Bound states in twisting tubes

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The wave equation subject to Dirichlet boundary conditions has a bound state in an infinite tube of constant cross section in any number of dimensions, provided that the tube is not exactly straight. We prove this result, develop Green's-function methods to find the energy eigenvalue, and solve some simple cases. We discuss the implications for quantum systems and electromagnetic waveguides.

I. INTRODUCTION

It is easy to see that the uncertainty principle can provide binding in quantum systems. Consider, for example, an infinite cylindrical tube with a bulge in the middle. A particle constrained to move in this tube can have lower transverse momentum and therefore lower transverse energy within the bulge, where it is less severely confined. A bound state results because the quantum particle would have to squeeze into the cylindrical section of the tube in order to propagate away to infinity. Such a system—a straight tube with a slowly changing radius—can be mapped into a one-dimensional problem in which the changing radius appears as a changing potential. A bulge corresponds to attraction, and in one dimension an attraction, no matter how weak, suffices to produce binding.

The object of this paper is to demonstrate that bends do as well as bulges. We will prove that an infinite tube (a precise definition of which will be given in Sec. II B) with a constant normal cross section *always* has a bound state if it bends. Apparently, a bend provides a region in which the quantum particle can relax, lowering its momentum in comparison with straight regions, though this is not as obvious as it is for bulges.

We will give a simple variational proof of our result in Sec. II. The proof is formulated for channels of constant width in two dimensions but the extension to tubes in three dimensions and to other situations is straightforward and is given Sec. II B. The proof does *not* require the tube to be in any sense narrow, nor must its curvature be small nor even continuous. The result applies to any system characterized by the wave equation with Dirichlet boundary conditions and therefore has application beyond quantum mechanics.

In Sec. III we develop the machinery necessary to find the bound-state energy under rather general conditions. We apply this formalism to the case of a very-small-angle bend in two dimensions. We also solve the special case of a right-angle bend which requires other methods.

In Sec. IV we address several issues surrounding the detection of these bound states. First, we discuss the existence of such bound states for radiation in waveguides. We prove that bound states exist in a class of bent waveguides. We cannot prove as general a result as in

the case of the Schrödinger equation. We suspect that bound states exist under much more general conditions but have not found a more general proof or example. Next we discuss the observation of these bound states. In practice all tubes have ends, and consequently our "bound states" can decay by tunneling out the ends of the tube. They are therefore resonances and can be excited by their coupling to the continuum. Alternatively, the bound states can be observed indirectly by their effect on scattering states in the tube. We show that the presence of the bound state has a significant effect on the transmission and reflection coefficients for waves propagating down the tube. For electrons in a metal, the transmission coefficient is related to the resistance measured across the ends of the tube, so a careful measurement of the resistance can detect the presence of the bound state.

Our interest in the problem was stimulated by Ref. 1 in which a particular model of quark confinement is recast as a problem of Schrödinger dynamics in a two-dimensional right-angle channel. This subject has been studied in a series of works by Exner, Šeba and collaborators and by others.[2] They proved the existence of bound states in two-dimensional channels of fixed width and small and slowly varying curvature, for which an adiabatic approximation applies. We have not been able to find any reference to this phenomenon in the extensive literature on electromagnetic waveguides.

II. EXISTENCE OF A BOUND STATE

In this section we give a simple variational proof of the existence of a bound state of the wave equation in the two-dimensional case. Afterwards we describe the generalization to three dimensions and briefly to other differential operators.

A. Variational proof in two dimensions

Our proof applies to an infinite *"channel"* of constant width in the plane. The channel is constructed as follows: Let C be a curve parametrized by its length. C is straight on both ends, say for $s < -s_1$ and $s > s_1$. In the middle, C curves in an arbitrary way. (For the sake of simplicity we will assume C does not cross itself and has no kinks—it has a unique tangent at each point—

although both of these restrictions can be relaxed.) At each point on C erect a unit normal on the same side of C. The tip of the normal traces out another curve C'. (The length of the normal is limited by the condition that C' does not cross itself and has no kinks.) The channel $\mathcal{C}$ is the region between C and C' as shown in Fig. 1.

We will prove that the wave equation,

$$(\nabla^2 + k^2)\psi(\mathbf{x}) = 0 , \qquad (2.1)$$

in $\mathcal{C}$, subject to the boundary condition $\psi(\mathbf{x}) = 0$ on C and C', has a bound state with the sole exception of the case when C (and C') is an infinite straight line. The proof employs the variational principle. Break up the channel into three regions: (I) $s < -s_1$, (II) $-s_1 \leq s \leq s_1$; (III) $s > s_1$. Let points in $\mathcal{C}$ be labeled by $\mathbf{x} = \mathbf{x}(s) + y\hat{\mathbf{n}}(s)$, where $\mathbf{x}(s)$ is the curve C, $\hat{\mathbf{n}}(s)$ is the unit normal to C at $\mathbf{x} = \mathbf{x}(s)$, and $0 \leq y \leq 1$, i.e., we choose the channel width as our unit of length. Choose a candidate Schrödinger wave function:

$$\psi(s,y) = e^{-\lambda(|s| - s_1)}\sin(\pi y) \quad \text{for} \quad |s| > s_1 \qquad (2.2)$$

with $\lambda > 0$. The only constraint on ψ in region II is $\psi(\pm s_1, y) = \sin\pi y$. The normal derivatives of ψ need not match at $|s| = s_1$. We must evaluate

$$E[\psi] = \frac{\int_{\mathcal{C}} d^2x |\nabla\psi|^2}{\int_{\mathcal{C}} d^2x \psi^2} . \qquad (2.3)$$

