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Separation of Variables in Deformed Cylinders[1]

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We study the Laplace operator subject to Dirichlet boundary conditions in a two-dimensional domain that is one-to-one mapped onto a cylinder (rectangle or infinite strip). As a result of this transformation the original eigenvalue problem is reduced to an equivalent problem for an operator with variable coefficients. Taking advantage of the simple geometry we separate variables by means of the Fourier decomposition method. The ODE system obtained in this way is then solved numerically, yielding the eigenvalues of the operator. The same approach allows us to find complex resonances arising in some noncompact domains. We discuss numerical examples related to quantum waveguide problems. The aim of these experiments is to compare the method based on the separation of variables with the standard finite-volume procedure. For the most computationally difficult examples related to domains with narrow throats one can clearly see the advantages of the proposed method.

Key Words: eigenvalue; resonance; Laplace operator; perturbation theory.

1. INTRODUCTION

The object of this study is the Dirichlet Laplacian in a deformed cylinder (i.e., a domain that is mapped onto a rectangle or an infinitely long strip, depending on whether the domain is compact or noncompact). A typical example of a deformed cylinder is a waveguide where the propagation of waves is governed by the Helmholtz equation. The two major types of waves observed in waveguides are referred to as trapped modes and resonance solutions. Both of these are eigenfunctions of the relevant differential equation and both satisfy the given boundary conditions. The trapped modes decay rapidly at infinity (the technical condition is that they lie in $\mathcal{L}^2$) and the corresponding eigenvalues are real. The resonances on the other hand satisfy a radiation condition at infinity. They represent quasistable states of the system and correspond to complex eigenvalues. Their real parts give the energies of the resonances while the inverses of the imaginary parts determine the lifetimes of the

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resonances. Resonances located close to the real axis are mathematically quite distinct from eigenvalues, but physically they have very similar effects on the behaviour of the system. It is quite common for a trapped mode to turn into a resonance with a small imaginary part when the region is slightly deformed.

There is a large literature studying resonances, particularly in quantum chemistry [20, 15, 19, 16] and acoustics [10, 17, 9, 6, 1, 18], to mention just the works most closely related to this paper. The subject also arises in the study of quantum waveguides, which are assuming increasing importance in the design of quantum-level electronic devices. We refer to the series of papers [13, 11, 12] where bound states and scattering in quantum waveguides are considered and to [22], where the authors address the problem of finding quantum resonances numerically for a particular waveguide.

Despite the extensive analysis carried out in the mentioned and other related literature, there still exist substantial problems in computing resonances close to the real axis. At the same time, resonances with small imaginary parts are often regarded as the most important case occurring in applications. It is this situation that interests us and motivates our study.

Waveguide phenomena are usually associated with either Dirichlet or Neumann boundary conditions. The former correspond to scattering problems in quantum theory, the latter appear in acoustics. The cited papers are concerned with either eigenvalues or resonances occurring in waveguides under specific conditions, or both of these. Our paper is very close in spirit to [6] and [1]. In the former the main issue is the resonance–eigenvalue connection, and the technique of the latter is also based on the separation of variables.

Our intention is to study the above-mentioned problems numerically. Dealing with both of them involves solving a boundary value problem for the Dirichlet Laplacian in two dimensions, which is either a self-adjoint eigenvalue problem or a non-self-adjoint resonance problem. Along with general numerical methods applicable in two dimensions, there exist techniques especially designed for cylinderlike domains, also called ducts in acoustics. We have already mentioned [1, 18], where such methods are developed. Both of these papers stress the importance of advanced methods specially designed for acoustic waveguides. It is hardly surprising that carefully performed numerical analysis is equally important for quantum problems. In [18] the authors apply a second-order finite-difference method and implement an iterative procedure for the resulting algebraic system. It is mentioned there that standard methods not using any preconditioning are likely to fail, especially when a large wave number is involved.

The numerical approach proposed in [1] is similar in spirit to that of our paper. In both cases the Helmholtz equation is reduced to the so-called coupled mode system of equations via the separation of variables. The main difference is that in [1] the coefficients of the ODE system have to be computed numerically, whereas our choice of the Fourier expansion functions allows us to find them in closed form. This substantially reduces the CPU time. The Dirichlet problem studied here is separable, as opposed to the much less straightforward Robin case. The examples in the cited paper are related to higher frequencies while we concentrate on the lowest oscillation mode only. On the other hand, the transfer method we use for the final ODE problem is able to handle a waveguide with narrow throats, such as that illustrated in Fig. 1—a situation not covered in [1].

The aim of this paper is to elaborate a method suitable for deformed cylinders that takes account of their geometry. The method based on the Fourier decomposition in one direction allows us to separate variables in the Helmholtz equation explicitly, leading to a system of ODEs. This is done for a fairly general geometry in the next section. In Section 3 we discuss

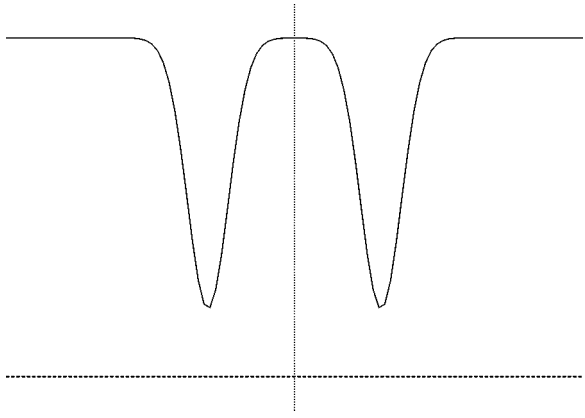

FIG. 1. Waveguide with indentations.

different boundary conditions involved. First we deal with standard self-adjoint conditions; then we concentrate on noncompact domains and define resonances by a specific boundary condition at infinity. What is often called the radiation condition in the literature is rewritten in terms of the resulting ODE system. We end up with a non-self-adjoint eigenvalue problem on a finite interval whose solution approximates that of the original resonance problem. Finally, we use the transfer method of [2] to find the eigenvalues of the two problems. Our numerical results illustrate the closeness of eigenvalues and resonances and are presented in Section 4, where we conclude by discussing the rate of convergence.

