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Confined modes in two-dimensional tubes

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We survey various numerical methods for finding solutions of quantum confined states. We especially consider states in two-dimensional (2D) tubes, or 2D surfaces that are confined in the transverse direction but are unconfined in the longitudinal direction. We first review existence proofs for bound states in long 2-D tubes. We then review various methods for finding such states and we discuss the significance of these eigenstates. © 2012 American Association of Physics Teachers. [<http://dx.doi.org/10.1119/1.4751875>]

I. INTRODUCTION

When inventing problems for introductory courses in quantum mechanics, it is common for instructors to avoid the complications of space-dependent potentials by dealing with motion in a region with constant (i.e., zero) potential, bounded by hard walls. By doing so, one can focus on the effects of the boundary conditions on the solutions. Thus, the student typically begins with a one-dimensional “box,” after which he/she can study a box in two or three dimensions. As we will show in this article, solutions on two-dimensional surfaces exhibit a number of interesting quantum properties, symmetries, and degeneracies. In this paper, we consider a number of simple two-dimensional (2D) hard-wall geometries, which can be straightforwardly solved numerically by undergraduates, and we give examples of the types of solutions that can be demonstrated for such systems.

One example of a 2D system that has been widely investigated is a 2D region where a particle is confined to a cavity. Such systems have a direct analog with electromagnetic waves in a 2D cavity. For electrons moving in a 2D cavity in a quantum heterostructure, such a state is commonly referred to as a “quantum dot.”¹ In this paper, our emphasis will be on particles moving in long tubes or channels, where the particle is confined in the transverse direction but can move freely in the longitudinal direction. Such states for electrons in quantum heterostructures are referred to as “quantum wires” or “electron waveguides.”¹ It has been relatively recently understood that under a rather general set of conditions, confined modes will exist in these 2D tubes, despite the fact that confined modes would not exist for classical particles in such a system.² As we will show, any localized bulge or bend in an otherwise straight channel or “quantum wire” will give rise to a stationary state which has a lower energy than the threshold energy for free motion down the channel; the corresponding wave function is thus localized. Two popular textbooks have posed problems dealing with these states (problem 7.20 in Ref. 3 and problem 8.21 in Ref. 4), but the approaches used in these problems involved variational methods or limiting cases, which are sufficient to demonstrate the existence of a confined mode but which can give a rather poor value for the energy. In this paper we discuss various numerical methods by which one can obtain accurate answers, and in certain cases extremely precise values, for the eigenstates in simple geometries.

We will survey some techniques for obtaining exact (numerical) solutions for these systems. Our aim is to demon-

strate the emergence of these very interesting results in simple 2D geometries, while keeping the level of complexity suitable for an undergraduate who wants to solve novel and nontrivial problems that require numerical computation but at the same time are not overly difficult.

II. MOTION IN SIMPLE TWO-DIMENSIONAL SYSTEMS

Consider a quantum particle confined to a flat two-dimensional surface. The easiest problem for us to consider is one in which a particle moves in a surface for which there is zero potential inside a particular region but an infinite potential on the walls of that region. This is simply the two-dimensional analog of the classic one-dimensional box problem that is a staple of introductory quantum mechanics courses. The wave function of a particle inside such a region will satisfy the time-independent Schrödinger equation (equivalently, the Helmholtz equation),

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + k^2 \right] \psi(x, y) = 0, \text{ where } k^2 = \frac{2mE}{\hbar^2}. \quad (1)$$

The hard-wall boundary condition requires $\psi|_S = 0$, where S is the outer boundary of the region.

Like the one-dimensional quantum box, such idealized 2D systems provide many interesting examples of quantum behavior. They are also directly relevant to several realistic situations. For example, in quantum heterostructures one is able to restrict the motion of electrons so that they travel predominantly in two dimensions. There are now several monographs that discuss experimental methods for producing these heterostructures and the properties of electron states in these low-dimensional systems.^{1,5–10}

One has an analogous situation for electromagnetic fields inside a resonating cavity. If we consider a thin cavity with conducting walls such that the height h along the vertical (which we define as the z direction) is small compared to any dimension in the base, then to lowest order the EM fields inside the cavity satisfy Maxwell’s equations in vacuum,

$$\nabla \times \mathbf{E} = i \frac{\omega}{c} \mathbf{B}; \quad i \frac{\omega}{c} \nabla \times \mathbf{B} = \frac{\omega^2}{c^2} \mathbf{E}. \quad (2)$$

In Eq. (2), the $\mathbf{E}$ and $\mathbf{B}$ fields in the interior are harmonic with angular frequency ω . The lowest-energy state in a thin cavity will be a TE mode where the $\mathbf{E}$ field has only a z

component, and that component will have no z dependence. Defining $\mathbf{E} = E_z(x, y)e^{-i\omega t}\hat{\mathbf{k}}$, Maxwell's equations for the $\mathbf{E}$ field then reduce to the equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\omega^2}{c^2} \right] E_z(x, y) = 0. \quad (3)$$

Comparing Eqs. (1) and (3), we see that there is an exact correspondence between the wave function for a quantum particle in a 2D surface and the electric field for the lowest TE mode in an identical surface, namely, that

$$\psi(x, y) = E_z(x, y), \quad \text{with } k^2 = \frac{\omega^2}{c^2}. \quad (4)$$