There is a bound state if we can show that for some ψ, $E[\psi] < \pi^2$ since π^2 is the energy of the lowest-energy traveling wave that can escape to $s = \pm\infty$. It is elementary to calculate

$$\int_{\mathcal{C}} d^2x \, \psi^2 = \frac{1}{2\lambda} + \int_{\text{II}} d^2x \psi^2 ,$$
$$\int_{\mathcal{C}} d^2x |\nabla\psi|^2 = \frac{\lambda}{2} + \frac{\pi^2}{2\lambda} + \int_{\text{II}} d^2x |\nabla\psi|^2 , \qquad (2.4)$$

where $\int_{\text{II}}$ refers to region II, where $|s| \leq s_1$. Let

$$I[\psi] = \int_{\text{II}} d^2x (\pi^2\psi^2 - |\nabla\psi|^2) , \qquad (2.5)$$

(independent of λ). From (2.3) and (2.4), a bound state exists if $I > \frac{1}{2}\lambda > 0$ and we can always choose $\lambda < 2I$, provided that $I > 0$.
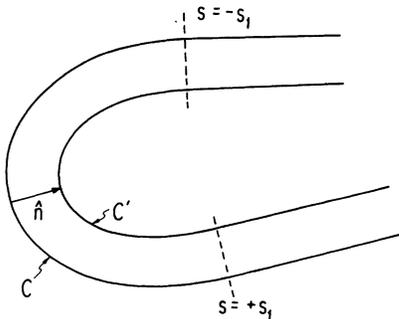
FIG. 1. A channel in two dimensions constructed from a curve, C, and its unit normal, $\hat{\mathbf{n}}$.

We parametrize the $I[\psi]$ in terms of the coordinates y and s. First note

$$\hat{\mathbf{t}} = \frac{d\mathbf{x}(s)}{ds} \qquad (2.6)$$

is the unit tangent to C, and

$$\frac{d\hat{\mathbf{t}}}{ds} = \kappa\hat{\mathbf{n}}, \quad \frac{d\hat{\mathbf{n}}}{ds} = -\kappa\hat{\mathbf{t}} \qquad (2.7)$$

defines the curvature, $\kappa(s)$. Then

$$|d\mathbf{x}|^2 = dy^2 + [1 - \kappa(s)y]^2 ds^2 , \qquad (2.8)$$

$$d^2x = ds\, dy[1 - \kappa(s)y] . \qquad (2.9)$$

Substituting the trial function $\psi_{\text{II}}(s,y) = \sin\pi y$ we obtain

$$I[\psi_{\text{II}}] = \pi^2 \int_{-s_1}^{s_1} ds \int_0^1 dy [1 - \kappa(s)y]$$
$$\times [\sin^2(\pi y) - \cos^2(\pi y)] = 0 . \qquad (2.10)$$

Finally we note that ψ_{II} is not stationary point of $I[\psi]$, from (2.8),

$$\nabla^2\psi_{\text{II}} + \pi^2\psi_{\text{II}} = \left[\frac{1}{1-\kappa y}\frac{\partial}{\partial y}(1-\kappa y)\right]\frac{\partial\psi_{\text{II}}}{\partial y} \neq 0 . \qquad (2.11)$$

Thus, there must exist some other trial function, ϕ, for which

$$I[\phi] > 0 , \qquad (2.12)$$

which is what we aimed to show.

This proof informs us that we can find useful (i.e., bound) estimates of the true ground state of the original problem in the space of functions satisfying $\psi = \sin(\pi y)$ at $|s| = 1$. The true ground state is a superposition of $\{\phi_n\}$ where

$$\phi_n(\mathbf{x}) \equiv \sin(n\pi y)e^{-\lambda_n|s|}, \quad \lambda_n^2 = n^2\pi^2 - k^2 \qquad (2.13)$$

for $|s| \geq s_1$, and n will appear as a channel (i.e., matrix) label on the Green's-function formulation of the problem. We see that useful estimates of the bound-state energy will be found within the truncated one-channel approximation to the problem.

B. Generalization to three dimensions

In three dimensions the theorem holds in "tubes" with constant normal cross sections. To be more precise, let $\mathcal{D}$ be a region in three-dimensional space which is swept out by the rigid motion of a two-dimensional disc D. The disc D may have arbitrary shape and may have holes. For the theorem to apply, $\mathcal{D}$ must have the additional property that the plane containing the disk D intersects the boundary of $\mathcal{D}$ normally. This is shown graphically in Fig. 2. It is equivalent to the statement that as the disk D tumbles through space sweeping out $\mathcal{D}$, at each instant its angular velocity ω lies in the plane of the disc D.