To be able to compare the method of the paper with others we look at the finite-volume method described, for example, in [21]. As discussed in Section 4, the proposed approach tested on our eigenvalue examples proved to be significantly more efficient than the standard two-dimensional procedure.

2. SEPARATION OF VARIABLES FOR THE LAPLACIAN

2.1. *Change of Variables*

Consider the operator $H := -\Delta$ acting on $\mathcal{L}^2(\Omega)$ subject to Dirichlet boundary conditions. The domain Ω is defined as

$$\Omega = \{(\xi, \eta)\colon a < \xi < b,\ 0 < \eta < \varphi(\xi)\} \tag{2.1}$$

in Cartesian coordinates (ξ, η). The possibility of a and b being infinite is not excluded here, so that Ω is not necessarily compact. The function $\varphi(\xi)$ is assumed to be smooth and to satisfy $\varphi(\xi) > 0,\ \xi \in [a, b]$. To find the spectrum of H we solve the Helmholtz equation

$$-\Delta f(\xi, \eta) = \lambda f(\xi, \eta), \quad (\xi, \eta) \in \Omega, \tag{2.2}$$

with the boundary conditions

$$f(\xi, \eta) = 0, \quad (\xi, \eta) \in \partial\Omega. \tag{2.3}$$

The change of variables

$$x = \xi, \quad y = \eta/\varphi(\xi) \tag{2.4}$$

maps the deformed cylinder Ω onto $\Omega_0 = \{(x, y)\colon a < x < b, 0 < y < 1\}$, which is either a rectangle or a strip (infinite or semiinfinite). We mention that a similar method has been used by Borisov *et al.* [7] to study bound states associated with a local perturbation of a strip or layer. In our case the deformation reduces the width of the strip locally, and there are no bound states. The transformation (2.4) can be expressed in the differential form as

$$\nabla_{\xi\eta} = W\nabla_{xy}, \quad \nabla_{xy} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix}, \quad W = \begin{pmatrix} 1 & -\frac{\varphi' y}{\varphi} \\ 0 & \frac{1}{\varphi} \end{pmatrix}.$$

The quadratic form corresponding to H is given by

$$J(f) = \int_\Omega [(\nabla_{\xi\eta} f, \nabla_{\xi\eta} f) - \lambda(f, f)]\, \mathrm{d}\xi\, \mathrm{d}\eta$$

or, equivalently, by

$$J(f) = \int_{\Omega_0} [(W\nabla_{xy} f, W\nabla_{xy} f) - \lambda(f, f)]\varphi(x)\, \mathrm{d}x\, \mathrm{d}y.$$

This can be rewritten as

$$J(f) = \int_{\Omega_0} [(A\nabla_{xy} f, \nabla_{xy} f) - \lambda(f, f)]\varphi(x)\, \mathrm{d}x\, \mathrm{d}y, \tag{2.5}$$

where

$$A = W^*W = \begin{pmatrix} 1 & -\frac{\varphi' y}{\varphi} \\ -\frac{\varphi' y}{\varphi} & \frac{(1+(\varphi' y)^2)}{\varphi^2} \end{pmatrix}. \tag{2.6}$$

Hence the Helmholtz equation in the new variables takes the form

$$(\varphi f_x)_x - (\varphi' y f_x)_y - (\varphi' y f_y)_x + ((1 + (\varphi' y)^2) f_y/\varphi)_y + \lambda\varphi f = 0. \tag{2.7}$$

Since we restrict ourselves to the Dirichlet case, no change in the boundary conditions is required here; the condition (2.3) is retained on $\partial\Omega_0$. However, in a generic situation one can still use (2.4) and (2.7), provided obvious changes are made to the original boundary conditions where necessary. For instance, instead of Neumann boundary conditions at $\eta = \varphi(\xi)$ one would have

$$((1 + \varphi'^2) f_y - \varphi\varphi' f_x)|_{y=1} = 0,$$

while Neumann boundary conditions at $x = a, b$ would become

$$(\varphi f_x - \varphi' y f_y)|_{x=a,b}.$$

Note that a similar transformation can be also done for a more general domain:

$$\Omega = \{(\xi, \eta)\colon a < \xi < b,\ \varphi_1(\xi) < \eta < \varphi_2(\xi)\}.$$

The change of variables

$$x = \xi, \quad y = \frac{\eta - \varphi_1}{\varphi_2 - \varphi_1}$$

leads to a quadratic form of type (2.5), whose coefficients are not quoted here, for brevity.

2.2. *Discretisation in the y-Direction*

The quadratic form (2.5) is related to the transformed operator on the weighted space $\mathcal{L}^2(\Omega_0, \varphi\, dx\, dy)$. Here and below we use the notation $\nabla = \nabla_{xy}$.

To discretise the form $J(f)$ in the y-direction let us separate the variables expanding f as

$$f(x, y) = \sum_{k=1}^{\infty} g_k(y) h_k(x). \tag{2.8}$$

Recall that we have Dirichlet boundary conditions everywhere so that our natural choice is to work with an orthonormal system of functions vanishing at the horizontal parts of the boundary. We therefore opt for

$$g_k = \sqrt{2}\sin(\pi k y).$$

Denote $f_0 = f$, $f_1 = f_x$, $f_2 = f_y$; then

$$f_i = \sum_{k=1}^{\infty} h_k^i(x) g_k^i(y),$$

where

$$g_k^0 = g_k^1 = g_k, \quad g_k^2 = \sqrt{2}\cos(\pi k y).$$

In this notation the x-dependence is determined by the functions

$$h_k^0 = h_k, \quad h_k^1 = h_k', \quad h_k^2 = \pi k h_k$$

(throughout the paper a prime denotes differentiation with respect to x).

