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Spectral algorithms for multiple scale localized eigenfunctions in infinitely long, slightly bent quantum waveguides

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ABSTRACT

A "bent waveguide" in the sense used here is a small perturbation of a two-dimensional rectangular strip which is infinitely long in the down-channel direction and has a finite, constant width in the cross-channel coordinate. The goal is to calculate the smallest ("ground state") eigenvalue of the stationary Schrödinger equation which here is a two-dimensional Helmholtz equation, $\psi_{xx} + \psi_{yy} + E\psi = 0$ where E is the eigenvalue and homogeneous Dirichlet boundary conditions are imposed on the walls of the waveguide. Perturbation theory gives a good description when the "bending strength" parameter ϵ is small as described in our previous article (Amore et al., 2017) and other works cited therein. However, such series are asymptotic, and it is often impractical to calculate more than a handful of terms. It is therefore useful to develop numerical methods for the perturbed strip to cover intermediate ϵ where the perturbation series may be inaccurate and also to check the pertubation expansion when ϵ is small. The perturbation-induced change-in-eigenvalue, $\delta \equiv E(\epsilon) - E(0)$, is $O(\epsilon^2)$. We show that the computation becomes very challenging as $\epsilon \to 0$ because (i) the ground state eigenfunction varies on both $O(1)$ and $O(1/\epsilon)$ length scales and (ii) high accuracy is needed to compute several correct digits in δ, which is itself small compared to the eigenvalue E. The multiple length scales are not geographically separate, but rather are inextricably commingled in the neighborhood of the boundary deformation. We show that coordinate mapping and immersed boundary strategies both reduce the computational domain to the uniform strip, allowing application of pseudospectral methods on tensor product grids with tensor product basis functions. We compared different basis sets; Chebyshev polynomials are best in the cross-channel direction. However, sine functions generate rather accurate analytical approximations with just a single basis function.

In the down-channel coordinate, $X \in [-\infty, \infty]$, Fourier domain truncation using the change of coordinate $X = \sinh(Lt)$ is considerably more efficient than rational Chebyshev functions $TB_n(X; L)$. All the spectral methods, however, yielded the required accuracy on a desktop computer.

1. Introduction

As reviewed in our previous article [1], there is considerable interest in the localized ground state eigenfunctions that arise when an infinitely long, uniform width quantum waveguide is perturbed by a localized bulge in the wall or by a sharp bend as shown schematically in Fig. 1. Perturbation theory, as developed in our article and by other articles we cite, is a good option when the perturbation parameter is very small. However, it is still desirable to develop numerical methods that can compute the eigenvalues and eigenfunctions with spectral accuracy.

The numerical computations have two large challenges. The eigenfunctions for the uniform, unperturbed waveguide are independent of the down-channel coordinate $x \in [-\infty, \infty]$ and are sinusoids in the cross-channel coordinate y. However, when the perturbation is very small but has a length scale comparable to the width of the waveguide (the usual case), the ground state eigenfunction has two widely disparate length scales. One is the $O(1)$ length scale of the wall perturbation. The other is the $O(1/\epsilon)$ length scale of the slow decay of the eigenfunction in the down-channel direction.

This is one numerical challenge, but verification of perturbation theory is also hard because, to provide any useful information about the accuracy of the perturbative approximation, the numerical method must accurately calculate the tiny *difference* between the perturbed and unperturbed eigenvalues.

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Table 1
Notation.

(x, y)	Cartesian coordinates for the physical domain
E	Schroedinger equation eigenvalue
$B(x, y)$	Boundary function: its zero isoline is the boundary
D	Total degree of a polynomial (for x^{m+n}, $D = m + n$)
H	Pseudospectral discretization matrix
$\mathcal{H}$	Laplace operator
L	Map parameter for rational Chebyshev functions TB_n
$\mathfrak{L}$	Map parameter for the sinh-Fourier method
M	Number of basis functions in X
N	Number of basis functions in Y, the cross-channel coordinate
N_{total}	Total number of functions in the tensor product basis, MN
P	Number of interpolation points
T	Parameter for parametric specification of the upper boundary curve
$\mathfrak{W}$	Boundary of the region $X \in [\mathfrak{W}, \infty]$ where asymptotic analysis yields an explicit approximation to the eigenfunction
X	Computational coordinate in the "down-channel" direction, $X \in [-\pi, \pi]$
Y	Computational coordinate perpendicular to the walls ("cross-channel coordinate"), $Y \in [0, 1]$
δ	Change in the ground state eigenvalue due to perturbation
ϵ	Perturbation parameter; strength of domain deformation
ν	Mode number for the y-dependent factor (cross-channel factor)
$\psi(x, y)$	Wavefunction [the unknown in the Schroedinger equation]
$\chi_n(X)$	One-dimensional basis in the down-channel computational coordinate X
$\Theta_n(Y)$	One-dimensional basis in the cross-channel computational coordinate Y
$\sigma(x, y)$	Metric factor in the PDE induced by conformal mapping