For analytic purposes it is convenient to construct $\mathcal{D}$ somewhat differently. First choose a curve C parametrized by $\mathbf{x}(s)$. Next erect the Frenet frame consisting of the unit tangent, the normal, and the binormal:
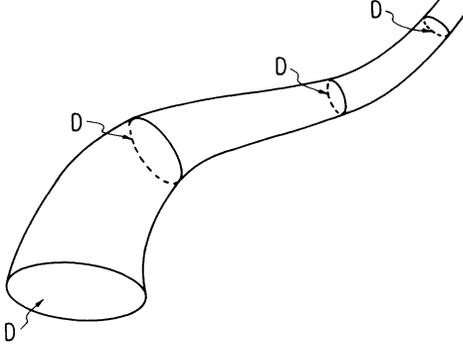
FIG. 2. A tube in three dimensions swept by the disc D as it tumbles through space.

$$\hat{\mathbf{t}}=\frac{d\mathbf{x}}{ds} ,$$

$$\hat{\mathbf{t}}'=\boldsymbol{\omega}\times\hat{\mathbf{t}}=\kappa(s)\hat{\mathbf{n}} ,$$

$$\hat{\mathbf{n}}'=\boldsymbol{\omega}\times\hat{\mathbf{n}}=-\kappa(s)\hat{\mathbf{t}}+\tau(s)\hat{\mathbf{b}} , \qquad (2.14)$$

$$\hat{\mathbf{b}}'=\boldsymbol{\omega}\times\hat{\mathbf{b}}=-\tau(s)\hat{\mathbf{n}} .$$

$\kappa(s)$ and $\tau(s)$ are the curvature and torsion of $\mathbf{x}(s)$. (' denotes d/ds.) $\boldsymbol{\omega}=\boldsymbol{\omega}(s)$ is the instantaneous angular velocity of the Frenet frame. In general $\boldsymbol{\omega}$ has a component along $\hat{\mathbf{t}}$. We define new unit vectors, $\hat{\mathbf{N}}$ and $\hat{\mathbf{B}}$, in the plane normal to C, by a rotation:

$$\hat{\mathbf{N}}=\cos[\theta(s)]\hat{\mathbf{n}}+\sin[\theta(s)]\hat{\mathbf{b}} ,$$

$$\hat{\mathbf{B}}=-\sin[\theta(s)]\hat{\mathbf{n}}+\cos[\theta(s)]\hat{\mathbf{b}} , \qquad (2.15)$$

and

$$\hat{\mathbf{N}}'=\boldsymbol{\Omega}\times\hat{\mathbf{N}}, \quad \hat{\mathbf{B}}'=\boldsymbol{\Omega}\times\hat{\mathbf{B}} . \qquad (2.16)$$

Now we choose $\theta(s)$ so that $\boldsymbol{\Omega}$ has no component in the direction of $\hat{\mathbf{t}}$. A brief calculation yields

$$\theta(s)=-\int_{-\infty}^{s}ds'\tau(s') \qquad (2.17)$$

and

$$\hat{\mathbf{N}}'=-\kappa(s)\cos[\theta(s)]\hat{\mathbf{t}} ,$$

$$\hat{\mathbf{B}}'=\kappa(s)\sin[\theta(s)]\hat{\mathbf{t}} , \qquad (2.18)$$

$$\hat{\mathbf{t}}'=\kappa(s)\{\cos[\theta(s)]\hat{\mathbf{N}}-\sin[\theta(s)]\hat{\mathbf{B}}\} .$$

The tube $\mathcal{D}$ is now constructed very simply: the disc D is mounted rigidly in the reference frame where $\hat{\mathbf{N}}$ and $\hat{\mathbf{B}}$ are at rest. $\mathcal{D}$ is swept out by D as it tumbles along with the $(\hat{\mathbf{t}},\hat{\mathbf{B}},\hat{\mathbf{N}})$ frame moving along the curve.

Points in the tube $\mathcal{D}$ may be parametrized by

$$\mathbf{x}(s,\xi,\eta)=\mathbf{x}(s)+\xi\hat{\mathbf{B}}+\eta\hat{\mathbf{N}} , \qquad (2.19)$$

and an elementary calculation shows that the volume element, d^3x, can be written

$$|d\mathbf{x}|^2=d\xi^2+d\eta^2+[1-\kappa(\eta\cos\theta-\xi\sin\theta)]^2ds^2 ,$$

$$d^3x=(1-\kappa(s)\{\eta\cos[\theta(s)]-\xi\sin[\theta(s)]\})ds\,d\xi\,d\eta . \qquad (2.20)$$

The variational argument proceeds much like the two-dimensional case. The tube is divided into straight sections, I and III with $|s|>s_1$, and an interior, curving section, II, with $|s|<s_1$. We take a trial function

$$\psi(s,\xi,\eta)=\begin{cases}\chi(\xi,\eta)e^{-\lambda(|s|-s_1)} & \text{for } |s|>s_1 \\ \chi(\xi,\eta) & \text{for } |s|=s_1 ,\end{cases} \qquad (2.21)$$

where χ is the lowest eigenfunction of the Dirichlet problem in the disc D,

$$\left[\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}+k_0^2\right]\chi(\xi,\eta)=0 \quad \text{in } D , \qquad (2.22)$$

$$\chi(\xi,\eta)=0 \quad \text{on } \partial D .$$

For convenience we choose units such that $k_0^2=1$. Then the existence of a bound state reduces to showing

$$\int_{\text{II}}d^3x(\psi^2-|\nabla\psi|^2)>0 \qquad (2.23)$$

for some trial function ψ, with $\psi(\pm s_1,\xi,\eta)=\chi(\xi,\eta)$.