We notice that the variables are separated in the coefficients of $J(f)$:

$$\varphi(x) A_{ij}(x, y) = B_{ij}(x) + C_{ij}(y) D_{ij}(x), \quad i, j = 1, 2. \tag{2.9}$$

The entries A_{ij} of the matrix A are defined by (2.6); the matrices B, C, and D satisfying the above decomposition are

$$B = \begin{pmatrix} \varphi & 0 \\ 0 & \frac{1}{\varphi} \end{pmatrix}, \quad C = \begin{pmatrix} 0 & y \\ y & y^2 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & -\varphi' \\ -\varphi' & \frac{\varphi'^2}{\varphi} \end{pmatrix}.$$

The formula (2.9) allows us to rewrite (2.5) in the form

$$J(f) = \int_a^b \int_0^1 \left[\sum_{i,j=1}^{2} (B_{ij} + C_{ij} D_{ij})\, \bar{f}_i\, f_j - \lambda\varphi |f|^2 \right] \mathrm{d}x\, \mathrm{d}y$$

$$= \int_a^b \left[\sum_{i,j=1}^{2} B_{ij} \int_0^1 \bar{f}_i\, f_j\, \mathrm{d}y + D_{ij} \int_0^1 C_{ij}\, \bar{f}_i\, f_j\, \mathrm{d}y - \lambda\varphi \int_0^1 |f|^2\, \mathrm{d}y \right] \mathrm{d}x$$

$$= \int_a^b \left[\sum_{i,j=1}^{2} B_{ij} E_{ij} + D_{ij} F_{ij} - \lambda\varphi G \right] \mathrm{d}x. \tag{2.10}$$

As we substitute the expansion (2.8) into the above integral, the coefficients E_{ij}, F_{ij}, G are readily computed:

$$E_{ij} = \int_0^1 \bar{f}_i\, f_j\, \mathrm{d}y = \int_0^1 \sum_k \bar{h}_k^i g_k^i \sum_r h_r^j g_r^j\, \mathrm{d}y$$

$$= \sum_{k,r} \bar{h}_k^i h_r^j \int_0^1 g_k^i g_r^j\, \mathrm{d}y = \sum_{k,r} \alpha_{kr}^{ij} \bar{h}_k^i h_r^j;$$

$$F_{ij} = \int_0^1 C_{ij}\, \bar{f}_i\, f_j\, \mathrm{d}y = \int_0^1 C_{ij} \sum_k \bar{h}_k^i g_k^i \sum_r h_r^j g_r^j\, \mathrm{d}y$$

$$= \sum_{k,r} \bar{h}_k^i h_r^j \int_0^1 C_{ij} g_k^i g_r^j\, \mathrm{d}y = \sum_{k,r} \beta_{kr}^{ij} \bar{h}_k^i h_r^j;$$

$$G = \int_0^1 \sum_k \bar{h}_k^0 g_k^0 \sum_r h_r^0 g_r^0\, \mathrm{d}y = \sum_k |h_k|^2.$$

To find α_{kr}^{ij} we use the orthogonality relations for g_k^i; in fact, we only need the diagonal elements $\alpha_{kr}^{jj} = \delta_{kr}$. The coefficients β_{kr}^{ij} are also calculated in the closed form:

$$\beta_{kr}^{11} = 0, \quad \beta_{kr}^{22} = \begin{cases} \frac{1}{3} + \frac{1}{2\pi^2 k^2}, & k = r, \\ (-1)^{k+r} \frac{4(k^2+r^2)}{\pi^2 (k^2 - r^2)^2}, & k \neq r, \end{cases}$$

$$\beta_{kr}^{12} = \beta_{rk}^{21} = \begin{cases} -\frac{1}{2\pi k}, & k = r, \\ (-1)^{k+r} \frac{2k}{\pi (r^2 - k^2)}, & k \neq r. \end{cases}$$

The quadratic form is now reduced to that of a one-dimensional differential problem.

2.3. *Canonical ODE System*

Having done the above calculations we finally arrive at

$$J(f) = \int_a^b \left[\sum_k |h_k'|^2 + \left(\left[\frac{\pi k}{\varphi} \right]^2 - \lambda \right) |h_k|^2 \right.$$

$$\left. + \sum_{k,r} \frac{\varphi'^2}{\varphi^2} \pi^2 k r \beta_{kr}^{22} \bar{h}_k h_r - \frac{\varphi'}{\varphi} \pi \left(r \beta_{kr}^{12} \bar{h}_k' h_r + k \beta_{rk}^{12} \bar{h}_k h_r' \right) \right] \varphi\, \mathrm{d}x.$$

The Euler equations are easily derived in the standard way. A simple calculation shows that the discretised form (2.10) is equivalent to the ODE system written in its canonical self-adjoint form as

$$-(Ph')' + Qh' - (Q^*h)' + Rh = 0. \tag{2.11}$$

Here the vector of unknowns is

$$h = (h_1, h_2, \ldots)^T;$$

the matrix coefficients are given by

$$P_{kr} = \varphi\delta_{kr}, \quad Q_{kr} = -\pi k\beta_{rk}^{12}\varphi',$$
$$R_{kr} = \pi^2 kr\beta_{kr}^{22}\frac{\varphi'^2}{\varphi} + \left(\frac{(\pi k)^2}{\varphi} - \lambda\varphi\right)\delta_{kr}, \quad k, r = 1, 2, \ldots .$$

For practical purposes we truncate the system to a finite number of equations, taking a sufficiently large N and keeping the same notation h, P, Q, R for the truncated matrices where $k, r = 1, \ldots, N$. This is justified by the fact that the Fourier coefficients involved in (2.8) are rapidly decaying in k and therefore higher order terms can be neglected. In [1] it has been suggested that N should be of order $h\sqrt{\lambda}$, where h denotes the mean width of the duct if the curvature of its boundary is not too large. In the examples in Section 4 the width of the waveguide varies greatly from point to point. The size of N is determined experimentally and is found to depend mainly on the width of the narrowest portion of the waveguide.