An extremely important feature of the Helmholtz equation (and also Maxwell's theory) is the fact that these systems obey simple scaling laws. For particles that obey the Helmholtz equation, if the lengths are scaled by some factor η , then the system will be invariant if the momentum k scales as $k' = k/\eta$ and the energy scales by $E' = E/\eta^2$. So without loss of generality, observables can be calculated at any convenient scale and the units rescaled to fit any physical device. Throughout this article will therefore work with a scaled Helmholtz equation, that is, we will remove the length scale a in the problem by working with dimensionless coordinates $x' = x/a$ and $y' = y/a$. After we find the eigenvalue k'^2 in the dimensionless Helmholtz equation

$$\left[\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} \right] + k'^2 \psi(x', y') = 0, \quad (5)$$

the energy eigenvalue of the original Schrödinger equation can be recovered from

$$E = \frac{\hbar^2 k'^2}{2ma^2}. \quad (6)$$

In Sec. III, we will work with dimensionless equations but drop the primes.

III. SOLUTIONS FOR MODES IN A TWO-DIMENSIONAL TUBE

We will confine our attention to infinitely long two-dimensional surfaces with simple geometries. These will serve as analogs of a “quantum wire,” or a long open two-dimensional surface. The simplest system we can envision is a long straight tube, which we scale to have unit width. If we define the x direction along the length of the tube and the y direction to be transverse with $0 \leq y \leq 1$, then we can expand solutions of the Helmholtz equation in terms of a series of transverse modes:

$$\psi(x, y) = \sum_{n=1}^{\infty} A_n e^{\pm i\alpha_n x} \sin(n\pi y); \quad \alpha_n = \sqrt{k^2 - (n\pi)^2}. \quad (7)$$

Since the lowest transverse mode ($n = 1$) has (dimensionless) transverse energy $k^2 = \pi^2$, the threshold for eigenmodes in the straight tube is $k_{\min} = \pi$, and we have a continuum of solutions that are sinusoidal in the longitudinal coordinate for any wave number $k > k_{\min}$. For a given value $k > k_{\min}$, one

or more of the longitudinal wave numbers α_n in Eq. (7) will be real and will represent sinusoidal solutions in the longitudinal direction. For higher values of n , in “closed” modes, the longitudinal wave number α_n for that mode will be imaginary and the wave functions in those modes will be exponentially damped. In waveguides, these are termed the “evanescent” modes.^{11,12} A tube of unit width that is straight everywhere will have no localized modes, and hence no solutions for $k < \pi$.

Consider next a long straight 2D tube with infinite confining walls and unit width everywhere, except for a local “bulge,” a finite region where the width is greater than 1. This is shown schematically in Fig. 1. For a sufficiently large bulge, the tube will contain one or more “confined” or localized modes, i.e., local solutions with wave number less than π ; such solutions will be trapped in the vicinity of the bulge as they cannot escape down the (unit) width of the straight tube. An interesting question is how large the bulge needs to be in order to support at least one confined mode. We may phrase the question in this way: Will any localized bulge, no matter how small, in a 2D tube of otherwise constant width support a locally confined mode? The answer (perhaps surprising) is yes: Any tube with hard walls that is otherwise straight, but contains a localized bulge, no matter what the shape or size of that bulge, will possess at least one confined mode.

We will give a heuristic proof that a tube with hard walls and a sufficiently gentle bulge will always possess at least one confined mode. Define $W(x)$ as the width of the tube at the point x . For large $|x|$, $W(x) = 1$ and $W(x) > 1$ in the bulge region. Choose a trial wavefunction $\psi_t(x, y)$ as given in the first line of Eq. (8). Inserting this trial function into the Schrödinger equation produces the second line of Eq. (8):

$$\begin{aligned} \psi_t(x, y) &= f(x) \sin \left[\frac{\pi y}{W(x)} \right] \\ &- \frac{d^2 f(x)}{dx^2} + \frac{\pi^2}{W(x)^2} f(x) \approx k^2 f(x). \end{aligned} \quad (8)$$

The final expression of Eq. (8) follows if we can enforce an “adiabatic” condition, namely that the bulge is sufficiently gentle that we can neglect all derivatives of $W(x)$. We then obtain a one-dimensional differential equation for $f(x)$ with an effective potential $\pi^2/W(x)^2$ that has a local minimum in the bulge region where $W(x) > 1$. As is well known, for the Schrödinger equation in one dimension, any local minimum in the potential will support at least one bound state. Obviously the “proof” we have provided is not general as it relies on the bulge satisfying an adiabatic condition. The proof that there exists a confined mode for any localized bulge in a 2D tube was given by Bulla *et al.*,¹³ who found a variational solution for the general problem.

Fig. 1. Schematic picture of a two-dimensional tube that is straight everywhere, with infinite potential walls on the outer surface, except for a localized “bulge.”

Fig. 2. Simple two-dimensional tubes. Left: L-shaped tube; we can choose the transverse dimension of this tube to be 1. Right: a tube shaped like a cross.

So a long otherwise straight tube with a bulge will always possess a confined mode or bound state. What about a long straight tube that has a local bend? First, consider an L-shaped tube, such as is shown in the left-hand side of Fig. 2. It was shown by Lenz *et al.*¹⁴ that a bound state existed in such a tube. Then Schult *et al.*¹⁵ found that a bound state existed in a cross geometry shown on the right-hand side of Fig. 2. Such observations were surprising; to the best of our knowledge, it had not been previously realized that such open systems would support a confined or bound state. Remembering the exact analogy between tubes and waveguides, this also implies that bent waveguides will possess a confined mode below the cutoff frequency. Carini *et al.*^{16,17} demonstrated that a waveguide in the form of an L-shaped tube possessed a confined mode below the cutoff frequency, at just the location predicted by numerical calculations.