For the trial function $\psi_{\text{II}}(s,\xi,\eta)=\chi(\xi,\eta)$, (2.23) reduces to

$$\int_{-s_1}^{s_1}ds\int_D d\eta\,d\xi[1-\kappa(\eta\cos\theta-\xi\sin\theta)](\chi^2-|\nabla_\perp\chi|^2) . \qquad (2.24)$$

Since χ satisfies (2.22),

$$\int_D d\eta\,d\xi(\chi^2-|\nabla_\perp\chi|^2)=0 . \qquad (2.25)$$

Also, it is easy to prove that

$$\int_D d\eta\,d\xi\,\mathbf{a}\cdot\mathbf{x}_\perp(\chi^2-|\nabla_\perp\chi|^2)=0 \qquad (2.26)$$

for any vector $\mathbf{a}$ which does not depend on ξ or η. (Note: it is essential that κ and θ depend only on s.) Together (2.25) and (2.26) imply

$$\int_{\text{II}}d^3x(\psi_{\text{II}}^2-|\nabla\psi_{\text{II}}|^2)=0 , \qquad (2.27)$$

and we complete the proof as we did in two dimensions, by arguing that ψ_{II} does not satisfy $\nabla^2\psi_{\text{II}}+\psi_{\text{II}}=0$ in II, so there must exist some $\phi(\mathbf{x})$ for which $\int_{\text{II}}d^3x(\phi^2-|\nabla\phi|^2)>0$.

When $\kappa(s)$ is small and slowly varying, it is easy to see how a bound state arises. From (2.20),

$$\nabla^2\psi=\frac{1}{h}\left[\frac{\partial}{\partial\xi}h\frac{\partial\psi}{\partial\xi}+\frac{\partial}{\partial\eta}h\frac{\partial\psi}{\partial\eta}\right]+\frac{1}{h}\frac{\partial}{\partial s}\frac{1}{h}\frac{\partial\psi}{\partial s} , \qquad (2.28)$$

where

$$h=1+\kappa\sin\theta\,\xi-\kappa\cos\theta\,\eta . \qquad (2.29)$$

With $\psi=h^{-1/2}\phi$ the wave equation becomes

$$\nabla_\perp^2\phi+\frac{1}{4}h^{-2}\kappa^2\phi+h^{-2}\frac{\partial^2\phi}{\partial s^2}+k^2\phi-2h^{-3}\frac{\partial h}{\partial s}\frac{\partial\phi}{\partial s}$$

$$-\frac{1}{2}h^{-3}\frac{\partial^2 h}{\partial s^2}\phi+\frac{5}{4}h^{-4}\left[\frac{\partial h}{\partial s}\right]^2\phi=0 . \qquad (2.30)$$

If κ and $\partial/\partial s$ are both of order $1/s_1$ with $s_1 \gg 1$ then to order $1/s_1^2$ the equation becomes

$$\nabla_1^2\phi + \frac{1}{4}[\kappa(s)]^2\phi + \frac{\partial^2\phi}{\partial s^2} + k^2\phi = 0 \; . \tag{2.31}$$

The solution is $\phi = \chi(\xi,\eta)u(s)$, where $u(s)$ is the bound-state wave function in the attractive one-dimensional potential

$$V(s) = -\tfrac{1}{4}[\kappa(s)]^2 \; . \tag{2.32}$$

For further elaboration of the adiabatic approximation see Ref. 2.

One further generalization is obvious at this point: The theorem applies equally to the case in which there is an arbitrary transverse potential energy, $V = V(\xi,\eta)$ in the disc D.

III. GENERAL SOLUTION AND SPECIAL CASES

In this section we set up a general formalism for finding bound states of the wave equation in channels with reflection symmetry. It is a straightforward application of Green's-function methods. We work nominally in three dimensions but the specialization to two dimensions is trivial and the generalizations to higher dimensions, to channels without reflection symmetry and to other differential operators are straightforward. We then use the general method to solve the example of a small-angle bend in two dimensions [Fig. 3(b)]. Finally we consider

(a)

(b)

(c)
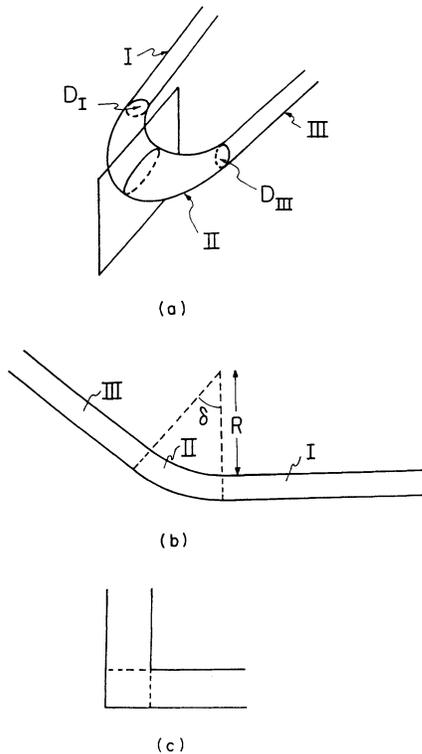
FIG. 3. (a) Domains relating to the mixed Green's-function formulation. (b) A small-angle bend constructed form concentric circles of radius R and $R + 1$; (c) A right-angle bend.

the right-angle channel [Fig. 3(c)] for which a different variant of the method of Green's functions is more suited.