Equivalently, we reduce (2.11) to the Hamiltonian system of $2N$ equations,

$$JH' = K(x, \lambda)H, \quad x \in \mathbb{R}, \tag{2.12}$$

where

$$H = \begin{pmatrix} h \\ Ph' + Q^*h \end{pmatrix} \in \mathcal{L}^2(\mathbb{R}), \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$
$$K = \begin{pmatrix} -R + QP^{-1}Q^* & -QP^{-1} \\ -P^{-1}Q^* & P^{-1} \end{pmatrix}.$$

The system (2.12) is self-adjoint with $P = P^* > 0$, $R = R^*$ for $\lambda \in \mathbb{R}$. We can therefore apply advanced numerical methods (see, for example, [2, 3]) to find the eigenvalues of the problem and the relevant solutions. Before proceeding to this task let us discuss the issue of boundary conditions.

3. BOUNDARY CONDITIONS

3.1. *The Self-Adjoint Problem*

To make sure the original boundary conditions are involved in the ODE problem, consider a generic situation when we have a functional

$$J(f) = \int_{\Omega_0} F(x, y, f, f_x, f_y)\, dx\, dy.$$

To derive the corresponding Euler equation we replace f with $f + \varepsilon\gamma$ and compute

$$\delta J = \varepsilon \int_{\Omega_0} \gamma \left(F_f - \frac{\partial}{\partial x} F_{f_x} - \frac{\partial}{\partial y} F_{f_y} \right) dx\, dy + \varepsilon \int_{\partial\Omega_0} \gamma \left(F_{f_x}\, dy - F_{f_y}\, dx \right).$$

Putting the first integral equal to zero we obtain the differential equation (2.7); the second is responsible for boundary conditions. For our class of problems $\partial\Omega_0 = \{y = 0\} \cup \{y = 1\} \cup \{x = a\} \cup \{x = b\}$. The conditions at different parts of the boundary are defined by

$$\int_a^b \gamma F_{f_y}\big|_{y=0;\,1}\, dx = 0; \quad \int_0^1 \gamma F_{f_x}\big|_{x=a;b}\, dy = 0.$$

Taking account of the obtained quadratic form, we get

$$\int_a^b \gamma f_y|_{y=0}\, dx = 0, \tag{3.1}$$

$$\int_a^b \gamma \left(\varphi'(x) f_x - \frac{1 + \varphi'^2}{\varphi} f_y \right)\Big|_{y=1} dx = 0 \tag{3.2}$$

on the horizontal lines. As pointed out in Section 2.1, Dirichlet boundary conditions remain unchanged in the new variables and are automatically taken into account by virtue of our choice of the functions $g_k(y)$ in (2.8). The above integrals (3.1) and (3.2) vanish because of the implied condition $\gamma = 0$. A difficulty would only occur if we had more complicated conditions at the curvilinear part of the boundary of Ω. Dirichlet boundary conditions are the ones relevant to quantum mechanical problems and they enable us to separate the variables in the quadratic form explicitly. We refer to [1], where the authors consider arbitrary boundary conditions of the form $(af + b\frac{\partial f}{\partial n})|_{\partial\Omega} = 0$ by using appropriate orthogonal curvilinear coordinates. The problem of this kind requires a more complicated expansion to be used instead of (2.8). In that case Fourier coefficients are not obtained in closed form but should be calculated numerically.

On the vertical parts of the boundary we have

$$\int_0^1 g(\varphi f_x - \varphi' y f_y)|_{x=a,\,b}\, dy = 0. \tag{3.3}$$

The Dirichlet case is as easy to treat as before: the conditions $h_k(a) = h_k(b) = 0$, $k = 1, \ldots, N$ are imposed on the solutions of (2.12). Consider also a domain where $\varphi'(a) = \varphi'(b) = 0$ — the situation typical for compactly perturbed strips and, in particular, for some waveguides. Here we are able to handle a more general case. For instance, Neumann boundary conditions at $x = a,\ b$ do not change and become $h_k'(a) = h_k'(b)$, $k = 1, \ldots, N$ in terms of the system (2.12). However, one cannot fully separate variables in generic Robin conditions of form (3.3).

3.2. *The Radiation Condition*

There are three technically distinct methods of defining resonances. The one which we give below involves imposing a so-called radiation condition at infinity on the eigenfunction. In many situations, including the present one, this is known to be equivalent to the definition via poles of the scattering matrix [8, 22, 6], but here we do not make essential use of this fact. One may also define resonances using a standard method referred to as (exterior) complex scaling. The resonances of the original operator become $\mathcal{L}^2$ eigenvalues of a new non-self-adjoint operator; once again one may show that this method yields the same set of resonances. See below for further comments on this method.

Turning to our particular resonance problem, let us consider a domain Ω such that, in the notation of Section 2.1, $x \in (a, \infty)$ and

$$\varphi(x) \sim 1, \quad x \geq X \tag{3.4}$$

for some $X > 0$. Similar assumptions are often made in papers dealing with scattering problems, for instance in [1, 18, 6]. We take Dirichlet boundary conditions on $\partial\Omega$ and require a different type of condition to be satisfied as $|x| \to \infty$. Namely, for a given $\lambda \in \mathbb{C}$ there always exists a unique solution of (2.2) that has the form

$$f(x, y) = (\exp(-t_1 x) + s_1 \exp(t_1 x))g_1(y) + \sum_{k=2}^{\infty} s_k g_k(y) \exp(t_k x), \quad x \geq X. \tag{3.5}$$

Here we denote

$$t_k = -\sqrt{(\pi k)^2 - \lambda}, \quad \operatorname{Re} t_k < 0;$$

g_k are the same as in Section 2.2. The coefficients $s_k, k = 1, 2, \ldots$ are defined by the formula (3.5) uniquely for each value of λ. We put $\omega = \sqrt{\lambda}$ and consider s_k as functions of ω. The function s_1, called the scattering coefficient of the problem, is involved in the definition of resonances. The reader will find their general definition in [8]. Note that when variables are separated the following construction proves to be more handy.

DEFINITION. If the scattering coefficient $s_1(\omega)$ has a pole at $\omega = \omega_0$ we say that $\lambda = \omega_0^2$ is a resonance.