Note that the tubes shown in Fig. 2 actually represent a combination of a “bend” and a “bulge.” For example, in the L-shaped tube, although the transverse width in the arms of the tube is 1, at the bend in the tube the length of the diagonal is $\sqrt{2}$. Consequently, we would suspect that there would exist at least one confined mode in each of these tubes, based on the proof for a tube with a bulge.¹³

How about the case of a tube of constant width with a localized bend? It may be surprising to the reader to learn that such tubes also always possess at least one confined mode. In 1992 Goldstone and Jaffe proved by variational techniques^{18,19} that any 2D tube of constant width with a local bend possesses at least one confined mode; their proof was extended by Renger and Bulla.²⁰

The existence of such localized modes in two-dimensional surfaces has many interesting consequences and potential applications. For example, a waveguide containing a bend will possess at least one confined mode below the cutoff frequency. An analogous situation occurs in photonic crystals, which may also have localized modes due to the prevention of light propagation by photonic band gaps;²¹ possible applications for such modes were reviewed in the monograph by Joannopoulos *et al.*²²

Electrons in “quantum wires” will possess at least one bound state if the wire contains a bend. An application using this property can be obtained by creating a series of identical bent quantum wires and stacking them vertically. An electron confined mode (bound state) will exist at the bend of each wire; the confined electron wave function will be large in the vicinity of the bend and will decay exponentially along the wire. Since the bound-state wave functions are identical for each wire, electrons allowed to move in these quantum heterostructures will produce one identical confined electron state at the bend in each wire. Wegscheider *et al.* produced a series of T-shaped intersections in GaAs systems.²³ When this system was exposed to an appropriately tuned laser

beam, stimulated optical emission was observed from electrons and holes in the T intersections. Finally, if one considers a series of coupled 2D cells, then the existence of confined modes can produce trapped modes localized in the vicinity of a defect in a periodic “quasicrystal.”^{24–26}

In the remainder of this article, we will examine the existence and properties of localized modes in bent 2D tubes. For examples, we will choose the simple geometries shown in Fig. 2. We will start by reviewing various methods for determining eigenmodes and eigenfunctions for the L-shaped tube and the “cross” geometry.

A. Variational method

Before turning to the more complicated (and accurate) numerical techniques, we review an interesting variational solution for the bound state of the crossed-wires geometry shown in Fig. 2. This example is homework problem 7.20 in the introductory quantum mechanics text by Griffiths.³

In the variational method, one finds a trial wave function $\psi_{\text{tr}}(x, y)$, which satisfies the boundary conditions for the problem. From this trial wave function, we can produce a variational energy E_{var} which can never be less than the lowest eigenmode energy. Thus we have

$$E_{\text{gs}} \leq E_{\text{var}} \equiv \frac{\langle \psi_{\text{tr}} | H | \psi_{\text{tr}} \rangle}{\langle \psi_{\text{tr}} | \psi_{\text{tr}} \rangle}, \quad (9)$$

from which we obtain an upper bound on the lowest eigenmode energy E_{gs} .

For convenience, we choose the half-width of the channel as the length scale (which we normalize to 1) and place the center of the coordinate system at the center of the cross, as shown in Fig. 3.

Then we introduce a trial wave function containing a single variable parameter α :

$$\psi_{\text{tr}}(x, y) = A \begin{cases} (1 - |xy|)e^{-\alpha}, & |x| \leq 1 \text{ and } |y| \leq 1 \\ (1 - |x|)e^{-\alpha|y|}, & |x| \leq 1 \text{ and } |y| > 1 \\ (1 - |y|)e^{-\alpha|x|}, & |x| > 1 \text{ and } |y| \leq 1 \\ 0, & \text{otherwise} \end{cases} \quad (10)$$

Fig. 3. Coordinates and regions for the 2D cross problem.

which like the wave function for the true ground state is symmetric under reflection about both the x and y axes. The trial function obeys the boundary conditions in that it is continuous and it vanishes on the channel boundaries; note, however, that the first derivative of the trial function has discontinuities (i.e., the trial function has “roof lines”). Taking the second derivatives of the trial wave function will produce delta functions that must be accounted for. When this is done one obtains the result

$$\frac{\langle \psi_{\text{tr}} | H | \psi_{\text{tr}} \rangle}{\langle \psi_{\text{tr}} | \psi_{\text{tr}} \rangle} = \frac{6(\alpha^2 + 2\alpha + 3)}{11\alpha + 6}. \quad (11)$$

Minimizing Eq. (11) with respect to α produces the result $E_{\text{var}} = 2.12$, which is below the threshold for wave propagation in a channel (since the scaled width of the channel is 2, the threshold energy is $E_{\text{thr}} = \pi^2/4 \approx 2.48$). The variational method demonstrates that this system must have at least one bound state, and the energy of the lowest confined mode must be less than $(0.85)E_{\text{thr}}$.