A. Solution via a mixed Green's function

We consider a three-dimensional domain consisting of two straight tubes (I and III) connected to a region (II) of arbitrary shape except for the condition that the whole system has a reflection symmetry about some plane [see Fig. 3(a)]. We seek to find the lowest eigenvalue of the wave equation. Its wave function will be the same in both straight tubes and will decay exponentially,

$$\psi(\mathbf{x}) = \sum_{n=1}^{\infty} a_n \chi_n(\alpha) e^{-\kappa_n s} \; . \tag{3.1}$$

Here, s is the distance along the channel and α denotes the coordinates in the disc D which sweeps out the channel. $\{\chi_n(\alpha)\}$ are eigenstates of

$$(\nabla_1^2 + k_n^2)\chi_n(\alpha) = 0 \tag{3.2}$$

in D, with

$$\chi_n(\alpha) = 0$$

on the boundary of D normalized so that

$$\int ds_\alpha \chi_m(\alpha)\chi_n(\alpha) = \delta_{mn} \; . \tag{3.3}$$

The $\{\kappa_n\}$ are fixed by the condition that

$$\kappa_n^2 = k_n^2 - k^2 \; . \tag{3.4}$$

A bound state exists if a solution exists with all κ_n real.

Region II consists of a reflection symmetric domain whose boundary, D_{II}, has two holes where the straight channels, I and III, are attached. We complete region II by attaching two copies of the disc, D_{I} and D_{III}, to fill the two holes. We define a Green's function for region II which is Dirichlet on D_{II} and Neumann on D_{I} and D_{III}:

$$(\nabla^2 + k^2)G(\mathbf{x},\mathbf{y},k^2) = -\delta^3(\mathbf{x} - \mathbf{y}) \quad \text{in II} \; ,$$

$$G(\mathbf{x},\mathbf{y},k^2) = 0 \quad \text{on } D_{\mathrm{II}} \; , \tag{3.5}$$

$$\partial_\alpha G(\alpha,\mathbf{y},k^2) = 0 \quad \text{on } D_{\mathrm{I}}, D_{\mathrm{III}} \; ,$$

where

$$\partial_\alpha f(\alpha) \equiv \lim_{\mathbf{x} \to \alpha \in D} \hat{\mathbf{n}}_\alpha \cdot \nabla f(\mathbf{x}) \tag{3.6}$$

and we take the outward normal. Then the wave function ψ in region II is given by

$$\psi_{\mathrm{II}}(\mathbf{x}) = \int_{D_{\mathrm{I}}+D_{\mathrm{III}}} ds_\alpha G(\alpha,\mathbf{x},k^2)\partial_\alpha\psi(\alpha) \; . \tag{3.7}$$

We obtain an eigenvalue condition on the $\{\kappa_n\}$ by demanding continuity of ψ and $\nabla\psi$ at the discs D_{I} and D_{III} which join region II to the straight channels. Let $\mathbf{x}$ approach $\beta \in D_{\mathrm{I}}$ in (3.7), substitute

$$\psi(\beta) = \sum_n a_n \chi_n(\beta) \; ,$$

$$\partial_\beta\psi(\beta) = -\sum_n a_n \kappa_n \chi_n(\beta) \; , \tag{3.8}$$

and "Fourier" expand by means of the orthonormality of the $\{\chi_m\}$, to obtain

$$a_m = \sum_n \Delta_{mn}(k^2)\kappa_n a_n \ , \tag{3.9}$$

where

$$\Delta_{mn}(k^2) = -\int_{D_I} ds_\alpha \int_{D_I + D_{III}} ds_\beta G(\beta, \alpha, k^2)\chi_m(\beta)\chi_n(\alpha) \ . \tag{3.10}$$

Equation (3.9) has solutions if and only if the determinant of the matrix $[\Delta_{mn}(k^2)\kappa_n - \delta_{mn}]$ vanishes when all κ_n are real, i.e., for $k^2 < k_1^2$.

The structure of Δ_{mn} can be made more apparent by expanding G in terms of the eigenfunctions of the problem defined in (3.5):

$$G(\mathbf{x}, \mathbf{y}, k^2) = \sum_p \frac{\phi_p(\mathbf{x})\phi_p(\mathbf{y})}{q_p^2 - k^2} \ , \tag{3.11}$$

where the ϕ_p obeys the homogeneous form of (3.5) with the eigenvalue q_p. Then

$$\Delta_{mn}(k^2) = \frac{1}{2}\sum_p \frac{g_{mp}g_{np}}{k^2 - q_p^2} \ , \tag{3.12}$$

where g_{mp} is the "channel coupling" of the pth eigenstate to be mth channel:

$$g_{mp} = \int_{D_I + D_{III}} ds_\alpha \chi_m(\alpha)\phi_p(\alpha) \ . \tag{3.13}$$

In general, of course, the eigenvalues of (3.9) can only be obtained by direct numerical analysis. This task is made easier under certain special circumstances, some examples of which are given in the following sections.