The above definition does not include all the resonances but only those lying on the first nonphysical sheet (see [8] for detailed explanation). We refer to [22, 6] for the equivalence of the two definitions. Apart from its simplicity, the approach based on (3.5) has another distinctive advantage. It is known from scattering theory that $s_1(\omega)\overline{s_1}(\overline{\omega}) = 1$ and that s_1 is analytic in the half-plane $\operatorname{Im}\omega < 0$. Therefore instead of seeking the poles of $s_1(\omega)$ one can look for its zeros located in the lower ω-half-plane. This is the approach we use here, along with the separation of variables in the deformed cylinder Ω.

Given the above definition, there is an obvious difference between the resonance problem and a classical spectral problem. Indeed, according to (3.5) here we are looking for a solution exponentially growing at infinity. Note, however, that the resonances we are interested in occur as perturbations of eigenvalues and are typically situated near the real axis. This means that the values of $|\operatorname{Im} t_k|$, $k = 1, 2, \ldots$, are rather small and therefore the corresponding solution grows slowly.

Combining (3.5) with (2.8) for a sufficiently large x we get

$$h_1(x) = \exp(-t_1 x) + s_1 \exp(t_1 x), \quad h_k'(x) = t_k h_k(x), \quad k = 2, 3, \ldots .$$

There are two ways to handle these conditions. One can solve the inhomogeneous problem (as has been done in [6] in two dimensions), then find the zeros of s_1. Alternatively one can put $s_1 = 0$ straight away, then solve the resulting eigenvalue problem with λ-dependent boundary conditions. The latter approach leads to the set of boundary conditions at X

$$\psi_X H(X) = 0, \quad \psi_X = (T - P^{-1}Q^*,\ P^{-1}), \quad T = \mathrm{diag}(t_1, -t_2 \ldots, -t_N). \tag{3.6}$$

This formula, known as the radiation or outgoing wave condition, singles out the solution whose first component grows and whose others decay exponentially at infinity. It is this solution that is sometimes called the resonance eigenfunction.

It should be mentioned here that our approach agrees with the one that uses exterior complex scaling (see, for example, [8]). In this technique one replaces the operator with a family of operators on the same domain, which depends analytically on a complex parameter. The operators are independent of the parameter for $x \le X$ and are associated with a space scaling for $x \ge X$. One computes the complex eigenvalues of this family acting in $\mathcal{L}^2(\Omega)$ and proves that they do not depend on the parameter, subject to certain conditions. It is known that the complex eigenvalues coincide with resonances defined via either the scattering coefficients or analytic continuation of the resolvent kernels. One may verify that exterior complex scaling yields the same boundary condition at $x = X$ as (3.6) (see [14]).

4. NUMERICAL EXAMPLES

4.1. *The Transfer Method*

Summarising the results of the first three sections let us formulate the problems to be solved numerically. We are looking for such values of λ that the system (2.12) has a nontrivial solution satisfying

$$\psi_a H(a) = 0, \quad \psi_b H(b) = 0,$$

where (i) $\psi_a = \psi_b = (I,\ 0)$ and (ii) $\psi_a = (I,\ 0)$, $\psi_b = \psi_X$, as defined by (3.6). Problem (i) provides approximations to the Dirichlet eigenvalues of a compact domain of kind (2.1); problem (ii) enables us to calculate complex resonances that may occur in an unbounded domain of the same type satisfying (3.4).

The method we apply to both problems is based on the orthogonal transfer of [2], which we briefly outline below. The manifold of the solutions of the system (2.12) satisfying the left boundary condition is determined by

$$\psi(x) H(x) = 0, \quad a \le x \le b,$$

where $\psi \in \mathbb{C}^{N \times 2N}$ solves the Cauchy problem

$$\psi' = \psi J K, \quad \psi(a) = \psi_a.$$

Theoretically one can integrate the above equation for a fixed λ, define

$$f(\lambda) = \det\begin{pmatrix} \psi(b;\lambda) \\ \psi_b(\lambda) \end{pmatrix}$$

and solve $f(\lambda) = 0$ to find the eigenvalues of the problem. This method is known to be hopelessly inefficient because $\psi(x)$, although formally of rank N, can have almost linearly dependent rows. Abramov [2] proposed replacing ψ with $\tilde{\psi}(x) = \nu(x)\psi(x)$, where $\nu \in \mathbb{C}^{N\times N}$, $\det \nu \neq 0$. The function ν is chosen to ensure $\tilde{\psi}(x)\tilde{\psi}^*(x) = \text{const}$. The transfer equation now takes the form

$$\tilde{\psi}' + \tilde{\psi} J A\Big(I - \tilde{\psi}^*\big(\tilde{\psi}\tilde{\psi}^*\big)^{-1}\tilde{\psi}\Big) = 0, \quad \tilde{\psi}(a) = \psi_a. \tag{4.1}$$

The RHS of (4.1) is bounded and the solution $\tilde{\psi}$ exists on the whole of $[a, b]$. By comparison with ψ, the matrix $\tilde{\psi}$ has the key advantage of being easily computed without loss of rank. The use of this idea proved essential to obtaining stable results for this problem.

Having calculated the smooth function $\tilde{\psi}$ we proceed to find the eigenvalues. For the resonance problem this is done along the lines of [4], where the idea of [2] has been applied to non-self-adjoint eigenvalue problems. As observed there,

$$\tilde{f}(\lambda) = \det\begin{pmatrix} \tilde{\psi}(b) \\ \psi_b \end{pmatrix} = f(\lambda)\det \nu,$$

so that the zeros of f and $\tilde{f}$ coincide. Moreover, the zeros of $\tilde{f}$ can be found using the method based on the argument principle, although $\tilde{f}$ does not have to be analytic in λ as opposed to f. Still the number of zeros of $\tilde{f}$ inside a contour Γ is

$$N = \frac{1}{2\pi}\oint_\Gamma d\,\operatorname{Arg}\tilde{f}(\lambda),$$

as shown in [4]. It is this computational formula that we use to locate the complex eigenvalues of problem (ii). Taking a shrinking sequence of contours Γ we find the zeros up to a chosen accuracy. We computed the contour integrals reliably for circles of radii down to 10^{-4} and made sure that if the centre was shifted by a similar order of magnitude, the integrals vanished. In the better conditioned case (i) we applied Newton's method, allowing us to calculate the eigenvalues of the self-adjoint problem.