The exact result was first found by Schult *et al.*¹⁵ by a relaxation method (to be described below) with the result $E_{\text{gs}} = (0.66)E_{\text{thr}}$ (the system possesses only a single confined mode). Note that the trial function in Eq. (10) accounts for only about half of the actual binding energy.

B. Mode matching methods

A quantitative method for obtaining eigenmodes and eigenvalues in a bounded two-dimensional surface is to expand the function in modes in the various sections of the tube, and then match the mode expansions at the section boundaries. We illustrate the method of mode matching in solving for eigenmodes and eigenvalues in the L-shaped geometry shown in Fig. 4. Here, the length scale a is the transverse width of the tube, so after normalizing to unit width we consider an L-shaped tube with two long straight sections of width 1 attached to a central square of side 1. The first proof that an L-shaped tube has a confined mode was by Lenz *et al.*¹⁴ Their method involved finding the poles of the P matrix which was introduced by Jaffe and Low.²⁷ Carini *et al.*^{16,17} subsequently solved this by mode-matching methods which we review here; they also carried out experimental

Fig. 4. Regions in the L-shaped tube.

studies of modes in bent waveguides and found the confined mode below threshold frequency, using the exact analogy between confined modes in a 2D tube and modes in a bent waveguide of the same shape.

We divide the tube into three regions labeled I, II, and III as shown in Fig. 4, and we place the origin of the coordinate system at the lower left-hand corner. Both the Helmholtz equation and the geometry of the tube are symmetric with respect to interchanging x and y (i.e., reflections about the line $x=y$); consequently all eigensolutions will be either symmetric or antisymmetric under the interchange $x \leftrightarrow y$. It is therefore sufficient to expand the solutions only in regions I and II; the solution for region III will either be equal to or opposite in sign to the reflected solution in region I.

We apply the mode matching method to calculate the confined eigenmode for the system. With this geometry we have only one confined mode, and the confined eigenfunction will be symmetric under the interchange $x \leftrightarrow y$. In the mode matching method, we expand the solution in region I in an infinite series of solutions each of which satisfies the Helmholtz equation and vanishes on the outer boundaries, $y=0$ and $y=1$. Because the state is confined it will vanish exponentially with increasing x . In region II, we find a solution that is symmetric under interchange of x and y and that vanishes on the boundaries $x=0$ and $y=0$, namely,

$$\begin{aligned} \psi_I(x, y; k) &= \sum_{n=1}^{\infty} A_n e^{-\alpha_n x} \sin(n\pi y), \\ \psi_{II}(x, y; k) &= \sum_{n=1}^{\infty} B_n [\sin(n\pi x) \sinh(\alpha_n y) + \sinh(\alpha_n x) \sin(n\pi y)], \\ \alpha_n &= \sqrt{(n\pi)^2 - k^2}. \end{aligned} \quad (12)$$

The coefficients A_n and B_n are determined by requiring that the eigenfunctions and their normal derivatives are continuous at the boundary between regions I and II, namely the line $x=1$. The first condition leads to the equality of two series:

$$\sum_{n=1}^{\infty} A_n e^{-\alpha_n} \sin(n\pi y) = \sum_{n=1}^{\infty} B_n \sinh \alpha_n \sin(n\pi y). \quad (13)$$

From Eq. (13) by the uniqueness of Fourier expansions we obtain

$$A_n = B_n e^{\alpha_n} \sinh \alpha_n. \quad (14)$$

Enforcing the continuity of the normal derivatives at $x=1$ gives the relation

$$\sum_{n=1}^{\infty} A_n (-\alpha_n) e^{-\alpha_n} \sin(n\pi y) = \sum_{n=1}^{\infty} B_n (n\pi) (-1)^n \sinh(\alpha_n y). \quad (15)$$

We then expand the function $\sinh(\alpha_n y)$ on the interval $0 < y < 1$ in a Fourier series

$$\begin{aligned} \sinh(\alpha_n y) &= \sum_k d_{nk} \sin(k\pi y), \quad \text{where} \\ d_{nk} &= \frac{-2k\pi (-1)^k \sinh \alpha_n}{\alpha_n^2 + (k\pi)^2}. \end{aligned} \quad (16)$$

Substituting into Eq. (15), we equate the coefficients of $\sin(k\pi y)$ on both sides of the equation. In doing so, we are assuming that when these equations are truncated the results will still converge properly; this was shown by Exner *et al.*²⁸ Once this is done we obtain a result that can be written in matrix form as

$$\mathbf{Z}(k) \mathbf{B} = 0, \text{ where}$$

$$Z_{mn}(k) = \frac{\alpha_n}{\sinh(\alpha_n)} \delta_{m,n} + \frac{m\pi(-1)^m e^{-\alpha_m}}{\sinh(\alpha_m)} d_{nm}. \quad (17)$$

The matrix $\mathbf{Z}$ depends explicitly upon the wave number k . Thus a sufficient condition for a confined mode is that the determinant of $\mathbf{Z}(k)$ vanish at that value of k . The symmetric confined eigenmode for the system can be located by constructing the matrix $\mathbf{Z}$ and finding the value of k for which the determinant of $\mathbf{Z}(k)$ vanishes. Once the confined eigenmode is determined, the corresponding eigenfunction can straightforwardly be constructed.

