SEPARATION OF VARIABLES IN PERTURBED CYLINDERS

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ABSTRACT. 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 non-compact domains. We discuss numerical examples related to quantum waveguide problems.

1. INTRODUCTION

The object of this study is the Dirichlet Laplacian in a perturbed cylinder, *i.e.* a domain that is mapped onto a rectangle or an infinitely long strip depending on the domain being compact or non-compact. A typical example of a perturbed 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. Mathematically trapped modes are described as the eigenfunctions of self-adjoint operators. These are $\mathcal{L}^2$ functions associated with bound states, as opposed to resonance solutions that correspond to the so-called scattering poles, or complex resonances. Despite their different nature, eigenvalues and resonances are sometimes closely connected with each other. For example, eigenvalues may generate resonances under small perturbations of the domain. It is this situation that interests us and motivates our study of resonances.

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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. We refer to the series of papers [13, 11, 12] where bound states and scattering in quantum waveguides are studied. In [17] the authors address the problem of finding quantum resonances numerically for a particular waveguide. For results on acoustic waveguides, both theoretical and numerical see, for instance, [10, 14, 9, 6, 1, 15]. The papers cited here 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, that 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 cylinder-like domains also called ducts in acoustics. We have already mentioned [1, 15] where such methods are developed. Both of these papers stress the importance of advanced methods specially designed for acoustic waveguides. It is hardly surpsising that carefully performed numerical analysis is equally important for quantum problems. In [15] 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. 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 a narrow throat — a situation not covered in [1].

The aim of this paper is to elaborate a method suitable for perturbed 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 different boundary conditions involved. First we deal with standard self-adjoint conditions, then concentrate on non-compact 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, *e.g.* in [16]. As discussed in section 4, the proposed approach tested on our eigenvalue examples proves 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

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

in the 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 satisfy $\varphi(\xi) > 0,\ \xi \in [a, b]$. To find the spectrum of H we solve the Helmholtz equation

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

with the boundary conditions

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

The change of variables

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

maps the perturbed cylinder Ω onto $\Omega_0 = \{(x, y) : \ a < x < b,\ 0 < y < 1\}$ which is either a rectangle or a strip (infinite or semi-infinite). 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

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

The quadratic form corresponding to H is given by

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

or, equivalently, by

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

This can be rewritten as

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

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

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

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), (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

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

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

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

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

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

The change of variables

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

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 $\mathcal{L}^2(\Omega_0, \varphi \mathrm{d}x\, \mathrm{d}y)$. 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 $f_0 = f,\ f_1 = f_x,\ f_2 = f_y$;

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

where

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

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

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

(throughout the paper $'$ denotes differentiation with respect to x).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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 (2.3) is equivalent to the ODE system written in its canonical self-adjoint form as

$$-(Ph')' + Qh' - (Q^*h)' + Rh = 0. \tag{2.10}$$

Here the vector of unknowns

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

the matrix coefficients are given by

$$P_{kr} = \varphi\delta_{kr}, \qquad Q_{kr} = -\pi k \beta^{12}_{rk}\varphi',$$

$$R_{kr} = \pi^2 kr\beta^{22}_{kr}\frac{\varphi'^2}{\varphi} + \left(\frac{(\pi k)^2}{\varphi} - \lambda\varphi\right)\delta_{kr}, \qquad k, r = 1, 2, \dots .$$

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 $k, r = 1, \dots, N$. 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 of section 4 the width of the waveguide varies greatly from point to point. The size of N is determined experimentally and found to depend mainly on the width of the narrowest portion of the waveguide.

Equivalently, we reduce (2.10) to the Hamiltonian system of $2N$ equations:

$$JH' = K(x, \lambda)H, \ x \in \mathbb{R} \tag{2.11}$$

where

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

$$K = \begin{pmatrix} -R + QP^{-1}Q^* & -QP^{-1} \\ -P^{-1}Q^* & P^{-1} \end{pmatrix}.$$

The system (2.11) 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. **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

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

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

$$\begin{aligned} \delta J &= \varepsilon \int_{\Omega_0} \gamma \left(F_f - \frac{\partial}{\partial x} F_{f_x} - \frac{\partial}{\partial y} F_{f_y} \right) \mathrm{d}x\mathrm{d}y \\ &+ \varepsilon \int_{\partial\Omega_0} \gamma \left(F_{f_x}\mathrm{d}y - F_{f_y}\mathrm{d}x \right). \end{aligned}$$

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

$$\begin{aligned} \int_a^b \gamma F_{f_y}\big|_{y=0;\,1} \mathrm{d}x &= 0; \\ \int_0^1 \gamma F_{f_x}\big|_{x=a;\,b} \mathrm{d}y &= 0. \end{aligned}$$

Taking account of the obtained quadratic form, we get

$$\int_a^b \gamma f_y\big|_{y=0} \mathrm{d}x = 0, \tag{3.1}$$

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

on the horizontal lines. As pointed out in subsection 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), (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 for 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 $\left(af + b\frac{\partial f}{\partial n}\right)\big|_{\partial\Omega} = 0$ 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

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

The Dirichlet case is as easy to treat as before: the conditions $h_k(a) = h_k(b) = 0$, $k = 1, \dots, N$ are imposed on the solutions of (2.11). 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 $h_k'(a) = h_k'(b)$, $k = 1, \dots, N$ in terms of the system (2.11). However, one cannot fully separate variables in generic Robin conditions of form (3.3).

