}{V_\Omega\gamma} + \sum_n' \frac{\phi_n(\mathbf{x})\phi_n(\mathbf{y})}{\epsilon_n + \gamma},$$

where V_Ω is the volume of the region Ω. Here, ϵ_n and ϕ_n are, respectively, the eigenvalues and eigenfunctions of the negative Laplacian on Ω, obeying the appropriate boundary conditions, and $\sum_n'$ is the sum over all possible modes, except the zero mode.

It is possible to expand the Green's function around $\gamma = 0$ as

$$G_\gamma(\mathbf{x}, \mathbf{y}) = \frac{1}{V_\Omega\gamma} + \sum_{q=0}^{\infty}(-1)^q\gamma^q G^{(q)}(\mathbf{x}, \mathbf{y}),$$

where

$$G^{(q)}(\mathbf{x}, \mathbf{y}) \equiv \sum_{n \neq 0} \frac{\phi_n(\mathbf{x})\phi_n(\mathbf{y})}{\epsilon_n^{q+1}}.$$

Observe that $G^{(0)}(\mathbf{x}, \mathbf{y})$ is the "regularized" Green's function discussed by the author in some earlier papers [4, 5] and, at this point, the current problem has been converted to the same form as in those papers. Therefore, the application of Theorem 2.1 using the shifted Green's function $G_\gamma(\mathbf{x}, \mathbf{y})$ could be used to obtain the power series expansions of the eigenvalue and the eigenfunction of the fundamental mode around

$\gamma = 0$. However, while this calculation is useful in the evaluation of the sum rules involving eigenvalues of $\hat{O}$ (see [6]), in the present case calculation of the first mode of $\hat{O}$ with a nonvanishing eigenvalue is emphasized.

First, Theorem 2.1 is applied to the shifted problem to obtain

$$\tilde{\Xi}^{(1)}(\mathbf{x}) = \sqrt{\Sigma(\mathbf{x})} \int_{\Omega_d} G_\gamma(\mathbf{x}, \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} \Xi^{(0)}(\mathbf{y}) \, d^d y. \tag{2.6}$$

Even if the starting ansatz is assumed to be independent of γ, $\tilde{\Xi}^{(1)}(\mathbf{x})$ contains terms which depend on $1/\gamma$. These terms, however, are only present if $\tilde{\Xi}^{(0)}(\mathbf{x})$ is not orthogonal to $\Phi_0(\mathbf{x})$. The effect of orthogonalizing $\tilde{\Xi}^{(1)}(\mathbf{x})$ with respect to $\Phi_0(\mathbf{x})$ is then to eliminate the factors which depend on $1/\gamma$. Moreover, if these terms are not present, one can work with the regularized Green's function $G^{(0)}$ rather than the full Green's function. As a matter of fact, the only way that the infinitesimal contributions of $G^{(q)}$ with $q = 1, 2, \dots$ could survive when $\gamma \to 0^+$ would be if they could interfere with divergent contributions going as $1/\gamma^q$, which, however, are absent due to the orthogonalization. As a result, equation (2.6) can be written in terms of the regularized Green's function $G^{(0)}$, and equations (2.4) and (2.5) follow.

At each iteration, the lowest energy components of the ansatz are inflated, and the component corresponding to the zero mode is removed by orthogonalization, which yields

$$\Psi_1(\mathbf{x}) = \lim_{p \to \infty} \frac{\Xi^{(p)}(\mathbf{x})}{\sqrt{\Sigma(\mathbf{x})}}.$$

This completes the proof of the theorem.   □

Theorems 2.1 and 2.2 are the extensions of the *power method (PM)* for approximating eigenvalues and eigenvectors of a finite Hermitian matrix to the case of a Hermitian operator (and, therefore, to the infinite-dimensional case).

As for the case of the PM, the rate of convergence of the iterated function towards the eigenfunction of the fundamental mode of equation (1.1) is essentially determined by the separation between the two largest eigenvalues of $\hat{O}^{-1}$.