In practice, one truncates the infinite matrix $\mathbf{Z}$ at some finite number of modes, and then searches for the value of k where the determinant of $\mathbf{Z}(k)$ changes sign. As the number N of expansion modes increases, the precision of the eigenmode increases until at some point the matrix becomes so large that determinant-finding algorithms begin to introduce errors. In this way, one can determine the confined eigenmode to a decent precision. One obtains $k^2 = 0.9296\pi^2$, where π^2 is the start of the continuum. Thus, one obtains a weakly bound state for the L-shaped tube. In Fig. 5, we plot the eigenfunction for the confined mode. As expected, it is large in the center and decays exponentially along the channels of the tube.²⁹

Exercise: Set up the mode-matching solution for the cross geometry of Fig. 3. Hint: If we use the same coordinates as in that figure, the wave function in the right arm should be a linear sum of functions of the form

$$\psi_{\text{right}} \sim e^{-\beta_n x} \cos(n\pi y/2), \text{ where } \beta_n = \sqrt{\frac{n^2 \pi^2}{4} - k^2}, \quad (18)$$

and the wave function in the center region should be a combination of terms of the form

$$\psi_{\text{center}} \sim [\sinh(\beta_n x) \cos(n\pi y/2) + \sinh(\beta_n y) \cos(n\pi x/2)]. \quad (19)$$

Fig. 5. The bound state eigenfunction for the L-shaped tube, corresponding to eigenmode value $k^2 = 0.9296\pi^2$.

Once you have the matrix $\mathbf{Z}(k)$, search for the value of k that gives a zero determinant. With this choice for the length scale, a bound state has a solution with $k^2 < \pi^2/4$.

C. Method of relaxation for a tube

The “method of relaxation” is so named because it begins with a trial solution to the Helmholtz equation and with repeated application of a particular operator the function evolves over time into the correct ground state solution for the problem. Relaxation methods involve splitting the sparse matrix that arises from finite differencing and iterating to obtain a solution. The general method is outlined in Section 17.5 of the book *Numerical Recipes*.³⁰

We begin with a trial solution $\psi(\mathbf{r})$ of the problem which satisfies the boundary conditions. (For our hard-wall cavities, $\psi = 0$ at the boundaries.) The scaled Hamiltonian $H = -\nabla^2$ (with boundary conditions) gives a complete set of eigenstates $\psi_0(\mathbf{r}), \psi_1(\mathbf{r}), \dots$ with eigenvalues $\varepsilon_0, \varepsilon_1, \dots$ and where ψ_0 is the unique ground state with energy ε_0 where $\varepsilon_0 < \varepsilon_n$ for $n \neq 0$. The trial function $\psi(\mathbf{r})$ has a unique expansion in terms of the complete set of eigenstates:

$$\psi(\mathbf{r}) = c_0 \psi_0(\mathbf{r}) + c_1 \psi_1(\mathbf{r}) + \dots \quad (20)$$

We introduce another variable τ (analogous to a time variable) and then consider τ -dependent solutions $\Psi(\mathbf{r}, \tau)$ of the equation

$$\frac{\partial \Psi}{\partial \tau} = \nabla^2 \Psi, \quad (21)$$

with “initial” condition $\psi(\mathbf{r}) = \Psi(\mathbf{r}, \tau = 0)$. Equation (21) is of the same form as the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H\Psi = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) \quad (22)$$

(for which the full bound-state wave functions are solutions), but where t has been replaced by $-i\tau$.

Separating the variables $\mathbf{r}$ and τ in the new problem and using the fact that we already have the complete set of eigenstates for the operator ∇^2 , we find that the τ -dependent function corresponding to our trial function $\psi(\mathbf{r})$ is

$$\Psi(\mathbf{r}, \tau) = c_0 \psi_0(\mathbf{r}) e^{-\varepsilon_0 \tau} + c_1 \psi_1(\mathbf{r}) e^{-\varepsilon_1 \tau} + \dots \quad (23)$$

While all of the terms in Eq. (23) will decay with time, the terms for the excited states have a greater rate of decay due to the larger values of ε_n , and we see that at large τ the function $\Psi(\mathbf{r}, \tau)$ relaxes to a function Ψ_∞ which will be some scalar multiple of the ground state $\psi_0(\mathbf{r})$. If desired, the solution can be normalized. The energy of the ground state ε_0 then comes from

$$\varepsilon_0 \approx -\frac{\int \Psi_\infty \nabla^2 \Psi_\infty d\mathbf{x}}{\int |\Psi_\infty|^2 d\mathbf{x}}. \quad (24)$$

The procedure is now to begin with $\Psi(\mathbf{r}, \tau = 0) = \psi(\mathbf{r})$ for some $\psi(\mathbf{r})$ satisfying the boundary conditions and find Ψ at very large values of τ . Making a discrete approximation for Eq. (21), we have

$$\frac{\Psi(\mathbf{r}, \tau + \Delta\tau) - \Psi(\mathbf{r}, \tau)}{\Delta\tau} = \nabla^2 \Psi(\mathbf{r}, \tau), \quad (25)$$

from which we get $\Psi(\mathbf{r})$ for the new value of τ :

$$\Psi(\mathbf{r}, \tau + \Delta\tau) = (1 + \Delta\tau \nabla^2) \Psi(\mathbf{r}, \tau). \quad (26)$$

In practice, $\Psi(\mathbf{r}, \tau)$ is defined on a grid and a discrete approximation for the operator ∇^2 is used, for example, a simple four-point approximation.