3.2. **Radiation condition.** Bearing in mind the resonance problem that is of main interest to us, let us consider a domain Ω such that, in notation of subsection 2.1 $x \in (a, \infty)$ and

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

for some $X > 0$. Similar assumptions are often made in papers dealing with scattering problems, for instance in [1, 15, 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

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

Here we denote

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

g_k are the same as in subsection 2.2. The coefficients s_k, $k = 1, 2, \dots$ 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. If the scattering coefficient $s_1(\omega)$ has a pole at $\omega = \omega_0$ we say that $\lambda = \omega_0^2$ is a resonance. This does not include all the resonances but only those lying on the first non-physical sheet (see [8] for detailed explanation). We refer to [17, 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 $s_1(\omega)\bar{s_1}(\bar{\omega}) = 1$ and that s_1 is analytic in the half-plane $\mathrm{Im}\omega < 0$. 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 perturbed 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 $|\mathrm{Im}\, t_k|$, $k = 1, 2, \dots$, are rather small and therefore the corresponding solution grows slowly.

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

$$h_1(x) \;=\; \exp(-tx) \;+\; s_1 \exp(tx), \qquad h_k'(x) \;=\; t_k h_k(x),\; k = 2, 3, \dots .$$

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

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

This formula known as the radiation, or outgoing wave condition singles out the solution whose first component grows and the 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 that using exterior complex scaling (see, for example, [8]). In this technique one replaces the operator by a family of operators on the same domain which depend 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).

4. NUMERICAL EXAMPLES

4.1. **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 (2.11) has a non-trivial solution satisfying

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

where

1 $\psi_a = \psi_b = (I,\, 0)$;
2 $\psi_a = (I,\, 0)$, $\psi_b = \psi_X$ as defined by (3.6).

Problem **1** provides approximations to the Dirichlet eigenvalues of a compact domain of kind (2.1); problem **2** 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] that we shall briefly outline below. The manifold of the solutions of the system (2.11) satisfying the left boundary condition is determined by

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

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

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

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 by $\tilde{\psi}(x) = \nu(x)\psi(x)$, where $\nu \in \mathbb{C}^{N\times N}$, $\det \nu \neq 0$. The function ν is chosen so that to ensure $\tilde{\psi}(x)\tilde{\psi}^*(x) = \text{const}$. The transfer equation now takes the form

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

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 obtain 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 by 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

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

as shown in [4]. It is this computational formula that we use to locate the complex eigenvalues of problem **2**. 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 **1** we applied Newton's method allowing us to calculate the eigenvalues of the self-adjoint problem.

Note that typically problem **2** is much harder to solve than **1**, 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

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

where α and γ are real positive constants (see fig. 1.1).

We shall be working in two different domains:

$$\Omega_{\mathbf{1}} = W \cap \{0 < \xi < \gamma\}, \qquad \Omega_{\mathbf{2}} = W \cap \{0 < \xi\}.$$

The domains $\Omega_{\mathbf{1}}$ and $\Omega_{\mathbf{2}}$ relate to problems **1** and **2** of the previous subsection, respectively. In the latter the resonance boundary condition is imposed at a sufficiently far point X as suggested in subsection 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. 1.2, so that the eigenvalue problem is decomposed into three separate problems. The