B. Small-angle bend in two dimensions

We consider the two-dimensional domain shown in Fig. 3(b) in the limit $\delta \to 0$, $R \to \infty$. We choose polar coordinates with $r = R + y$ so that $0 \le y \le 1$, $0 \le \theta \le \delta$. The eigenfunctions $\{\phi_p\}$ have two integer labels, l and j:

$$\phi_p(\mathbf{x}) \to A_{lj}f_l(q_{lj}y)\cos(l\pi\theta/\delta) \ , \tag{3.14}$$

where

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{l^2\pi^2}{\delta^2(R+y)^2} + q_{lj}^2\right]f_l(q_{lj}y) = 0 \ , \tag{3.15}$$

and $f_l(0) = f_l(q_{lj}) = 0$ fixes the eigenvalue q_{lj}. The eigenfunctions f_l are Bessel functions of order $l\pi/\delta$. In the limit $\delta \to 0$ only $l = 0$ contributes. As $R \to \infty$, $f_0(q_j y)$ $(q_j \equiv q_{l=0,j})$ can be expressed in terms of trigonometric functions:

$$f_0(q_j) \sim \sqrt{2/(1-R)}\sin(j\pi y) \tag{3.16}$$

with

$$q_j^2 = j^2\pi^2 - 1/4R^2 \ . \tag{3.17}$$

The factor $1/4R^2$ in (3.17) is the only residue of the circular geometry. The channel eigenfunctions, $\chi_m(\alpha)$, are also trigonometric,

$$\chi_m(\alpha) \to \sqrt{2}\sin(m\pi y) \tag{3.18}$$

so that the matrix $\Delta_{mn}(k^2)$ is easily computed in the limit $(\delta \to 0, R \to \infty)$

$$\Delta_{mn}(k^2) \approx -\frac{2}{\alpha R}\frac{1}{n^2\pi^2 - k^2 - 1/4R^2}\delta_{mn} \ . \tag{3.19}$$

With Δ of this form, (3.9) has solutions in the vicinity of $k^2 = n^2\pi^2$ with $a_n \ne 0$ and all $a_m = 0$ for $m \ne n$. Consider, for example, the lowest eigenstate with eigenvalue $\lesssim \pi^2$. Equation (3.9) yields the condition

$$\frac{1}{\kappa_1} \approx \Delta_{11}(k^2) \approx -\frac{2}{8R}\frac{1}{\pi^2 - k^2 - 1/4R^2} \ . \tag{3.20}$$

The limiting solution (as $\delta \to 0$) is $1/\kappa_1 = \Delta_{11}(\pi^2)$ or $\kappa_1 = \delta/8R$. This result can be checked using the adiabatic approximation developed in Sec. II where it corresponds to the eigenenergy of a particle in a one-dimensional square well of depth $1/4R^2$ and width δR.

C. Right-angle channel in two dimensions

Next we consider the right-angle channel shown in Fig. 3(b). This problem is treated with different methods in the last entry of Ref. 2. Strictly speaking this is not a channel as we have defined it: it does not have constant normal cross section. Nevertheless it was the original geometry which motivated the study of this problem[1] and its solution is quite instructive. The separability of the wave equation in Cartesian coordinates results in the "discs" D_I and D_{III} being described by different coordinates, $y = 1$ for D_I and $x = 1$ for D_{III}. This renders the expansion of Δ_{mn} in the channel space slowly convergent and suggests that we seek a Green's function better suited to this particular problem. The proper choice is the Dirichlet Green's function as explained by Lenz et al. when they considered variants of this problem in Ref. 1. It will become clear, however, that this method is of limited use.

The analysis which led to (3.9) in the previous case leads to the *inverse* equation in this case,

$$\kappa_m a_m = \sum_n \Delta_{mn}^{-1}(k^2)a_n \ . \tag{3.21}$$

$\Delta^{-1}(k^2)$ can be written in terms of the Dirichlet Green's function in a fashion similar to (3.10),

$$\Delta_{mn}^{-1}(k^2) = 2\int_0^1 dy \int_0^1 dy' \sin(m\pi y)\sin(n\pi y')\frac{\partial^2}{\partial x \partial x'}G_D(x, y; x', y', k^2)\bigg|_{x = x' = 1}$$

$$+ 2\int_0^1 dx' \int_0^1 dy \sin(m\pi x')\sin(n\pi y)\frac{\partial^2}{\partial x \partial y'}G_D(x, y; x', y', k^2)\bigg|_{x = y' = 1} \ . \tag{3.22}$$

The eigenfunction expansion for G_D cannot be used directly because the derivatives $\partial^2/\partial x\partial x'$ cannot be interchanged with the sum over eigenfunctions. In the special case at hand (region II is a square), the eigenfunction expansion can be subtracted and rendered more convergent:

$$G_D(x,y;x'y',k^2)$$

$$=4\sum_{pq}\frac{\sin(p\pi x)\sin(q\pi y)\sin(p\pi x')\sin(q\pi y')}{\pi^2(p^2+q^2)-k^2}\quad(3.23)$$

and

$$\frac{\partial^2}{\partial x\partial x'}G_D(x,y;x',y',k^2)\bigg|_{x=x'=1}$$

$$=-2\sum_q\kappa_q\coth(\kappa_q)\sin(q\pi y)\sin(q\pi y')\ .\quad(3.24)$$

The "subtraction" is embodied in the dispersion representation of $x\coth x$

$$x\coth x=1+2x^2\sum_{p=1}^{\infty}\frac{1}{x^2+p^2\pi^2}\ ,\quad(3.25)$$

which replaces the divergent (and useless) result,

$$2\sum_{p=1}^{\infty}\frac{p^2\pi^2}{x^2+p^2\pi^2}\ ,$$

which follows from manipulating $G_D(x,y;x',y',k^2)$ naively. For more general geometries the usefulness of the Dirichlet Green's function is limited by our ability to perform this subtraction. If, for example, we subtract at $k^2=0$, so that