Note that typically problem (ii) is much harder to solve than is (i), and our examples are no exception. When resonances are situated near the real axis the scattering coefficient s_1 has a pole and a zero close to one another. Naturally, the closer they are, the less stable the problem is.

4.2. *Results of Computations*

As an example we consider a quantum waveguide with indentations defined in the Cartesian coordinates (ξ, η) as

$$W = \big\{-\infty < \xi < \infty,\ 0 < \eta < \varphi(\xi) = 1 - \alpha\big(e^{-(\xi-\gamma)^2} + e^{-(\xi+\gamma)^2}\big)\big\},$$

where α and γ are real positive constants (see Fig. 2a).

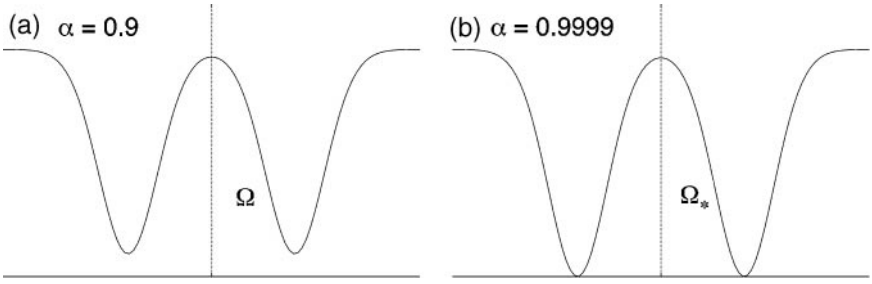

FIG. 2. Narrow-throated domains.

We work in two different domains:

$$\Omega_1 = W \cap \{0 < \xi < \gamma\}, \quad \Omega_2 = W \cap \{0 < \xi\}.$$

The domains Ω_1 and Ω_2 relate to problems (i) and (ii) of the previous section, respectively. In the latter the resonance boundary condition is imposed at a sufficiently far point X, as suggested in Section 3.2. In our experiments we put $\gamma = 2$, so that it suffices to take $X \geq 5.4$ to ensure $\varphi'(X) < 10^{-4}$.

In this example there exists $\alpha = \alpha_* \approx 1$ such that the two parts of $\partial\Omega$ touch one another near $\xi = \gamma$. For this value of α the domain Ω consists of three disjoint parts, as shown in Fig. 2b, so that the eigenvalue problem is decomposed into three separate problems. The Laplacian considered in the compact domain Ω_* has infinitely many real eigenvalues accumulating at infinity. As we decrease α joining the three subdomains, one expects the eigenvalues to disappear, generating resonances in their neighbourhood. A similar phenomenon, where resonances originate from eigenvalues as the domain is perturbed, has been observed in [6], although the mechanism by which they emerge is different here.

Clearly, both domains Ω_1 and Ω_2 satisfy the conditions of Section 2.1 for $\alpha < \alpha_*$. We compute resonances (i.e., eigenvalues of problem (ii) for a range of α) using the deformed cylinder approach. In the self-adjoint example the eigenvalues of problem (i) are found for the same values of α. The ODE problem is solved by the transfer method described in the previous section. An important question is how to choose the number of terms to be retained in (2.8) or, in other words, the dimension of the system (2.12). This number should depend on α: indeed, for α close to α_* the width of the domain is small near $\xi = \gamma$, so one needs to keep a larger number of terms $g_k(y)$ in (2.8). There are two possibilities here. One is to increase repeatedly the number of terms by one and solve the system with the corresponding constant number of unknowns until the answers converge. Or, instead of keeping a large number of terms throughout the interval, one can start off with a smaller N in (2.12). Moving along the x-interval one changes N gradually, adding or removing variables $h_k(x)$ depending on the size of $\varphi(x)$. We have used both techniques in different situations, ensuring that the results coincide within the chosen accuracy for two subsequent values of N. For reasonably small values of α it suffices to take smaller N: for instance, when $\alpha = 0.8$ the results obtained for $N = 4$ and greater coincide up to the tolerance of 10^{-4}. The maximal number of terms taken in our computations is $N = 30$ for $\alpha = 0.97$ (the largest value considered).

There is an important connection between problems (i) and (ii) which makes us study them within the same framework. Namely, as $\alpha \to \alpha_*$ both the eigenvalues of Ω_1 and the resonances of Ω_2 converge to the Dirichlet eigenvalues of the domain Ω_*. These cannot be found using the same method because Ω_* has a cusp at $\xi = \gamma$ and is not a deformed cylinder in our terminology. In this case one could still separate variables in the Helmholtz equation in a similar way, arriving at a singular ODE problem. This question requires a separate consideration, which is beyond the subject of our paper. Recall that the aim of our numerical experiments is to calculate resonances occurring in this example and find out how they are related to eigenvalues. To be able to make proper comparisons we have used the finite-volume method to discretise the operator on Ω_* and find its spectrum. To know the limit eigenvalue is also helpful, as it serves as an initial guess for the eigenvalues of problems (i) and (ii).

4.2.1. The self-adjoint problem. We applied both the finite-volume method and the ODE technique to a series of problems of type (i) to compare the effectiveness of the two approaches. The comparisons are in favour of the proposed method, which appears to be more efficient than the conventional one. The relative benefits of our technique are more spectacular for larger values of α. For $\alpha > 0.9$ the finite-volume method becomes very unstable and does not provide accurate results any longer, while the new method works safely for a wider range, up to $\alpha = 0.97$. The two methods agree with each other for $\alpha \leq 0.9$. Everything else being equal, the closer α gets to its critical value, the more advantageous the deformed cylinder approach is in comparison with the finite-volume method.

Of course if one were to use commercial packages, one could surely treat an α somewhat bigger than 0.9 by using standard methods, but the same comment could be made about our method: if it were developed at a commercial level several further elaborations could be incorporated to improve its performance.

The numerical results presented below are related to the lowest Dirichlet eigenvalue of Ω_* and are quoted in terms of the wave number $\omega = \sqrt{\lambda}$ (we retain the term eigenvalue for the wave numbers). The smallest eigenvalue corresponding to the domain with the cusp is $\omega_* = 4.6252$; it is included in the diagrams to illustrate the convergence of our results.