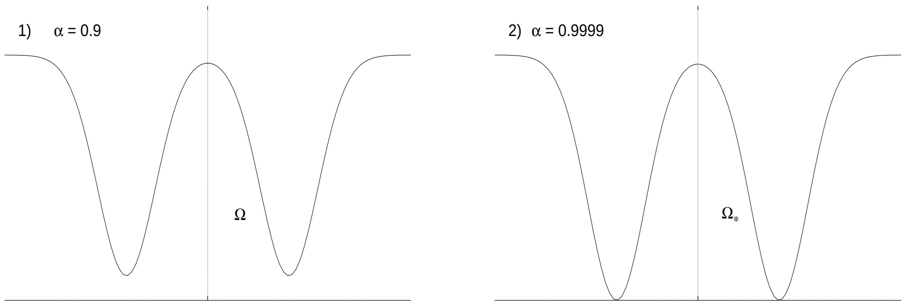

Figure 1. Waveguide with indentations

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 $\Omega_{\mathbf{1}}$ and $\Omega_{\mathbf{2}}$ satisfy the conditions of subsection 2.1 for $\alpha < \alpha_*$. We compute resonances, *i.e.* eigenvalues of problem **2** for a range of α using the perturbed cylinder approach. In the self-adjoint example the eigenvalues of problem **1** are found for the same values of α. The ODE problem is solved by the transfer method described in the previous subsection. 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 (2.11). This number should depend on α: indeed, for α close to α_* the width of the domain is small near $\xi = \gamma$ so that one needs to keep a larger number of terms $g_k(y)$ in (2.8). There are two possibilities here: first, to increase repeatedly the number of terms by one and solve the system with the corresponding constant number of unknowns until the answers converge. Secondly, instead of keeping a large number of terms throughout the interval one can start off with a smaller N in (2.11). 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 been using 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 the two problems **1** and **2** which makes us study them within the same framework. Namely, as $\alpha \to \alpha_*$ both the eigenvalues of $\Omega_{\mathbf{1}}$ and the resonances of $\Omega_{\mathbf{2}}$ converge to the Dirichlet eigenvalues of the domain Ω_*. These cannot be found by the same method because Ω_* has a cusp at $\xi = \gamma$ and is not a perturbed 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 **1** and **2**.

We applied the finite volume method to a series of problems of type **1** to compare the effectiveness of the two approaches. As expected, the comparisons are in favour of the discussed method, which appears to be several times faster than the conventional one. The benefits of our technique are more spectacular for larger values of α. For example, when $\alpha = 0.8$ it takes twice as long to get accurate results by the finite volume method, while for $\alpha = 0.9$ the new method is almost four times faster. Everything else being equal, the closer α gets to its critical value the more advantageous the perturbed cylinder approach is.

The numerical results presented below are related to the lowest Dirichlet eigenvalue of Ω_* and quoted in terms of the wave number $\omega = \sqrt{\lambda}$ (we shall 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. 2 a series of the eigenvalues of problem **1** 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 (2.11) depend on α linearly.

The resonances $\omega_{\mathbf{2}}$ emerging from the lowest eigenvalue as α decreases can be found in table 1. They are also shown in fig. 3 where their real parts are plotted against their imaginary parts. They definitely converge to ω_*. The problem is, of course, very sensitive to perturbations near the critical value of $\alpha = \alpha_*$, or $\varepsilon = 0$. However,

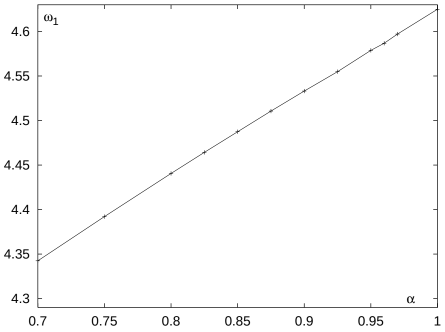

FIGURE 2. Eigenvalues of problem **1** for a range of α

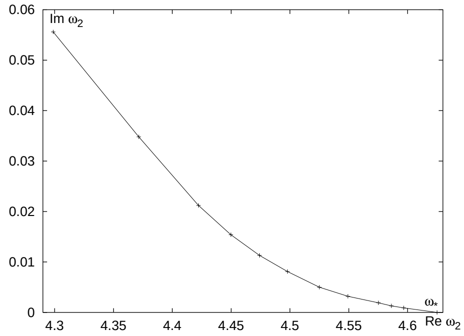

FIGURE 3. Resonances generated by ω_*

we believe that for $\alpha \le 0.97$ our computations are relatively stable and provide reliable results. For larger values of α we have observed various instability effects preventing us from computing resonances accurately. The system (2.11) 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 subsection, 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_*.

The α-dependence of the real and imaginary parts of the resonance originating from ω_* is shown in fig. 4. The real part is found to depend on the perturbation parameter linearly, whereas the imaginary part

TABLE 1. Resonances $\omega_{\mathbf{2}}$

α	$\omega_{\mathbf{2}}$	α	$\omega_{\mathbf{2}}$
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	$4.5967 + 0.0008i$

