Bound states and resonances in waveguides and quantum wires

John P. Carini
Department of Physics, Indiana University, Bloomington, Indiana 47405

J. T. Londergan
Department of Physics, Indiana University, Bloomington, Indiana 47405
and Nuclear Theory Center, Indiana University, 2401 Milo Sampson Lane, Bloomington, Indiana 47408-0768

Kieran Mullen
Department of Physics, Indiana University, Bloomington, Indiana 47405

D. P. Murdock
Nuclear Theory Center, Indiana University, 2401 Milo Sampson Lane, Bloomington, Indiana 47408-0768
and Department of Physics, Tennessee Technological University, Cookeville, Tennessee 38505
(Received 31 August 1992)

We present experimental and theoretical results on bound states in quantum wires (narrow, two-dimensional quantum channels). We study rectangular systems of constant width, varying the bend angle. This system is realized by propagation of TE-mode microwaves in flat rectangular waveguides; resonant frequencies for absorption of power are measured for various bend angles, and compared with theoretical results for bound-state (resonant) eigenvalues.

It is possible to produce very narrow two-dimensional surfaces that allow electrons to propagate in the channels formed by these surfaces, but require their wave functions to vanish on the surfaces. Such systems, called quantum wires (alternatively called quantum waveguides by Exner and Seba[1]), have been used extensively to study quantum interference effects.[2–5] One can imagine surfaces that have infinite extent; the general types of systems considered in this paper are shown in Fig. 1(b). Since such surfaces have no "classically forbidden" region, the discovery by Schult, Ravenhall, and Wyld[6] that such systems possess a bound state was rather surprising.

The existence of bound states in such systems has several implications for possible application to low-dimensional electron systems with similar boundary conditions. These have been discussed at length in previous papers.[2–5] Perhaps even more remarkable were recent results of Goldstone and Jaffe[7] (anticipated by earlier work of Exner[1,8]), namely, that at least one bound state will appear for *all* two-dimensional surfaces of constant width (except a surface of constant curvature, which possesses no bound state). Indeed, the results of Goldstone and Jaffe are valid for an infinite tube of constant cross section in any number of dimensions. As is well known, a bulge in a two-dimensional waveguide can be mapped into one dimension where the transverse bulge appears as an effective attraction, which always produces a bound state in one dimension. The fact that "bends do as well as bulges"[7] is quite surprising and at first sight counterintuitive.

The existence of these bound states can be understood qualitatively. Consider a rectangular system of constant width as shown in Fig. 1(a) (without loss of generality, normalize the width to unity). Requiring the wave function to vanish on the surface of the system, together with the separability of the Hamiltonian, forces the y dependence of the wave function in the right-hand leg of the system to be of the form $\sin(n\pi y)$ for integer n. The continuum starts at π^2, reflecting the quantization of the transverse wave number in the legs of the rectangle, $\lambda_n = 2/n$ (we use units where $\hbar^2/2m \equiv 1$). In the center of the waveguide, one can support wavelengths longer than the maximum allowed for continuum waves but

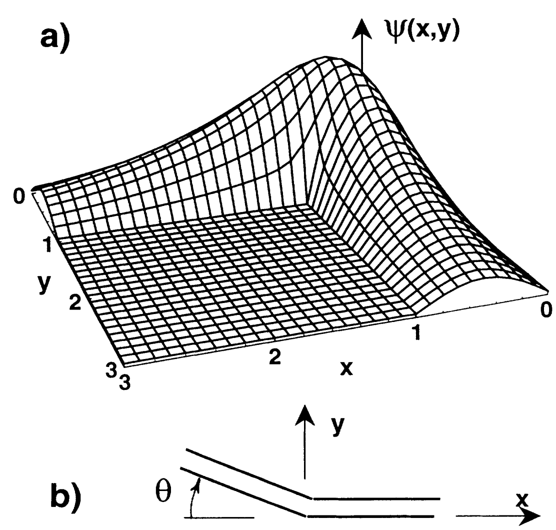

FIG. 1. (a) Bound state of a right-angle quantum wire. The vertical coordinate in the three-dimensional plot represents the amplitude for the bound-state wave function ψ in the quantum wire (or the amplitude of the transverse electric field for the resonant mode below the cutoff frequency of the $TE_{1,0}$ mode in the straight rectangular waveguide sections). (b) Schematic diagram of bent-waveguide geometry; θ denotes the angle by which the waveguide deviates from a straight channel.