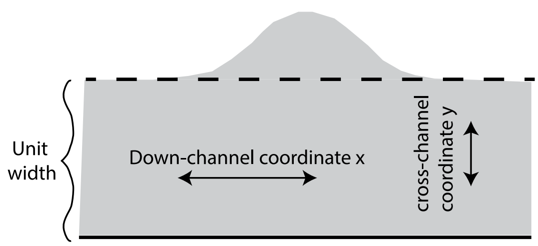

Fig. 1. Schematic of a bent waveguide. The unperturbed waveguide is a strip which is infinitely long in the "down-channel" coordinate x. The waveguides considered here are perturbed by bulges in one wall and are not actually bent. The jargon "bent waveguide" has become a shorthand for the class of "waveguides that are perturbations of a uniform-width, infinitely long rectangle by bend, bulging walls or other deformation that allows a bound state of finite energy".

Thus, a low order method is quite useless. All the algorithms applied here are spectrally accurate.

Spectral methods applied to a phenomenon with a single spatial scale are well understood as cataloged in [2–4]. However, applying spectral methods when there are multiple spatial scales is still an application on the research frontier. SIAM founded its *Journal of Multiscale Modeling and Simulation* not because multiple scales are passé, but because multiple scale methods are the frontier.

The eigenproblem is

$$\psi_{xx} + \psi_{yy} + E\psi = 0, \qquad \psi(x, y) = 0 \ \forall (x, y) \in \partial\Omega \tag{1}$$

where E is the eigenvalue and we impose homogeneous Dirichlet boundary conditions on the walls of the waveguide $\partial\Omega$. Important symbols are listed in Table 1. Note that subscripts with respect to a coordinate denote partial differentiation with respect to that coordinate, a convention employed throughout this article.

2. Strategies for an asymmetric channel

Many strategies have been applied to complicated domains, but we concentrate on approaches that are well-suited to perturbed rectangular domains: conformal mapping and the immersed boundary method. Both transform the waveguide from the "physical coordinates" (x, y) to computational coordinates (X, Y) where the domain is a channel of uniform unit width in the cross-channel coordinate Y, but extending indefinitely in the down-channel X coordinate. Thus, like the unperturbed domain, the computational domain in the coordinates (X, Y) is a rectangle.

We shall now briefly describe each strategy.

In the conformal mapping method, the computational domain is the infinite, uniform width channel in the coordinates (X, Y). This is the image of a non-rectangular domain under a conformal mapping. Because the mapping is conformal, the coordinate transformation merely multiplies the eigenvalue term in the Schrödinger equation by the metric factor. The "crowding" or "Geneva Effect", that is, a highly nonuniform grid, is fatal to most efforts at grid generation by conformal mapping [5]. Here, crowding is not an issue because the map is a *small perturbation* of the *identity transformation*. The conformal mapping used here is given by a simple analytical expression. However, an explicit conformal map may not be available. What then? One option is to calculate conformal maps using perturbation theory as in [6,7]. Another is to apply PDE-solvers that do not require a conformal mapping as elaborated below.

The key idea of an "immersed boundary" method is to embed the physical domain inside a computational domain which, in this case, is an infinite strip of uniform width [8–10]. Boundary conditions are imposed by Krylov's method [6]. That is, if the boundary is specified implicitly as the union of the zero isolines of a function $B(x, y)$, then homogeneous Dirichlet boundary conditions are enforced by writing the approximation as

$$\psi(x, y) = B(x, y)v(x, y) \tag{2}$$

where $v(x, y)$ is an unconstrained sum of tensor product basis functions.

An alternative to these approaches is to map the perturbed waveguide into the channel of uniform unit width using a non-conformal mapping. The bad news is that the metric factors will be numerous, significantly extending the debugging time. However, relaxing conformality opens up a vast spectrum of grid generation techniques for future studies.

3. A typical asymmetric channel

In the rest of the article, we focus on an example that is representative of a broad class of bent waveguides – more accurately described as "bulging waveguides" – in which the perturbation is a distortion of the shape of the upper boundary, $y = 1$. We shall concentrate on a particular distortion, but the methods applied are general. In our case, the perturbation is generated by the conformal map

$$F(z) = z + \epsilon \tanh(z), \qquad \epsilon \ll 1. \tag{3}$$

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