Ideally, for sufficiently small $\Delta\tau$, the discrete approximation Eq. (25) will be accurate enough that repeated application of the operator on the right side of Eq. (26) will produce Ψ_∞ . In practice, some care is required for the procedure to produce a precise (or indeed any) answer:

- Because *all* of the terms in Eq. (23) die off as τ increases during the evolution, one must periodically multiply by some overall scalar to normalize the function and make sure, it does not vanish or pick up too much noise due to round-off error.
- If the value of $\Delta\tau$ chosen for Eq. (26) is too small, the computation time will be correspondingly longer.
- If the value of $\Delta\tau$ chosen is too large, then numerical inaccuracies will ruin the calculation; in particular, the value of ε_0 calculated in Eq. (24) will not strictly decrease to some asymptotic value but eventually will increase.

Exercise: Try the method outlined above to find the ground state energy for a particle confined to a square of side a (which is scaled to 1, as in Sec. II). The exact (dimensionless) answer is $E = \pi^2$; try to obtain this with various spatial grids and choices for $\Delta\tau$. You might try $\Delta x = \Delta y = 0.02$ and $\Delta\tau = 0.0001$ to start off.

The relaxation method is useful for finding the energy eigenvalue for a nontrivial (closed) shape, and we have done this for the finite L geometry of Fig. 7 where the length of the shorter side is scaled to 1.

Later we will discuss a method for getting the eigenvalue for this geometry to 8 digits of accuracy, but we found that with the very simple relaxation method given above, with a grid of $\Delta x = \Delta y = 0.01$ and $\Delta\tau = 1.0 \times 10^{-5}$, we get a scaled energy of $E = 9.644$ which compares well with the true value of $E = 9.640$.

For the tubes considered in this article it is simplest to approximate the wire as having closed ends, in which case the correct eigenvalues for the open wire are obtained in the limit where the length of the legs goes to infinity. The relaxation method was applied to the crossed wires geometry in Schult *et al.*¹⁵ and to quantum wires similar to the L geometry but with bend angles other than 90° in Carini *et al.*^{16,17,31}

The problems with stability for the simple relaxation method given above can be avoided with the Crank-Nicholson relaxation method (described in Section 17.2 of *Numerical Recipes*³⁰). This method combines forward and backward “time” propagation to give better behavior for convergence, at the expense of a more complicated operator that produces $\Psi(\mathbf{r}, \tau + \Delta\tau)$ from $\Psi(\mathbf{r}, \tau)$.

D. Method of particular solutions in a cavity

In this section, we discuss a powerful method of solving the Helmholtz equation for finite regions in two dimensions, called the “method of particular solutions” (MPS). It was introduced by Fox, Henrici, and Moler (FHM),³² who used

an L-shaped cavity or membrane to present numerical examples of their method. We will outline the method of particular solutions here, discuss difficulties with this method if one wants to achieve great precision in identifying eigenmode energies, and then introduce an improved method that surmounts these difficulties.

First, imagine that we have a function that vanishes on the boundary of a two-dimensional region. In particular, imagine that one portion of the boundary consists of a corner, i.e., two straight lines with an interior angle π/α , as shown in Fig. 6. Defining the interior corner as the origin of our coordinate system and using radial coordinates, it is straightforward to show that solutions of the Helmholtz equation that vanish on the sides of this corner are Fourier-Bessel functions of the form

$$u^{(j)}(r, \theta) = J_{\alpha j}(kr) \sin(\alpha j \theta), \quad (27)$$

where j takes on positive integer values. We have thus identified a set of solutions that satisfy the Helmholtz equation and are guaranteed to vanish on the sides of this particular corner. However, these functions also illustrate an issue that has been neglected up to this point. Note that if one starts at $\theta = 0$ and then rotates by 360° to return to the same point, the function $u^{(j)}(r, \theta)$ will return to its starting value only if α is an integer. Consequently, for all angles where α takes on noninteger values (called “singular corners”), the wave function is not analytic at the corner, and so the corner will be a branch point.

Let us apply this to an L-shaped cavity, shown in Fig. 7. We choose the origin of the coordinate system as the upper right-hand corner of the L. The interior angle of that corner corresponds to angle π/α where $\alpha = 2/3$; from our previous discussion, the resulting eigenfunctions will have a branch point at this corner. Since the functions of Eq. (27) satisfy the Helmholtz equation, vanish on the sides of this corner, and properly produce a branch point at the origin, we can use them as basis functions for an expansion in modes. Thus, we approximate the eigenfunction inside the cavity in terms of N Fourier-Bessel functions:

$$\psi^{(N)}(r, \theta) \approx \sum_{j=1}^N c_j^{(N)} u^{(j)}(r, \theta). \quad (28)$$

The coefficients $c_j^{(N)}$ in Eq. (28) are obtained by imposing a series of constraints on the eigenfunction. One way to do this is to choose N points on the boundary of the cavity (except

Fig. 6. The corner of a cavity with interior angle π/α of a cavity; the Fourier-Bessel function $u^{(j)}(r, \theta)$ defined in Eq. (27) vanishes on the sides. If α is not an integer then this will represent a singular corner.

Fig. 7. An L-shaped cavity. In the method of particular solutions we choose the origin of the coordinate system to be the upper right-hand corner of the L. One chooses N_B boundary points on which the wave function must vanish, and in addition N_I interior points.

on the interior corner, where the function is guaranteed to vanish) and require that the function vanish on all of those points.