In Fig. 3 a series of the eigenvalues of problem (i) for $\alpha \in [0.7,\ 0.97]$ is shown. They converge to ω_* as $\alpha \to \alpha_*$. The linear rate of convergence is in agreement with standard perturbation theory: the principal correction term is of order $\varepsilon = \alpha_* - \alpha$ since the coefficients of (2.12) depend on α linearly.

4.2.2. The resonance problem. We showed in Section 3.2 that the problem of finding resonances effectively reduces to a non-self-adjoint boundary value problem in a truncated, compact domain. The resonances can then be computed using various methods, for instance a non-self-adjoint version of the finite-volume method. An example similar to those of our paper has been numerically studied in [6], where the reader can also find a detailed description of the method put in the relevant context. It is that procedure that we use to benchmark the separation-of-variables approach and make further comparisons.

The resonances ω_2 emerging from the lowest eigenvalue as α decreases can be found in Table I. They are also shown in Fig. 4, where their real parts are plotted against their imaginary parts. The quoted resonances are obtained using the new method and they agree with those found using the finite-volume method up to the chosen accuracy for $\alpha \leq 0.9$, beyond which the finite-volume method becomes unstable. On the other hand the resonances

TABLE I

Resonances ω_2

α	ω_2	α	ω_2
0.7	$4.2988 + 0.0545i$	0.9	$4.5250 + 0.0050i$
0.75	$4.3715 + 0.0348i$	0.925	$4.5492 + 0.0032i$
0.8	$4.4223 + 0.0212i$	0.95	$4.5755 + 0.0017i$
0.825	$4.4498 + 0.0154i$	0.96	$4.5864 + 0.0012i$
0.85	$4.4741 + 0.0113i$	0.97	$4.5967 + 0.0008i$

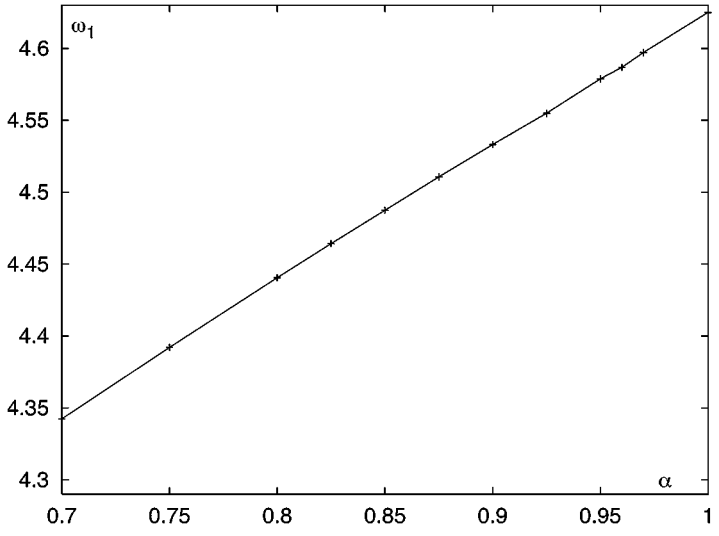

FIG. 3. Eigenvalues of problem (i) for a range of α.

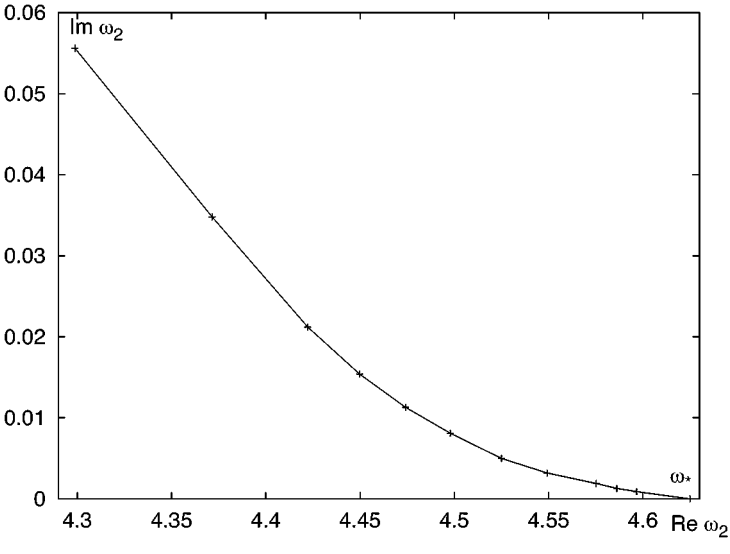

FIG. 4. Resonances generated by ω_*.