which satisfy the boundary conditions [e.g., imagine a half sine wave running diagonally across the square in the central region of Fig. 1(a)]. Waves exceeding the maximum allowed continuum wavelength will be "trapped" in the interior. The extra space in the bend of such systems supports these long wavelengths, which make up the bound state.

The systems we consider are interesting examples of wave systems whose bound states do not arise from the "traditional" picture, where a binding potential creates classically allowed and forbidden regions. Here the boundary conditions (vanishing of the wave function on the waveguide boundaries) give an effective confining potential that produces a minimum (cutoff) energy for continuum solutions (bands of propagating states). Similar models have been used to describe several physical systems, for example, chemical rearrangement processes.[9,10] Most previous studies did not predict the existence of a bound state; the presence of bound states in such systems was noticed by Lenz *et al.*,[11] who considered this system as one example of models where confinement and scattering in multiquark systems were reformulated as a two-dimensional scattering problem. For the rectangular two-dimensional surfaces we consider, there is an exact correspondence between the eigenenergies and wave functions for electrons, and the z component of the electric-field vector for the $TE_{n,0}$ modes of a rectangular waveguide of identical width.

Upon seeing the bound-state predictions of Goldstone and Jaffe,[7] we reexamined bound states in bent rectangular waveguides as shown in Fig. 1(b), with bend angle θ. Present fabrication techniques produce curved quantum wires of constant area as discussed by Goldstone and Jaffe, but rectangular quantum wires with sharp corners might be produced in the near future.[12] In the limit as the bend angle θ goes to zero, the bound-state energy approaches the continuum π^2; with increasing θ the bound-state energy decreases, and for sufficiently large θ the system will support more than one bound state; we will describe theory and experiment for such systems in a subsequent paper.

We now outline a model for a waveguide with one bend that allows us to compare numerical and experimental determination of the bound-state energy. Consider an electron wave function satisfying the Schrödinger (or Helmholtz) equation with no potential in two dimensions,

$$\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+k^2\right]\psi(x,y)=0\ , \tag{1}$$

where ψ vanishes on the boundaries of the waveguide as shown in Fig. 1. To identify the bound state for this system, note that the Hamiltonian is symmetric under reflection about the diagonal, so we need consider only half the system. For a right-angle bend using the method of Schult, Ravenhall, and Wyld,[6] we predict a bound state with $k^2=0.929\pi^2$. A plot of the bound-state wave function ψ is shown in Fig. 1(a); ψ is concentrated about the center of the bend, vanishes on the boundary, and decreases exponentially in the waveguide legs.

To see the bound state in a real waveguide bend, we constructed a simple realization for microwaves of the variable-angle bend geometry shown in Fig. 1(b). Pairs of aluminum bars (0.953-cm thick) held between two large, milled aluminum plates form the sides of two straight waveguide sections, approximately 15-cm long when assembled. Removable, milled aluminum parallels 1.905-cm wide define the width a of the straight waveguide sections while the bend is constructed. One end of each of the inner 0.953-cm-thick bars was machined to a 30° angle so that in contact they produce the sharp (inner) corner between the waveguide section. Although we expect intense microwave magnetic fields near such a corner, mechanical contact should be sufficient to observe the bound state; for a TE mode with a maximum amplitude on the symmetry axis, no current will flow from one waveguide section to the other. The outer bars are machined to overlap to form the complementary angle on the outside of the bend. The calculated cutoff frequency for the waveguide sections is $f_{co}=c/2a$, approximately 7.87 GHz with an uncertainty from machining tolerances of 0.01 GHz.