These theorems apply to arbitrary regions in d dimensions, although they require the knowledge of the Green's function of the homogeneous problem corresponding to that region, and therefore of the spectrum of the associated homogeneous problem. In two dimensions, however, one can always reduce the original problem to an equivalent problem over a suitable region (that is, a region where a basis of functions is known) with the use of an appropriate conformal map.

3. Applications

Some applications of the theorems in Section 2 will be discussed in this section. The first two applications in one and two dimensions are simple, but they serve to illustrate the methods discussed in this paper to higher orders, obtaining highly precise results; the third application, which concerns one-dimensional heterogeneous systems with a highly oscillatory density and different boundary conditions, illustrates the effectiveness of this approach.

3.1. A string with parabolic density Let us consider a string with density [2]

$$\Sigma(x) = (1 + \alpha x)^2, \tag{3.1}$$

where $\alpha \leq 2/a$ and $|x| \leq a/2$. This particular density is chosen to illustrate the implementation of our theorems by limiting the technical difficulties. In the following calculations, it is assumed that $a = 1$ and $\alpha = 2$.

First, consider the case of Dirichlet boundary conditions and choose the ansatz

$$\xi^{(0)}(x) = \frac{\sqrt{105}}{8}(2x + 1)(1 - 4x^2).$$

In this case, it is straightforward to perform a very large number of iterations because of the polynomial form of the functions involved, and 105 iterations have been easily calculated, obtaining an estimate for the energy of the fundamental mode which is accurate up to 130 digits.

The precise value of $E_0^{(\text{exact})}$ after 100 iterations of Theorem 2.1 is

$$\begin{aligned}
E_0^{(\text{exact})} \approx\ & 7.73333653346596686390263803336783830309161196987161763020 \\
& 52519574462099730694722359688473360319830646138755000 \\
& 75565385500030558828\ldots.
\end{aligned}$$

Next, consider the case of Neumann boundary conditions and use the initial ansatz

$$\xi^{(0)}(x) = 2x + 1. \tag{3.2}$$

The precise value of $E_0^{(\text{exact})}$ after 105 iterations of Theorem 2.2 is

$$\begin{aligned}
E_0^{(\text{exact})} \approx\ & 12.1871394680951290047505723560039674407200495183458 \\
& 591999323057450689688696123459800390650121512407 \\
& 90737876149983\ldots.
\end{aligned}$$

Finally, consider the case of periodic boundary condition, using the same initial ansatz of equation (3.2).

The precise value of $E_0^{(\text{exact})}$ after 105 iterations of Theorem 2.2 is

$$\begin{aligned}
E_0^{(\text{exact})} \approx\ & 26.59255582932000052713762021489743577931546820189393\ldots.
\end{aligned}$$

3.2. A rectangular drum with density which varies along one direction Now Theorem 2.1 is applied to the two-dimensional problem of a rectangular region $(x, y) \in (-a/2, a/2) \times (-b/2, b/2)$ with Dirichlet boundary conditions at the border and with density as in equation (3.1).

In this case, the Green's function is

$$G^{(D)}(x, y; x', y') = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \frac{\psi_{n_x}^{(D)}(x)\phi_{n_y}^{(D)}(y)\psi_{n_x}^{(D)}(x')\phi_{n_y}^{(D)}(y')}{\epsilon_{n_x}^{(D)} + \eta_{n_y}^{(D)}}.$$
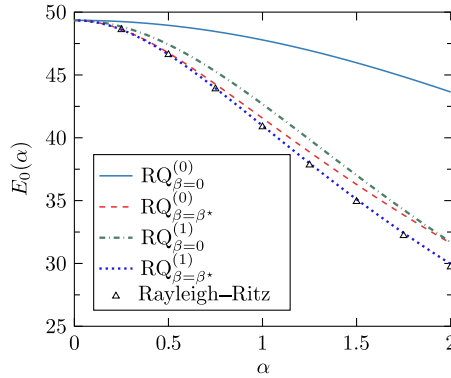
FIGURE 1. Approximate energy of the fundamental mode of a rectangular membrane with sides $a = 1$ and $b = 1/2$, with density (3.1). The solid and dashed lines are the values obtained using the bounds of equations (3.3) and (3.4), respectively, setting $\beta = 0$. The dot-dashed and dotted lines are the values obtained using the bounds of equations (3.3) and (3.4), respectively, setting $\beta = \beta^\star$. The triangles are the precise results obtained using the Rayleigh–Ritz method with 800 basis functions.