Thus, we choose a set of points (r_i, θ_i) , with $i = 1 \dots N$, on the boundary. The boundary condition $\psi^{(N)}(r_i, \theta_i) = 0$ is equivalent to the matrix equation

$$Z_{ij}(k) c_j^{(N)} = 0, \quad \text{where} \quad Z_{ij}(k) = J_{\alpha_j}(kr_i) \sin(\alpha_j \theta_i), \quad (29)$$

for $(i, j) = 1 \dots N$. The eigenmodes for this cavity will occur at those values of k for which the determinant of the matrix $\mathbf{Z}(k)$ vanishes. In this method, one chooses a value of N and then searches for values of k where the determinant of $\mathbf{Z}(k)$ vanishes.

Exercise: Try the method outlined above for the lowest mode for a particle trapped in a square cavity. Here there are no singular corners, but choose one corner around which to make the expansion in Eq. (28). Choose about 20 total points, evenly spaced around the boundary, and solve Eq. (29) for k . (Of course, the exact solution for a square of unit side is $k^2 = 2\pi^2$.)

In practice, if we employ the method of particular solutions as outlined by FHM, as we increase the number of boundary points N_B , at first the precision with which we can obtain a given cavity mode increases. However, at some point $N_{\min}$ one reaches the maximum precision available; when $N_B > N_{\min}$ the convergence breaks down, and actually becomes worse with increasing N . The breakdown of convergence occurs because there is an additional solution to the Helmholtz equation that vanishes everywhere on the boundary, and this is the null solution $\psi(r, \theta) = 0$, i.e., a solution that is zero everywhere both on and inside the boundary of the cavity. With increasing N_B , the FHM method eventually latches onto the null solution.

We want a solution that vanishes everywhere on the boundary, but that is nonzero inside the boundary. Such a solution was found by Betcke and Trefethen,^{33,34} and we will summarize their method here. In this procedure, one chooses N_B points on the boundary of the cavity, and N_I points in the interior. Again one expands the wave function in a Fourier-

Bessel expansion using N basis functions as given in Eq. (28). Evaluating this on both the boundary and interior points gives a new matrix equation for the coefficients,

$$\mathbf{Z}(k)\mathbf{c} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ - \\ x_1 \\ \vdots \\ x_{N_I} \end{pmatrix}. \quad (30)$$

In Eq. (30), $\mathbf{c} = (c_1, c_2, \dots, c_N)$, and the column matrix $\mathbf{Z}$ has $N_B + N_I$ rows and N columns. The column matrix on the right side of Eq. (30) contains N_B zeroes followed by N_I unknown nonzero points (we arrange the rows so that the boundary points come first, followed by the interior points).

We can divide Eq. (30) into two parts, one for the boundary and one for the interior, namely,

$$\mathbf{Z}_B(k)\mathbf{c} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}; \quad \mathbf{Z}_I(k)\mathbf{c} = \begin{pmatrix} x_1 \\ \vdots \\ x_{N_I} \end{pmatrix}. \quad (31)$$

Since we must avoid the null solution, we solve this for unit vectors $\mathbf{c}$. The matrix $\mathbf{Z}$ can be decomposed into the product of an orthogonal matrix $\mathbf{Q}$ and an upper diagonal matrix $\mathbf{R}$ (as described in Section 11.3 of *Numerical Recipes*³⁰). Following Eq. (31), the orthogonal matrix $\mathbf{Q}$ can itself be split into a piece $\mathbf{Q}_B$ corresponding to the boundary and a piece $\mathbf{Q}_I$ for the interior, and therefore the first expression in Eq. (31) can be written

$$\mathbf{Q}_B(k)\mathbf{R}\mathbf{c} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (32)$$

We now define $\mathbf{v} = \mathbf{R}\mathbf{c}$ and normalize so that $\mathbf{v}$ is a unit vector. Our problem then reduces to finding unit vectors that satisfy

$$\mathbf{Q}_B(k)\mathbf{v} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (33)$$

Betcke and Trefethen solve Eq. (33) using the singular value decomposition (see Section 2.9 of *Numerical Recipes*³⁰). The matrix $\mathbf{Q}_B$ can be written as the product

$$\mathbf{Q}_B = \mathbf{U}\mathbf{S}. \quad (34)$$

In Eq. (34), $\mathbf{U}$ is an $N_B \times N$ orthogonal matrix; $\mathbf{S}$ is an $N \times N$ diagonal matrix containing the singular values; and $\mathbf{V}$ is an $N \times N$ matrix, whose columns are the right singular vectors corresponding to the singular values contained in $\mathbf{S}$. All of these quantities depend upon the eigenvalue k . For a given value of k , let $\sigma(k)$ be the smallest element of $\mathbf{S}$ for that value of k . The eigenmodes of this problem are thus found by varying k and finding the minimum of $\sigma(k)$.

All of the operations here can be accomplished using standard routines in the program MATLAB. Here, the “QR” decomposition of a matrix is effected by the routine `qr`; the singular value decomposition is obtained by calling the routine `svd`.

