Bound states of two-dimensional nonuniform waveguides

M. Andrews and C.M. Savage
Department of Physics and Theoretical Physics, The Australian National University, Australian Capital Territory 0200, Australia
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We consider the theoretical problem of finding the bound eigenstates of an infinite nonuniform two-dimensional waveguide with Dirichlet boundary conditions. Using a coordinate transformation we show that this is equivalent to finding the eigenstates of a uniform waveguide with a potential proportional to the eigenvalue. Hence there is a sense in which the bound states occurring in nonuniform waveguides are analogous to bound states due to potentials in uniform waveguides.

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I. INTRODUCTION

It has recently been noted that infinite nonuniform waveguides with Dirichlet boundary conditions can have bound states [1–4]. The relevant mathematical problem is the solution of the Helmholtz equation with the eigenfunction zero on the waveguide boundary B:

$$\nabla^2\psi + k^2\psi = 0; \quad \psi(\mathbf{x}) = 0, \quad \mathbf{x} \in B. \tag{1}$$

Bound states can occur when the waveguide is bent [1], has an intersection [2], or a bulge [3]. The novel bound states can have eigenvalues below the continuum cutoff for the corresponding uniform waveguide. In this paper we provide a physical picture of these bound states, for the case of two spatial dimensions. This picture also facilitates their numerical computation.

The Helmholtz equation with Dirichlet boundary conditions arises in a variety of physical problems. For example, the TM modes of microwave waveguides satisfy it. The bound states correspond to nonpropagating eigenmodes below the propagation cutoff.

The time-independent Schrödinger equation for a free particle is just the Helmholtz equation. A steep potential barrier will approximate Dirichlet boundary conditions since it forces the wave function towards zero. Such a potential barrier is provided for atoms by the light shift potential in evanescent light fields [5–7]. These occur on the walls of hollow optical fibers and hence could be used to make atomic waveguides [8]. Nonuniformities in the evanescent field could then produce bound atomic states [9]. Such structures could be alternatives to the atomic cavities already proposed [10–12].

Two-dimensional waveguides for electrons may be formed by lateral confinement of two-dimensional electron gases at suitable heterojunctions. Bound states are predicted in nonuniform channels when the electron de Broglie wavelength, and coherence length, exceed the channel width [13].

The bound states can be understood by noting that for a uniform waveguide the eigenmodes are products of transverse and longitudinal sinusoids. The propagation cutoff is due to the existence of a longest transverse wavelength satisfying the boundary conditions. For a wider waveguide a longer wavelength, and lower eigenvalue, is possible. Bends, intersections, and bulges produce a region of the waveguide with a greater effective width, around which the bound state is localized.

In the following we provide another view of the origin of bound states. We will show that after a suitable coordinate change they can be regarded as arising from an effective potential in a uniform waveguide. A similar result was obtained by Goldstone and Jaffe for three-dimensional waveguides in the limit of slowly twisting waveguides [4].

This paper is organized as follows. In Sec. II we describe our transformation from the Helmholtz equation with nonuniform boundaries to a certain eigenvalue problem with uniform boundaries *and* a potential. In Sec. III we show how the transformation can be applied to the numerical calculation of the ground bound state of a waveguide with a bulge. The Appendix describes details of the numerical calculations.

II. THE TRANSFORMATION

We construct a new coordinate system (u, v) in which the waveguide boundaries are coordinate curves of v. Hence in the (u, v) system the boundaries are straight lines of constant v. The required transformation uses the solution $v(x, y)$ of Laplace's equation, $\nabla^2 v = 0$, which is a different constant on each boundary of the waveguide. Such a function is guaranteed to exist. From v one can construct another solution $u(x, y)$ of Laplace's equation, such that the coordinate system (u, v) is orthogonal. This is done as follows: the vector field $(\partial v/\partial y, -\partial v/\partial x)$ has no curl and therefore there exists a function u such that

$$\nabla u = \left(\frac{\partial v}{\partial y}, -\frac{\partial v}{\partial x}\right). \tag{2}$$

It follows that $\nabla^2 u = 0$ and also that $(\nabla u)^2 = (\nabla v)^2$. Geometrically, u is constructed to be constant along trajectories orthogonal to the curves of constant v, and u

increases along curves of constant v at a rate such that $|\nabla u| = |\nabla v|$.