Here, $\psi_{n_x}(x)$ and $\phi_{n_y}(y)$ are the Dirichlet eigenfunctions of the one-dimensional negative Laplacian on $x \in (-a/2, a/2)$ and $y \in (-b/2, b/2)$, respectively, and $\epsilon_{n_x}^{(D)}$ and $\eta_{n_y}^{(D)}$ are the corresponding eigenvalues. The explicit expression for the two-dimensional Green's function can be found in the literature [4, 13].

The choice of the initial ansatz

$$\Xi^{(0)}(x, y) = (1 + \beta x) \sqrt{\Sigma(x, y)} \psi_1^{(D)}(x) \phi_1^{(D)}(y)$$

yields the upper bound for the energy of the fundamental mode as

$$E_0 \le E_0^{(\text{var})}(\beta) = \frac{\int \Xi^{(0)} \hat{O} \Xi^{(0)} \, dx \, dy}{\int \Xi^{(0)} \Xi^{(0)} \, dx \, dy}, \tag{3.3}$$

which has a minimum at a particular value, $\beta = \beta^\star$ (the explicit expressions of $E_0^{(\text{var})}(\beta)$ and $\beta^\star$ have been calculated explicitly, but those are not reported here for saving space).

A stricter bound for the energy of the fundamental mode can be derived using the function obtained after one iteration of Theorem 2.1:

$$E_0 \le \frac{\int \Xi^{(1)} \hat{O} \Xi^{(1)} \, dx \, dy}{\int \Xi^{(1)} \Xi^{(1)} \, dx \, dy}. \tag{3.4}$$

The explicit expressions for $\int \Xi^{(1)} \hat{O} \Xi^{(1)} \, dx \, dy$ and $\int \Xi^{(1)} \Xi^{(1)} \, dx \, dy$ are not reported here because of their lengthy form.

In Figure 1, the approximate energy of the fundamental mode of a rectangular membrane is plotted, with sides $a = 1$ and $b = 1/2$, and density given in equation (3.1). The solid and dashed lines are the values obtained using the bounds of equations (3.3)

and (3.4), respectively, setting $\beta = 0$. Similarly, the dot-dashed and dotted lines are the values obtained using the bounds of equations (3.3) and (3.4), respectively, setting $\beta = \beta^{\star}$. The triangles are the precise results obtained using the Rayleigh–Ritz method with 800 basis functions.

3.3. A string with rapidly oscillating density

The iterative methods that are described here can be applied to the study of inhomogeneous systems with a density which varies on a much smaller scale than the scale of the system itself. In particular, the behaviour of the system when the period of the density tends to zero is discussed here.

For simplicity, the present discussion is restricted to one dimension, and the Helmholtz equation

$$-\frac{d^2\psi}{dx^2} = E_n \Sigma_\epsilon(x) \psi_n(x) \tag{3.5}$$

is studied for an inhomogeneous system with density

$$\Sigma_\epsilon(x) \equiv \Sigma(x/\epsilon),$$

where $\Sigma(x)$ is a periodic function. The eigenfunctions $\psi_n(x)$ obey specific boundary conditions (such as Dirichlet, Neumann, periodic or mixed Dirichlet–Neumann).

The physical properties of the composite materials which can be modelled by these equations will depend both on the *microscale* (that is, the typical scale where the density changes) and on the *macroscale* of the system (that is, the typical size of the system itself). However, a numerical study of these systems is challenging, because the size associated with the discretization of the problem must clearly be much smaller than the size of the microscale, thus leading to a huge number of grid points. The *homogenization method* has been developed over the past 40 years to obtain an effective description of these systems (see, for example, [10, 18, 24]), which have important applications in several areas of physics and applied mathematics.