When Betcke and Trefethen applied this method to the L-shaped cavity, they found a dramatic increase in the precision with which they could obtain the eigenvalues.³³ For example, for the first mode in this cavity, using the original method of particular solutions of FHM, they could obtain the eigenvalue to only four significant figures. However, using the improved method of particular solutions that we have outlined here and increasing the number of expansion points N , Betcke and Trefethen could obtain the first eigenvalue to 14 digits of accuracy. Specifically, the scaled eigenvalues of the lowest two cavity eigenmodes (the second mode being antisymmetric under $x \leftrightarrow y$) are

$$E_1 = 9.6397238, \quad E_2 = 15.197252. \quad (35)$$

E. Method of particular solutions in a tube

The numerical method outlined in Sec. III D can be extended to the calculation of bound states in quantum wires. Our description is complicated, but the difficulty here is primarily in keeping the book-keeping straight. Taking the 90° bent wire with unit width as a simple example, we can again divide the wire into “corner” and “leg” regions (I, II, and III), as shown in Fig. 8. We expand the wave function in region I as outlined in Sec. III:

$$\psi_I(x, y) = \sum_{j=1}^{\infty} a_j \sin(j\pi y) e^{-\alpha_j x} \equiv \sum_{j=1}^{\infty} a_j v^{(j)}(x, y; k), \quad (36)$$

with a similar expansion in region III. This sum will be truncated to N_1 terms.

In region II, the wave function is written as a Fourier–Bessel expansion, as Sec. III D:

$$\psi_{II}(r, \theta) = \sum_{j=1}^{\infty} c_j J_{\alpha_j}(kr) \sin(\alpha_j \theta) \equiv \sum_{j=1}^{\infty} c_j u^{(j)}(r, \theta; k), \quad (37)$$

where we will truncate this series to N_2 terms.

Fig. 8. MPS method applied to a tube: N_{B1} points on the matching boundary, N_{B2} points on the walls, and N_I interior points. Basis functions u and v use the two coordinate systems as shown.

We choose a total of N_{B1} points on the I–II and III–II boundaries (on which we impose continuity conditions), N_{B2} points on the hard walls where the wave function must vanish, and finally N_I points interior to region II.

Define the vectors $\mathbf{c}$ and $\mathbf{x}$ as

$$\mathbf{c} \equiv \begin{pmatrix} a_1 \\ \vdots \\ a_{N_1} \\ c_1 \\ \vdots \\ c_{N_2} \end{pmatrix} \quad \text{and} \quad \mathbf{x} \equiv \begin{pmatrix} 0 \\ \vdots \\ 0 \\ x_1 \\ \vdots \\ x_{N_I} \end{pmatrix}. \quad (38)$$

The continuity conditions for the wave function $\psi(\mathbf{r})$ on the N_{B1} boundary points $\mathbf{r}_{B1}$ on the I–II and I–III boundaries are

$$\psi_I(\mathbf{r}_{B1}) - \psi_{II}(\mathbf{r}_{B1}) = 0, \quad \left. \frac{\partial \psi_I}{\partial x} \right|_{\mathbf{r}_{B1}} - \left. \frac{\partial \psi_{II}}{\partial x} \right|_{\mathbf{r}_{B1}} = 0, \quad (39)$$

which together give $2N_{B1}$ relations between the N_1 coefficients a_j and the N_2 coefficients c_j . (Note: The second relation in Eq. (39) is appropriate for points on the I–II boundary; on the III–II boundary one would use the operator $\partial/\partial y$.)

Along with the N_{B2} conditions that the wave function vanishes on the hard-wall boundary and the conditions that the N_I interior points have nonzero values, we can construct a matrix $\mathbf{Z}$ to get an equation of the form

$$\mathbf{Z}\mathbf{c} = \mathbf{x}, \quad (40)$$

where $\mathbf{Z}$ has $2N_{B1} + N_{B2} + N_I$ rows and $N_1 + N_2$ columns. From here one follows the same matrix operations as in the case of the cavity: Separate off the homogeneous part of the equations, do a QR decomposition, and find the smallest singular value. The advantage of using the particular solutions method here is that it can be applied to a wire of arbitrary shape and it is not necessary to approximate the sections as having finite length. This method was extended by Tuegel³⁵ to cover the case of a bent wire (i.e., a wire with an arbitrary value for the interior angle), which was initially calculated by Carini *et al.*^{16,17,31} using series expansion and relaxation methods.

IV. CONCLUSION

Two-dimensional systems provide a large number of interesting examples of confined modes and scattering problems. In this article, we have focused on some properties of open tubes (or “quantum wires”). The simplest such system is the 2D analog of the 1D square well, a 2D state with zero potential inside the tube and infinite potentials on the walls. In particular, we have reviewed the proof that a long 2D tube of constant width but with any local bulge always possesses at least one confined mode. We summarized the physical results in a few of these examples and showed some numerical methods for calculating these confined modes. In particular, we summarized how one can solve for these states using variational methods, the method of relaxation, mode-matching methods, and the method of particular solutions. For this last method, we reviewed a recent improvement by Betcke and Trefethen that allows one to calculate these modes with extremely high precision.

All of these methods are amenable to calculation by undergraduates using numerical techniques. They are particularly straightforward if one uses routines built into mathematical software such as MATHEMATICA, MAPLE, or MATLAB. Although we have focused on the question of confinement in quantum wire geometries, similar methods can be extended to 2D cavities ("quantum dots"), or systems with multiple bends in quantum wires, coupled systems of quantum dots, etc. One can also extend these methods to study scattering problems, or continuum systems, to find reflection and transmission amplitudes for waves propagating in 2D systems.

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