Now for any function $\psi(x,y)$, write $\phi(u,v) = \psi(x,y)$. Then

$$\nabla^2\psi = \frac{\partial^2\phi}{\partial u^2}(\nabla u)^2 + \frac{\partial^2\phi}{\partial v^2}(\nabla v)^2 + \frac{\partial\phi}{\partial x}(\nabla^2 u) + \frac{\partial\phi}{\partial y}(\nabla^2 v) = h(u,v)\nabla^2\phi, \quad (3)$$

where

$$h(u,v) = (\nabla u)^2 = (\nabla v)^2. \quad (4)$$

Thus in the new coordinates the waveguide is straight and the Helmholtz equation (1) becomes

$$\nabla^2\phi + k^2\phi = k^2[1 - h^{-1}(u,v)]\phi = V_k\phi, \quad (5)$$

where we have defined the effective potential

$$V_k \equiv k^2[1 - h^{-1}(u,v)]. \quad (6)$$

This potential depends on the eigenvalue k^2 and is hence not a physical potential. Nevertheless, restricting our consideration to a particular eigenfunction we can understand its form as arising from its potential V_k. Such a view could be useful, for example, in the analysis of the decay of a quasibound state when the waveguide is not infinite. In that case other eigenfunctions are not involved.

The existence of the potential suggests an interesting possibility. A periodic boundary will generate a periodic potential. Such a potential has Bloch type eigenfunctions and the possibility of band gaps. For example, we might expect to find atomic band structure in a hollow optical fiber atomic waveguide with a periodic evanescent field [14]. Such a field would result from the interference of counterpropagating light waves.

III. AN EXAMPLE

In this section we apply our transformation to a specific nonuniform waveguide. We start from the observation that the real, u, and imaginary, v, parts of any analytic function $F(z)$ of the complex variable $z = x + iy$,

$$F(z) = u(z) + iv(z), \quad u,v \in \{\text{real functions}\}, \quad (7)$$

satisfy Laplace's equation. This provides candidate functions $v(x,y)$ for defining waveguide boundaries. Furthermore, the Cauchy-Riemann equations tell us that since $v(x,y)$ is the imaginary part of an analytic function, the real part $u(x,y)$ defines the required coordinate orthogonal to v.

In particular the real and imaginary parts of the analytic function

$$F(z) = z\left(1 - \frac{a}{1+z^2}\right) = u + iv, \quad (8)$$

are suitable orthogonal coordinates. We will use the parameter value $a = 0.25$ in all our calculations. The coordinate lines u = const and v = const are shown in Fig. 1(a). We consider a nonuniform two-dimensional waveguide bounded by the coordinate lines $v = 0.3$ and $v = -0.3$. This waveguide has a bulge at its center and hence has a bound state localized there. In terms of the (x,y) coordinates v is given by

$$v = y + \frac{ay(x^2+y^2-1)}{4x^2y^2 + (1+x^2-y^2)^2}. \quad (9)$$

So in (x,y) coordinates the waveguide boundary is defined implicitly by the solutions of this equation for $v = \pm 0.3$. In terms of the (x,y) coordinates u is given by

$$u = x - \frac{ax(1+x^2+y^2)}{4x^2y^2 + (1+x^2-y^2)^2}. \quad (10)$$

Note that as $x \to \infty$ the (u,v) coordinates approach the (x,y) coordinates.

We now give numerical solutions for the ground bound state of this waveguide. These will be compared to those for the transformed problem. The ground state eigenvalue for this waveguide is $k^2 \approx 19.6$. This may be compared to the cutoff for a uniform waveguide of width 0.6 units which is $k^2 = (\pi/0.6)^2 \approx 27.4$. As expected the ground state eigenvalue is below the uniform waveguide