The approach described in this paper allows one to obtain systematic approximations to the lowest part of the spectrum of systems described by equation (3.5). For simplicity, let us consider a string of unit length with a rapidly oscillating density

$$\Sigma_\epsilon(x) = 2 + \sin\left[\frac{2\pi}{\epsilon}(x + \eta/2)\right], \tag{3.6}$$

where $\epsilon \to 0^+$ is the parameter determining the typical size of the oscillations of the density and η is an arbitrary phase.

This problem has been originally studied by Castro and Zuazua [9] for the case $\eta = 1$, obtaining explicit expressions for the lowest eigenvalues of this string up to order ϵ^3 using the WKB method. The author has reproduced these results [3] and has obtained the fundamental eigenvalue of the string up to order ϵ^5 [2].
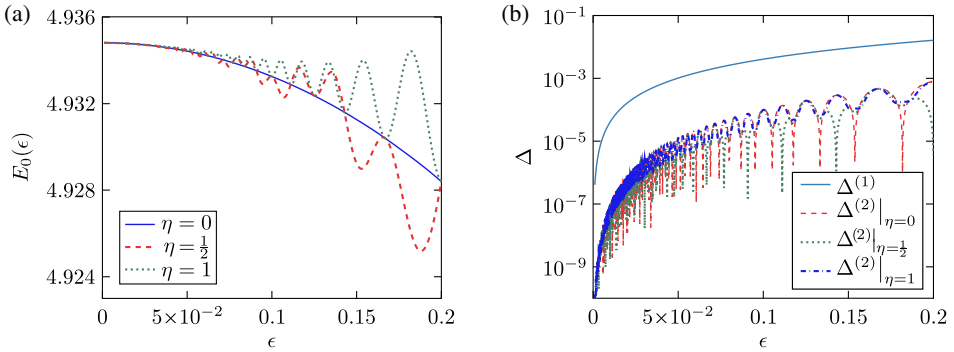
FIGURE 2. (a) Equation (3.8) for three different values of η; (b) mean square deviations obtained after one and two iterations for the string with density (3.6) using the initial ansatz (3.7).

3.3.1 *Dirichlet boundary conditions.* Here, the same ansatz [3]

$$\xi^{(0)}(x) = \sqrt{\Sigma(x)}\psi_1^{(DD)}(x) \tag{3.7}$$

is used, where

$$\psi_n^{(DD)}(x) \equiv \sqrt{2}\sin n\pi(x + 1/2)$$

are the Dirichlet eigenfunctions of the negative one-dimensional Laplacian.

In analogy with the previous calculation [3], applying Theorem 2.1 yields an expression for the lowest eigenvalue of the string, which is exact up to order ϵ^5 after two iterations:

$$\begin{aligned}
E_0 \approx {} & \frac{\pi^2}{2} - \frac{1}{64}\pi^2\epsilon^2 + \frac{1}{4}\pi\epsilon^3 \sin\left(\frac{\pi}{\epsilon}\right)\sin\left(\frac{\pi\eta}{\epsilon}\right) - \frac{15\pi^2\epsilon^4}{1024} \\
& + \frac{1}{512}\pi\epsilon^5\left[116\sin\left(\frac{\pi}{\epsilon}\right)\sin\left(\frac{\pi\eta}{\epsilon}\right) + 5\sin\left(\frac{2\pi}{\epsilon}\right)\cos\left(\frac{2\pi\eta}{\epsilon}\right)\right] \\
& + \cdots .
\end{aligned} \tag{3.8}$$

For $\eta = 1$, this result reduces to the one obtained in the paper [3]. The behaviour of E_0 for three different values of η is plotted in Figure 2.

Note that the Rayleigh quotients obtained using Theorem 2.1 form a monotonically decreasing sequence which converges to the exact eigenvalue of the fundamental mode as the number of the iterations goes to infinity. For this reason, the study of the Rayleigh quotient around $\epsilon = 0$ clearly leads to a hierarchy of contributions which correspond to the different powers of ϵ, possibly multiplied by functions which are not analytical at $\epsilon = 0$, but are bounded (see, for example, (3.8)). At a given iteration, it may happen, depending on the initial ansatz used, that the first few coefficients of the expansion have converged to the exact value; in this case, the contribution of the first term which has not yet converged must decrease at the next iteration. Since this must happen in an infinitesimal interval containing $\epsilon = 0$, it means that only even terms in ϵ

may decrease in the whole interval; in other words, the convergence of a term which is even in ϵ forces the convergence of the subsequent term in the expansion, which is odd in ϵ. This is observed in equation (3.8), which is exact up to the order ϵ^5.