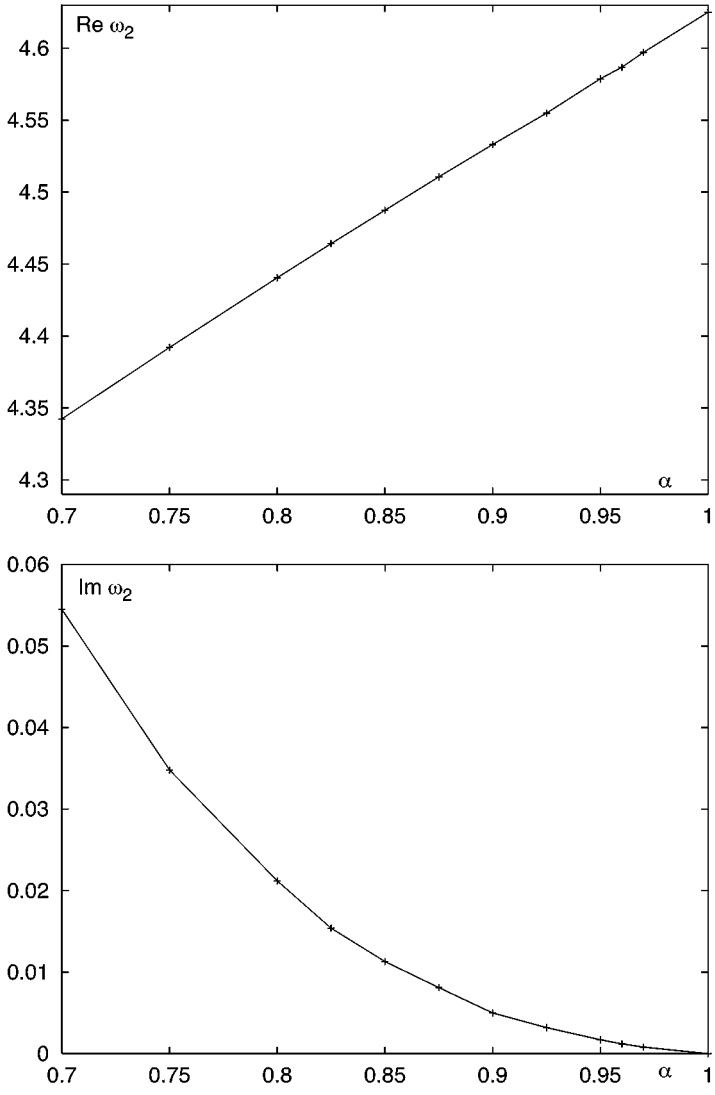

FIG. 5. Real and imaginary parts of resonances: α-dependence.

calculated by the separation-of-variables approach definitely converge to ω_*. The problem is, of course, very sensitive to perturbations near the critical value of $\alpha = \alpha_*$, or $\varepsilon = 0$. However, we found that for $\alpha \leq 0.97$ our computations are relatively stable and believe that they provide reliable results. For $\alpha > 0.97$ we have observed various instability effects, preventing us from computing resonances accurately. The system (2.12) is difficult to solve for values of ω close to ω_* (and, consequently, the corresponding resonance) because its coefficients change very rapidly for $\alpha \approx \alpha_*$. Even methods suitable for stiff systems fail to produce satisfactory results when ε is too small. As discussed in the previous section, another reason why the problem is likely to be unstable is the closeness of resonances to the real axis. These two factors make calculations slow and inefficient for α close to α_*. Once again the non-self-adjoint analogue of the finite-volume method proves to be less robust than our new procedure. The range of values of α, for which the results obtained using the two methods are comparable, is the same as in the self-adjoint problems of the

TABLE II

The Values of $\delta = \omega_1 - \mathrm{Re}\,\omega_2$

ε	0.3	0.25	0.2	0.175	0.15
δ	0.0436	0.0256	0.0182	0.0144	0.0123
ε	0.1	0.075	0.05	0.04	0.03
δ	0.0081	0.0044	0.0015	0.0008	0.0004

previous section. For $\alpha > 0.9$ one cannot trust the standard discretisation technique, but the deformed cylinder approach works for α up to about 0.97.

The α-dependence of the real and imaginary parts of the resonance originating from ω_* is shown in Fig. 5. The real part is found to depend on the perturbation parameter linearly, whereas the imaginary part seems to be of order ε^p, with $p \approx 3/2$ for $\varepsilon < 0.2$. A different behaviour has been observed in [6], where for a different geometry the authors derived an asymptotic formula for the imaginary part of the resonance. The resonances in the example of that paper are shown to be analytic in the domain perturbation parameter, their imaginary parts depending quadratically on the parameter.

One generally expects that if one perturbs an eigenvalue which is embedded in the continuous spectrum, then it is transformed into a resonance near the real axis. In many cases one can even write out a perturbation expansion, and a general theory for some such cases was described by Agmon [5]. However in our situation the natural parameter ε can only take positive values, for obvious reasons. Therefore even if the resonance depends analytically on ε for $\varepsilon > 0$, there is no proof that it has an expansion with finite coefficients around $\varepsilon = 0$, nor even that the resonance converges to the eigenvalue as $\varepsilon \downarrow 0$. The numerical experiments do, however, suggest that not only does it converge, but its real and imaginary parts also may be expanded in powers of $\varepsilon^{1/2}$ as $\varepsilon \downarrow 0$.

In Table II the eigenvalues of problem (i) are compared with the real parts of the resonances related to the same values of α. We tabulate the difference $\delta = \omega_1 - \mathrm{Re}\,\omega_2$ between the Dirichlet eigenvalue and the real part of the associated resonance and observe that this quantity decreases very rapidly as $\varepsilon \downarrow 0$. One might hope to deduce the rate of convergence of $\delta(\varepsilon)$ from asymptotic perturbation formulae. The question of how to obtain such formulae for the resonance still remains open.

5. CONCLUSIONS

The main idea of this paper was to reduce an eigenvalue problem in a two-dimensional deformed cylinder to an ODE problem. Complex resonances occurring in deformed strips were also dealt with in the same way.

The method of this paper allowed us to discretise the problem in one direction, taking into account the geometry of the domain. This was especially important for the highly distorted domains of Section 4. We could of course have considered only perturbed cylinders (i.e., cylinders for which the throat is quite wide), but in this case a variety of different numerical codes would have yielded the same results without difficulty. The case of very narrow throats is much more challenging. The intrinsic instability of the problem might in principle be handled either by the use of finite meshes, which are highly refined near the throat, or by normalisation to a straight cylinder, in which case one must accept the appearance of large

coefficients in the relevant differential operator. Eventually any method will fail, and the issue is how close one can get to the critical value. The relative advantage of our method relies upon the special techniques available for one-dimensional systems, which are highly developed at a theoretical level and easy to implement numerically. Standard finite-difference methods would require a significant mesh refinement in the narrow part of the considered waveguide. For comparison purposes we also computed the eigenvalues and resonances using the finite-volume method. As discussed in the previous section, the latter proved to be substantially less efficient than the method based on the separation of variables for the class of problems studied here. The new method works faster and, more importantly is able to treat a wider range of problems. This is in agreement with the already mentioned results of [1, 18], where other advanced methods were designed to suit similar problems. We believe that our approach is competitive and recommend it for ill-conditioned eigenvalue and resonance problems. Our confidence is supported by the strong agreement between numerical results and analytic expectations. Indeed, the convergence of both eigenvalues and resonances to their limit value (computed by an independent method) confirms the reliability of the proposed technique.

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