$$G_D(\mathbf{x},\mathbf{x}',k^2)=G_D(\mathbf{x},\mathbf{x}',0)+k^2\sum_n\frac{\psi_n(\mathbf{x})\psi_n(\mathbf{x}')}{k_n^2(k_n^2-k^2)}\ ,\quad(3.26)$$

then the normal derivatives may be taken under the sum:

$$\partial_\alpha\partial_{\alpha'}G_D(\alpha,\alpha',k^2)=\partial_\alpha\partial_{\alpha'}G_D(\alpha,\alpha',0)$$

$$+k^2\sum_n\frac{\partial_\alpha\psi_n(\alpha)\partial_{\alpha'}\psi_n(\alpha')}{k_n^2(k_n^2-k^2)}\ .\quad(3.27)$$

But this representation is only useful if we, independently, have a representation for the "subtraction constant" $\partial_\alpha\partial_{\alpha'}G(\alpha,\alpha',0)$—i.e., for the normal derivatives of the Dirichlet Green's function for the Laplacian.

Returning to the right angle, we insert (3.24) and (3.22) and evaluate $(\partial^2/\partial x\partial y')G_D$ straightforwardly (it needs no subtraction), to obtain

$$\Delta_{mn}^{-1}(k^2)=-\delta_{mn}\kappa_m\coth\kappa_m+2\frac{(-1)^{n+m}nm\pi^2}{\pi^2(n^2+m^2)-k^2}\ .$$

$$(3.28)$$

The eigenvalues of (3.21) can be found numerically. The single-channel approximation yields the transcendental equation

$$\kappa_1+\kappa_1\coth\kappa_1-2\pi^2/(\kappa_1^2+\pi^2)=0$$

whose solution is $\kappa_1=0.7276$ so that $k^2=9.340$. As the

number of channels is increased the eigenvalue falls monotonically. For $N=2$, 3, and 4 we obtain $k^2=9.255$, 9.224, and 9.208, respectively. Thus the channel expansion of the Dirichlet Green's function converges quite rapidly for this case.

IV. DISCUSSION

In this section we discuss several issues which are important if the bound state we have found is to be observed experimentally. First, we discuss the existence of such a bound state for light, and second we describe how to observe the bound state by a scattering experiment.

A. Electromagnetism

We consider an idealized waveguide with infinite conductivity realized by the boundary conditions $\hat{n}\cdot\mathbf{B}=0$ and $\hat{n}\times\mathbf{E}=0$. We have not been able to extend our general variational proof to this case. However, there is a special case of sufficient generality to be of interest. Let $\mathcal{D}$ be a three-dimensional tube constructed by taking a two-dimensional channel, $\mathcal{C}$, in the x-y plane, and translating it normally in the z direction (see Fig. 4). In this case the proof of the theorem in two dimensions is directly generalizable because there exists a scalar field $\phi(x,y)$ obeying $(\nabla^2+k^2)\phi=0$ in $\mathcal{D}$ and $\phi=0$ on the boundary of $\mathcal{D}$ with $\mathbf{A}=\phi\hat{z}$, $\mathbf{B}=-\hat{z}\times\nabla\phi$, $\mathbf{E}=ik\phi\hat{z}$, and $\nabla\cdot\mathbf{A}=\hat{z}\cdot\nabla\phi=0$. We believe that in more complicated geometries the existence and nature of bound states depend more delicately on the shape and curvature than in the scalar case.

Of course, physical conductors have only finite conductivity so that even if this bound state could be formed, it would dissipate very rapidly. This brings us to the final subject in our analysis: How can this bound state be observed, either for light in a waveguide or for electrons in some solid-state device?

B. Effect of the bound state on scattering

In practice, tubes are of finite length. Consider one long enough so that the bound state is only slightly perturbed by the finiteness of the tube. Since the bound-state wave function decays exponentially down the long straight sections, the result is an exponentially small amplitude for the bound state to "tunnel" down the straight sections and out into the continuum. The bound state has become a resonance centered close to the infinite tube energy with a small but non-negligible width. Such a resonance can be excited by exposing a finite tube to an external source (of radiation or particles). The resonance will appear as a sharp increase in the absorption of power

FIG. 4. A tube in three dimensions obtained by translating a planar channel normally in the $\hat{z}$ direction.

(or, equivalently, a decrease in reflection) by the tube at a frequency below the critical cutoff. In the case of radiation, the power is then dissipated in resistive losses in the (imperfect) conductor from which the tube is fabricated. This effect has recently been observed by Carini,[3] who observed resonant absorption of microwave radiation by a right-angle elbow at a frequency within a fraction of a percent of the value predicted by the analysis of Sec. III.