Alternatively, one can obtain a bound on the error in the eigenvalue by calculating the mean square deviation using the function obtained after k iterations, $\xi^{(k)}(x)$ (clearly, Theorem 2.1 implies that $\lim_{k\to\infty} \Delta^{(k)} = 0$):

$$\Delta^{(k)} \equiv \sqrt{\frac{\int \xi^{(k)}(x)\hat{O}^2\xi^{(k)}(x)\,dx}{\int [\xi^{(k)}(x)]^2\,dx} - \left[\frac{\int \xi^{(k)}(x)\hat{O}\xi^{(k)}(x)\,dx}{\int [\xi^{(k)}(x)]^2\,dx}\right]^2}.$$

The mean square deviation corresponding to the first iteration is

$$\Delta^{(1)} = \tfrac{1}{64}\sqrt{7}\pi^2\epsilon^2 + O[\epsilon^3]$$

and it is plotted in Figure 2(b) together with $\Delta^{(2)}$.

Now, the ansatz of equation (3.7) is generalized to arbitrary states:

$$\xi_n^{(0)}(x) = \sqrt{\Sigma(x)}\psi_1^{(DD)}(x).$$

Although Theorem 2.1 only holds for the lowest state, it is useful to check if the functions obtained after one iteration are good approximations to the higher eigenmodes for $\epsilon \to 0$. Applying equation (2.1), $\xi_n^{(1)}(x)$ has been obtained explicitly, which is not reported here. To see if $\xi_n^{(1)}(x)$ are good approximations, the mean square deviation is estimated using these states; if we let $\epsilon \to 0^+$ keeping n fixed,

$$\Delta_n^{(1)} \approx \frac{\sqrt{7}}{64}\pi^2\epsilon^2 n^4 + O(\epsilon^3).$$

Therefore, $\xi_n^{(1)}(x)$ are good approximations if $\Delta_n^{(1)} \ll 1$, implying that $n \ll 1.25/\sqrt{\epsilon}$. Using this limit, an estimation is obtained for the eigenvalues of the lowest part of the spectrum by evaluating the expectation value of $\hat{O}$:

$$E_n \approx \langle\hat{O}\rangle_{\xi_n^{(1)}} \approx \frac{\pi^2 n^2}{2} - \frac{1}{64}\pi^2\epsilon^2 n^4 + \frac{1}{4}\pi\epsilon^3 n^4 \sin\left(\frac{\pi}{\epsilon}\right)\sin\left(\frac{\pi\eta}{\epsilon}\right) + O(\epsilon^4).$$

For $\eta = 1$, this result reproduces the estimate obtained in previous papers [3, 9].

3.3.2 *Neumann–Dirichlet and Dirichlet–Neumann boundary conditions.* Working in analogy with what we have done for Dirichlet boundary conditions in the previous case, we use the ansatz

$$\xi^{(0)}(x) = \sqrt{\Sigma(x)}\psi_1^{(ND)}(x),$$

where $\psi_n^{(ND)}(x)$ are the Dirichlet eigenfunctions of the negative one-dimensional Laplacian on $x \in (-1/2, 1/2)$.

Now Theorem 2.1 is applied and after two iterations the expressions for the eigenvalue of the fundamental mode have converged to order ϵ for $\epsilon \to 0$ as follows:

$$E_0^{(ND)} \approx \frac{\pi^2}{8} - \frac{1}{16}\pi\epsilon \cos\left(\frac{\pi(1-\eta)}{\epsilon}\right) + O(\epsilon^2). \tag{3.9}$$
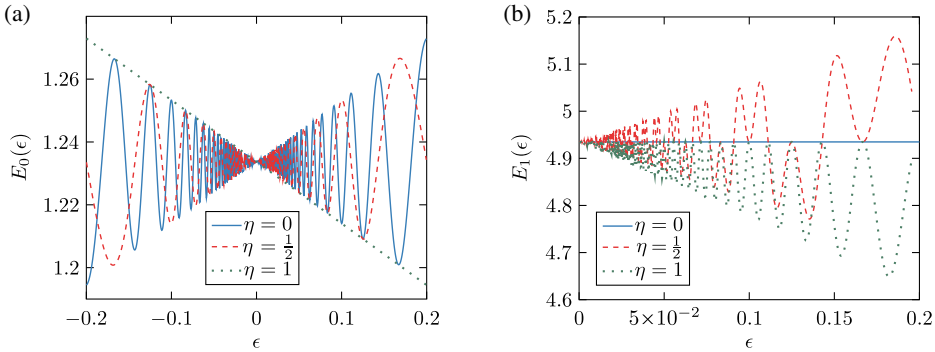
(a)

(b)

FIGURE 3. (a) Equation (3.9) for three different values of η; (b) equation (3.10) for three different values of η.

Notice that the convergence in this case is slower than that in the Dirichlet boundary conditions.

Observe that for $\epsilon \to -\epsilon$ and $\eta \to -\eta$, one gets $\Sigma(x) \to \Sigma(-x)$ to obtain the energy of the lowest mode for Dirichlet–Neumann boundary conditions:

$$E_0^{(DN)} \approx \frac{\pi^2}{8} + \frac{1}{16}\pi\epsilon \cos\left(\frac{\pi(\eta+1)}{\epsilon}\right) + O(\epsilon^2).$$

In Figure 3(a), we have the diagram for equation (3.9) for three different values of η (the curves for $\epsilon < 0$ may be viewed as the asymptotic expression for $E_0^{(DN)}$ with phase $-\eta$). As for the case of Dirichlet boundary conditions, the mean square deviations after one iteration is

$$\Delta^{(1)} = \left|\epsilon \cos\left(\frac{\pi(\eta-1)}{\epsilon}\right)\right| \frac{\pi}{64} \sqrt{\frac{1}{6}(\pi^4 - 96)} + O(\epsilon^2).$$

For a general state, the initial ansatz $\xi_n^{(0)}(x) = \sqrt{\Sigma(x)}\psi_n^{(ND)}(x)$ can be used, which yields the approximate expression for the nth eigenvalue after one iteration:

$$E_n^{(ND)} \approx \frac{\pi^2}{8}(1 - 2n)^2 - \frac{\pi}{16}\epsilon(1 - 2n)^2 \cos\left(\frac{\pi}{\epsilon} - \frac{\pi\eta}{\epsilon}\right) + O(\epsilon^2).$$

The corresponding mean square deviation in this case is

$$\Delta_n^{(1)} = \frac{\pi(1 - 2n)^2}{64\sqrt{6}} \sqrt{(\pi^4(1 - 2n)^4 - 96)} \left|\epsilon \cos\left(\frac{\pi(\eta-1)}{\epsilon}\right)\right| + O(\epsilon^2),$$

which, therefore, requires $n \ll \epsilon^{-1/4}$.

3.3.3 *Neumann boundary conditions.* This case is slightly more complicated, since the spectrum contains a zero mode. The implementation of the iterative method is done following Theorem 2.2 and using an initial ansatz orthogonal to the zero mode:

$$\xi^{(0)}(x) = \sqrt{\Sigma(x)}\psi_{1,2}^{(NN)}(x) - \frac{\int_{-a/2}^{a/2} \psi_{1,2}^{(NN)}(x)\Sigma(x)\,dx}{\int_{-a/2}^{a/2} \Sigma(x)\,dx} \sqrt{\Sigma(x)},$$
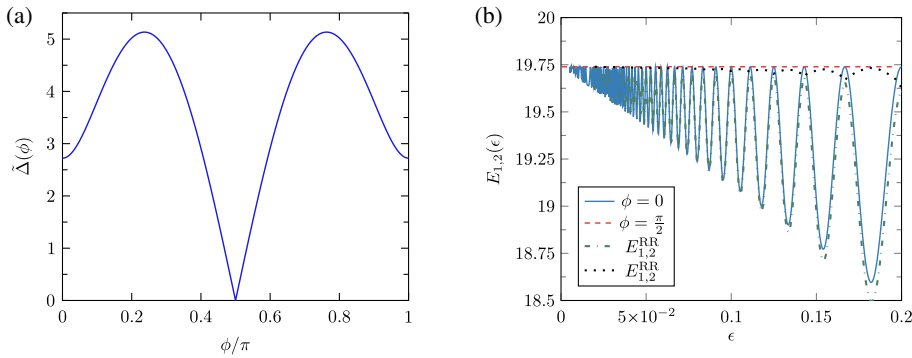
FIGURE 4. (a) Reduced mean square deviation $\tilde{\Delta}$ as a function of ϕ; (b) asymptotic behaviour of $E_{1,2}(\epsilon)$ for $\eta = 1$ obtained using Theorem 2.2 and numerical results obtained with the Rayleigh–Ritz method.

where $\psi_{n,u}^{(NN)}(x)$ are the eigenfunctions of the negative one-dimensional Laplacian, obeying Neumann boundary conditions. After one iteration,

$$E_0^{(\mathrm{NN})} \approx \frac{\pi^2}{2} - \frac{\pi\epsilon}{2} \sin\left(\frac{\pi}{\epsilon}\right) \sin\left(\frac{\pi\eta}{\epsilon}\right) + O(\epsilon^2). \tag{3.10}$$

Notice that for $\eta = 1$, this agrees with the approximate expression obtained by the author in an earlier work [4, equation (53)].

3.3.4 *Periodic boundary conditions.* In this case, the ansatz

$$\xi^{(0)}(x) = \sqrt{\Sigma(x)}(\cos\phi\,\psi_{1,1}^{(\mathrm{PP})}(x) + \sin\phi\,\psi_{1,2}^{(\mathrm{PP})}(x))$$
$$- \frac{\int_{-a/2}^{a/2}(\cos\phi\,\psi_{1,1}^{(\mathrm{PP})}(x) + \sin\phi\,\psi_{1,2}^{(\mathrm{PP})}(x))\Sigma(x)\,dx}{\int_{-a/2}^{a/2}\Sigma(x)\,dx}\sqrt{\Sigma(x)}$$

is used, where $\psi_{n,u}^{(\mathrm{PP})}(x)$ are the eigenfunctions of the one-dimensional negative Laplacian obeying periodic boundary conditions. Remember that these eigenfunctions are twice degenerate for $n > 0$; the ansatz is expressed in terms of the lowest two degenerate states.

Applying Theorem 2.2, after one iteration for $\epsilon \to 0$ the Rayleigh quotient provides the estimate for the lowest nontrivial eigenvalues as

$$E_{1,2}^{(\mathrm{PP})} = 2\pi^2 - 2\pi\epsilon\sin\left(\frac{\pi}{\epsilon}\right)\cos^2(\phi)\sin\left(\frac{\pi\eta}{\epsilon}\right) + O(\epsilon^2). \tag{3.11}$$

Using $\xi^{(1)}(x)$ for $\epsilon \to 0$, the mean square deviation is

$$\Delta^{(1)} = \frac{1}{3}\sqrt{\frac{2}{5}}\pi\left|\epsilon\cos(\phi)\sin\left(\frac{\pi}{\epsilon}\right)\sin\left(\frac{\pi\eta}{\epsilon}\right)\right|\sqrt{\pi^4 - 45\cos(2\phi) - 45} + O(\epsilon^2).$$

Figure 4(a) displays the quantity $\tilde{\Delta} \equiv |\cos(\phi)|\sqrt{\pi^4 - 45\cos(2\phi) - 45}$ as a function of the parameter ϕ, which controls the mixing of the degenerate states in the initial ansatz. As shown in the figure, the mean square deviation vanishes to order ϵ at $\phi = \pi/2$, while

it has a local minimum at $\phi = 0$. This suggests that the two lowest degenerate states of the homogeneous problem split at a finite ϵ into a state with constant energy (up to order ϵ) and a state with oscillating energy. Figure 4(b) displays the asymptotic formulas (3.11) for $\eta = 1$ (corresponding to $\phi = 0$ and $\phi = \pi/2$) and these can be compared with the numerical results obtained using the Rayleigh–Ritz method with a set of 101 states. The agreement between the analytical and the numerical results is evident. A similar agreement was also observed for the cases $\eta = 0$ and $\eta = 1/2$, although no figure has been included for these cases.