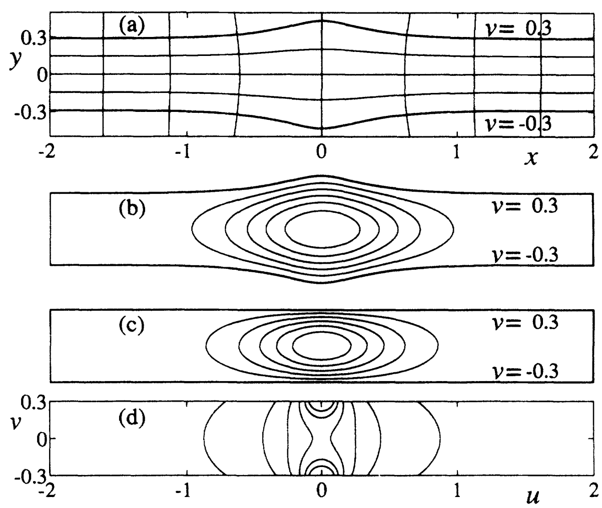

FIG. 1. The example waveguide and bound state in natural (x,y) and transformed (u,v) coordinates. The coordinates are chosen so that the propagation direction for a uniform waveguide would be along x or u. (a) The (u,v) coordinate curves defined by Eqs. (9) and (10). The waveguide boundaries are $v = \pm 0.3$. (b) Contour plot of the ground bound state $\psi(x,y)$ in (x,y) coordinates. The waveguide boundaries $v(x,y) = \pm 0.3$ and $x = \pm 2$ are shown by thick lines. (c) Contour plot of the ground bound state $\phi(u,v)$ in (u,v) coordinates. The waveguide boundaries $v = \pm 0.3$ and $u = \pm 2$ are shown by thick lines. (d) Contour plot of the effective potential $V_k(u,v)$ defined by Eq. (6). The contour levels are from 0 to -1.25 in steps of 0.25.

cutoff. The ground bound state is shown in Fig. 1(b). It was found numerically by the pseudotime method described by Schult *et al.* [2]. This method is based on the conversion of the elliptic Helmholtz equation into a parabolic equation. Then all the Helmholtz equation eigenfunctions decay in pseudotime, but the ground state decays most slowly and hence dominates the solution after a sufficiently long pseudotime. Renormalization of the solution is used to prevent it decaying to zero. Computational details are discussed in the Appendix.

A similar numerical method can be applied to the transformed Helmholtz equation. Equation (5) is an unsuitable form because it requires the eigenvalue to be known. A suitable form for numerical work is found by multiplying Eq. (5) through by $h(u, v)$:

$$h(u,v)\nabla^2\phi + k^2\phi = 0. \tag{11}$$

The boundary conditions are now that the wave function is zero on the coordinate lines $v = \pm 0.3$, which are of course straight lines in the (u, v) coordinate system. This simplifies the numerical implementation of the boundary conditions and is an advantage of the transformed Helmholtz equation. We have numerically solved the transformed equation (11) and obtained the eigenvalue $k^2 = 19.4$, which is within 1% of the value obtained in the (x, y) coordinate system. The eigenfunction is shown in Fig. 1(c). By transforming back to (x, y) coordinates we confirmed that it is identical to the eigenfunction obtained by solving the original Helmholtz equation.

The effective potential V_k, Eq. (6), for this waveguide is shown in Fig. 1(d). It approaches zero for large v and is most negative at $u = 0$ and $v = \pm 0.3$. As previously discussed the ground bound state Fig. 1(c) can be viewed as arising from this potential.

In conclusion we note that the two forms of the transformed Helmholtz equation, Eqs. (5) and (11), embody the two advantages of the transformation to straight boundaries. The first form, Eq. (5), allows us to understand bound states in terms of a confining potential instead of in terms of nonuniform boundaries. The second form, Eq. (11), simplifies the treatment of the boundaries in numerical solutions.

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APPENDIX A: COMPUTATIONAL DETAILS

The function h is defined by Eq. (4) to be a function of (x, y). However to use it in the transformed Helmholtz equations (5) and (11) we need it as a function of (u, v). Hence the equations $u = u(x, y)$, $v = v(x, y)$ must be (numerically) solved to obtain x and y as functions of u and v. Once this is done a substitution yields $h(u, v)$ from $h(x, y)$.

The infinite waveguide must be truncated for computations. Hence Dirichlet boundaries were put at the ends; at $x = \pm 2$ and at $u = \pm 2$. Moving these boundaries confirmed that this was far enough out not to affect the ground state.

The bound state in Fig. 1(b) was obtained with an (x, y) grid spacing of 0.01 units. The computed eigenvalue was $k^2 = 19.9$. Decreasing the grid spacing to 0.005 units gave $k^2 = 19.6$.

The bound state in Fig. 1(c) was obtained with a (u, v) grid spacing of 0.01 units. The computed eigenvalue was $k^2 = 19.4$. Decreasing the grid spacing to 0.005 units also gave $k^2 = 19.4$.

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