Another way to detect the bound state is to observe its effect on the propagation of radiation or electrons above the continuum threshold. In general, bound states just below the continuum have striking influence on scattering amplitudes. The bound state we are considering can be detected by its influence on the phase of the waves propagating down the tube in exactly the same fashion that the deuteron can be detected in very low energy p-n scattering. The formulation of the scattering problem mimics multichannel scattering in one dimension. Consider a tube with a wave incident from the "left" $(s \ll -s_1)$:

$$\psi_m^+(\mathbf{x},k)=\frac{\chi_m(\boldsymbol{\alpha})}{\sqrt{q_m}}e^{iq_m s}+\sum_{n=1}^{\infty}R_{mn}(k)\frac{\chi_n(\boldsymbol{\alpha})}{\sqrt{q_n}}e^{-iq_n s},$$
$$s < -s_1 \quad (4.1)$$

where $k^2=q_m^2+k_m^2$ and k_m^2 is the mth eigenvalue of the transverse wave operator [see (3.1)–(3.4)]. Equation (4.1) corresponds to an incident wave in the mth mode of transverse oscillation and reflection in all modes. For n large enough, q_n becomes imaginary, in which case $q_n \equiv i|q_n|$. In region III the corresponding wave is

$$\psi_m^+(\mathbf{x},k)=\sum_{n=1}^{\infty}\frac{T_{mn}(k)}{\sqrt{q_n}}e^{+iq_n s}, \quad s > s_1 . \quad (4.2)$$

If the wave is incident from the "right" $(s \gg s_1)$, we have

$$\psi_m^-(\mathbf{x},k)=\frac{\chi_m(\boldsymbol{\alpha})}{\sqrt{q_m}}e^{-iq_m s}$$
$$+\sum_{n=1}^{\infty}R'_{mn}(k)\frac{\chi_n(\boldsymbol{\alpha})}{\sqrt{q_n}}e^{iq_n s}, \quad s > s_1 \quad (4.3)$$

$$=\sum_{n=1}^{\infty}T'_{mn}(k)\frac{\chi_n(\boldsymbol{\alpha})}{\sqrt{q_n}}e^{-iq_n s}, \quad s < -s_1 \quad (4.4)$$

We define the S matrix by

$$S_{mn}=\begin{bmatrix} R_{mn} & T'_{mn} \\ T_{mn} & R'_{mn} \end{bmatrix} \quad (4.5)$$

and find that unitarity requires $S^\dagger S = 1$.

The effects we are interested in occur at such low energy that only the lowest channel momentum, q, is real, so that it suffices to consider a "reduced" S matrix,

$$S=\begin{bmatrix} R_{11} & T'_{11} \\ T_{11} & R'_{11} \end{bmatrix} \quad (4.6)$$

which is separately unitary. Time reversal (in this basis) requires $S^T=S$ or $T_{11}=T'_{11}$. Together with unitarity this allows us to parametrize S as follows:

$$S \equiv \begin{bmatrix} -\eta e^{i\delta_1} & \sqrt{1-\eta^2}e^{i(\delta_1+\delta_2)/2} \\ \sqrt{1-\eta^2}e^{i(\delta_1+\delta_2)/2} & -\eta e^{i\delta_2} \end{bmatrix} . \quad (4.7)$$

Consider, now, a tube with curvature characterized by some length l_0 (e.g., radius of curvature). At incident momenta large compared with l_0 (but still below threshold for the second channel momentum, q_2) it can be shown that δ_1 and δ_2 are small (analogous to the Born expansion). At small incident momenta the pole at $k=i\kappa_1$ dominates the scattering amplitude. A trivial calculation yields

$$\delta_1=\delta_2\equiv\delta\cong\tan^{-1}(\kappa_1/k) \quad (4.8)$$

for $k \sim \kappa_1$. So at the lowest energy $(k \to 0)$ $\delta \to \pi/2$. As k increase $\delta(k)$ falls to zero over momentum scales of order $\kappa_1 \sim 1/l_0$. Likewise the transmission coefficient $|T|^2$, which is unity at large momentum, drops to zero like $k^2/(k^2+\kappa_1^2)$ as $k \to 0$. This striking effect, no phase shift at high incident momentum followed by a sudden change to $\delta=90°$ at momenta small compared to $1/l_0$ would give strong experimental evidence of the bound state.

In the case of electrons moving in a strip fabricated as a semiconductor nanostructure,[4] the transmission coefficient, $|T|^2$, can be directly measured by making a measurement of the conductance, σ, across ends of the strip. $|T|^2$ and σ are related to each other under conditions of ballistic transport (low impurity levels and low temperatures) by Landauer's formula[5]

$$\sigma=\frac{2e^2}{h}\widetilde{\mathrm{Tr}}|T|^2=\frac{2e^2}{h}\sum_{mn}\theta(E-E_n)T_{nm}^\dagger T_{mn} , \quad (4.9)$$

where E is the Fermi energy in the leads connected to the ends of the strip. $\widetilde{\mathrm{Tr}}$ denotes the trace over open channels. There has been considerable interest of late in the behavior of σ at low energy for straight strips and apertures of various shapes.[4] Sudden jumps of $2e^2/h$ in σ at successive transverse channel thresholds, as suggested by (4.9), have been observed. The bound state we are considering would modify the shape of the step in σ at the lowest threshold for a curved strip. Furthermore, at each successive threshold there should appear a resonance—actually a bound state in the mth channel just below the mth threshold and decaying into lower channels—and a characteristic variation of σ near threshold. The scale of these effects would be determined by the curvature of the strip.

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