4. Conclusions

An iterative method has been devised which allows one to obtain arbitrarily precise solutions to the lowest eigenvalues and eigenfunctions of the Helmholtz equation for a heterogeneous medium in d dimensions, obeying different boundary conditions. The method requires the knowledge of the Green's function for the corresponding homogeneous problem and, therefore, it is limited to certain classes of domains (in two dimensions, however, one can apply it to arbitrary simply connected domains, which can be conformally mapped to a circle or to a square, and for which explicit expressions for the homogeneous Green's functions are available). A sequence of approximations which converges to the targeted solution is obtained by iteratively applying the inverse operator of equation (A.1) to an initial arbitrary ansatz with a finite overlap with the targeted state. Some applications in one and two dimensions are used to illustrate the method. In particular, an asymptotic behaviour of the lowest part of the spectrum of a string with a rapidly oscillating density is obtained when the size of the microstructure goes to zero for Dirichlet, Dirichlet–Neumann, Neumann and periodic boundary conditions.

Acknowledgements

Appendix A. Inverse operator

The spectrum of the operator

$$\hat{O} = \frac{1}{\sqrt{\Sigma(\mathbf{x})}} (-\Delta) \frac{1}{\sqrt{\Sigma(\mathbf{x})}}$$

on a d-dimensional region Ω_d is considered, where its eigenfunctions obey appropriate boundary conditions; depending on the boundary conditions, the spectrum may contain a zero mode.

Let us first consider the case in which a zero mode is not present, and let $G(\mathbf{x}, \mathbf{y})$ be the Green's function of the negative Laplacian on Ω_d, corresponding to the specific boundary conditions. We assume that $G(\mathbf{x}, \mathbf{y})$ is known exactly (which, in general, is

not true). Under these assumptions, it is straightforward to check that the operator

$$\hat{P}f = \sqrt{\Sigma(\mathbf{x})} \int G(\mathbf{x}, \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y \tag{A.1}$$

is the inverse of $\hat{O}$. In fact,

$$
\begin{aligned}
\hat{O}\hat{P}f &= \frac{1}{\sqrt{\Sigma(\mathbf{x})}}(-\Delta) \int G(\mathbf{x}, \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y \\
&= \frac{1}{\sqrt{\Sigma(\mathbf{x})}} \int \delta(\mathbf{x} - \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) = f(\mathbf{x}) \, d^d y.
\end{aligned}
$$

The case of a zero mode being present is more delicate. There, it is assumed that $G(\mathbf{x}, \mathbf{y})$ is the regularized Green's function, which does not contain the divergent contribution of the zero mode. This yields

$$(-\Delta)G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) - \frac{1}{V_\Omega}$$

and

$$
\begin{aligned}
\hat{O}\hat{P}f &= \frac{1}{\sqrt{\Sigma(\mathbf{x})}}(-\Delta) \int G(\mathbf{x}, \mathbf{y}) \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y \\
&= \frac{1}{\sqrt{\Sigma(\mathbf{x})}} \int \left[\delta(\mathbf{x} - \mathbf{y}) - \frac{1}{V_\Omega} \right] \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y \\
&= f(\mathbf{x}) - \frac{1}{V_\Omega} \frac{1}{\sqrt{\Sigma(\mathbf{x})}} \int \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y.
\end{aligned}
$$

Therefore, for a generic f, the operator $\hat{P}$ is not the inverse of $\hat{O}$. However, if $f(\mathbf{x})$ is orthogonal to the zero mode, whose eigenfunction is precisely $\sqrt{\Sigma(\mathbf{x})}$, then it follows that $\int \sqrt{\Sigma(\mathbf{y})} f(\mathbf{y}) \, d^d y = 0$, and $\hat{P}$ behaves as $\hat{O}^{-1}$.

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