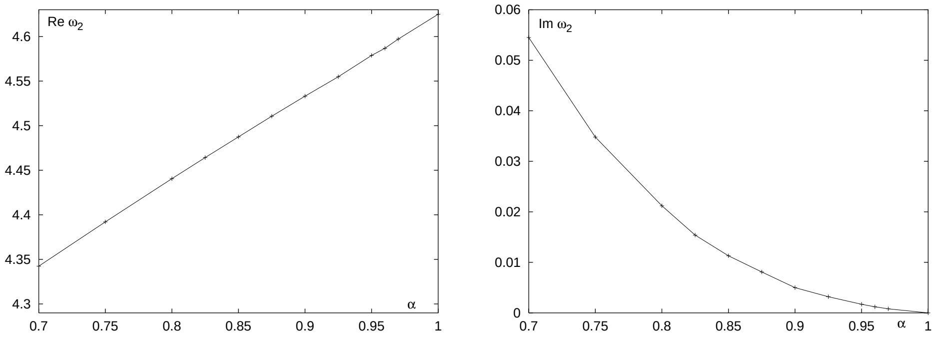

FIGURE 4. Real and imaginary parts of resonances: α-dependence

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 also that its real part and imaginary parts are expanded in powers of $\varepsilon^{1/2}$, $\varepsilon \downarrow 0$.

In the table below the eigenvalues of problem **1** are compared with the real parts of the resonances related to the same values of α. We

TABLE 2. The values of $\delta = \omega_{\mathbf{1}} - \operatorname{Re}\omega_{\mathbf{2}}$

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

tabulate the difference $\delta = \omega_{\mathbf{1}} - \operatorname{Re}\omega_{\mathbf{2}}$ between the Dirichlet eigenvalue and the real part of the associated resonance and observe that this quantity decreases as $\varepsilon \downarrow 0$. One might hope to deduce the rate of convergence of $\delta(\varepsilon)$ from asymptotic perturbation formulae. The question 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 perturbed cylinder to an ODE problem. Complex resonances occurring in perturbed 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 irregularly shaped domains of section 4. 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 of problem **1** by the finite volume method. As discussed in the previous section, it proved to be substantially more time-consuming than the method based on the separation of variables for the class of problems studied here. This is in agreement with the already mentioned results of [1, 15] 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.

REFERENCES

[1] L. Abrahamsson and H.-O. Kreiss. Numerical solution of the coupled mode equations in duct acoustics. *J. comput. Phys.*, 111:1–14, 1994.

[2] A. A. Abramov. A version of the pivotal condensation method. *Zh. vychisl. Mat. mat. Fiz. (Russian)*, 1:349–351, 1961.

[3] A. A. Abramov. A method of finding the eigenvalues and eigenfunctions of a self-conjugate differential problem. *Comp. Maths Math. Phys.*, 31:27–36, 1991.

[4] A. A. Abramov and L. F. Yukhno. Determining the number of eigenvalues of a spectral problem. *Comp. Maths Math. Phys.*, 34:671–677, 1994.

[5] S. Agmon. A perturbation theory of resonances. *Communs on Pure and Appl. Maths*, LI:1255–1309, 1998.

[6] A. Aslanyan, L. Parnovski, and D. Vassiliev. Complex resonances in acoustic waveguides. *Q. Jl Mech. appl. Math.*, 53:429–447, 2000.

[7] D. Borisov, P. Exner, R. Gadylshin, and D. Krejčiřík. Bound states in weakly deformed strips and layers. *(to appear)*, 2000.

[8] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon. *Schrödinger operators; with application to quantum mechanics and global geometry.* Texts and Monographs in Physics. Springer–Verlag, Berlin, 1987.

[9] E. B. Davies and L. Parnovski. Trapped modes in acoustic waveguides. *Q. Jl Mech. appl. Math.*, 51:477–492, 1998.

[10] D. V. Evans, M. Levitin, and D. Vassiliev. Existence theorems for trapped modes. *J. Fluid Mech.*, 261:21–31, 1994.

[11] P. Exner and D. Krejčiřík. Quantum waveguides with a lateral semitransparent barrier: spectral and scattering properties. *J. Phys. A*, 32:4475–4494, 1999.

[12] P. Exner and D. Krejčiřík. Waveguides coupled through a semitransparent barrier: a Birman–Schwinger analysis. *(to appear)*, 2000.

[13] P. Exner, P. Šeba, M. Tater, and D. Vaněk. Bound states and scattering in quantum waveguides coupled laterally through a boundary window. *J. Math. Phys.*, 37:4867–4887, 1996.

[14] H. D. Maniar and J. N. Newman. Wave diffraction by a long array of cylinders. *J. Fluid Mech.*, 339:309–330, 1997.

[15] K. Otto and E. Larsson. Iterative solution of the Helmholtz equation by a second-order method. *SIAM J. Matrix Anal. Appl.*, 21:209–229, 1999.

[16] R. S. Varga. *Matrix Iterative Analysis.* Prentice-Hall, Englewood Cliffs, 1962.

[17] P. Šeba, I. Rotter, M. Müller, E. Persson, and K. Pichugin. Collective modes in an open microwave billiard. *Physical Review E*, 61:66–70, 2000.

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