We send microwave power into the bend region through a 0.141-in. semirigid coaxial line that passes through a 9/64-in. clearance hole in the top aluminum plate. The center conductor of the coax protrudes five millimeters beyond the outer conductor in order to serve as an electric dipole antenna. We adjust the coupling of the coax to the waveguide by varying the length of the protusion that extends into the waveguide. We use a Hewlett-Packard 8510B network analyzer to measure $R(f)$, the ratio of the microwave power reflected from the end of the coax (terminated by the antenna) to the incident power as a function of frequency. A bound state appears as a sharp decrease in reflected power, that is, as a resonant absorption of power, for microwave frequencies below the cutoff frequency. To determine the bound-state frequency, we decrease the coupling of the coax until (1) it is much less than critical coupling (when all incident power is absorbed) and (2) further decrease does not affect the resonant frequency or bandwidth of the resonance.

Figure 2 shows $R(f)$ for the 90° bend with a low coupling strength between coax and waveguide. The bound state appears as the prominent minimum in $R(f)$ at 7.585 GHz, shown by the left arrow in the figure. The resonance occurs well below the calculated cutoff frequency, indicated by the right arrow. We estimate the decay length of the mode as 2.3 cm, so the length of the straight waveguide sections is more than six times the decay length. The bandwidth of the resonance is 0.062 GHz, implying a rather low Q of approximately 125. Resistive losses in the mechanical joints between the walls and floor of the cavity will dominate radiation losses to the coax (which we can decrease) or out of the ends of the waveguide sections (which is strongly attenuated due to the expected exponential decay of the fields away from the region of the bend).

Analytic approaches for arbitrary bend angles often suffer from poor convergence. However, the bound states can be calculated numerically in a straightforward manner. To find the ground state, we consider the equation

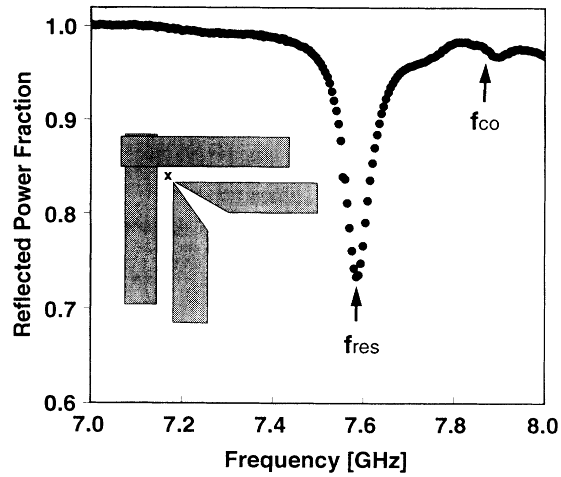

FIG. 2. Experimentally measured ratio of reflected power to incident power as a function of incident frequency in GHz, for right-angle waveguide bend. Arrows denote the resonant frequency $f_{\rm res}$ and cutoff frequency $f_{\rm co}$ (i.e., the beginning of the continuum) for straight waveguide sections of width 1.905 cm. Inset: Top view of experimental geometry. Waveguide sections were formed from parallel aluminum bars held between two large aluminum plates (not shown). Microwaves were radiated into the waveguide bend from a coaxial line with a protruding center conductor inserted through a hole in the top aluminum plate at the position marked "x."

$$-\frac{\partial}{\partial t}\psi(x,y,t)=\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\psi(x,y,t)\ , \tag{2}$$

starting from a random, noisy initial condition ψ_0. Such an initial condition is, in general, a mixture of all of the eigenstates $\phi_k(x,y)$ of the Hamiltonian so that $\psi_0=\sum_k a_k\phi_k(x,y)$. Then the solution of Eq. (2) is

$$\psi(x,y,t)=\sum_k a_k\phi_k(x,y,)e^{-E_k t}\ ,$$

where E_k is the eigenenergy of the kth state. Each component decays to zero exponentially; the state with the lowest energy will decay at the slowest rate. If we periodically normalize the wave function, then at large times the state with the lowest energy will dominate.

We approximate the two-dimensional wave function with one evaluated on a discrete set of points. These points are on the interstices of a rectilinear mesh with sides parallel to the boundaries of the waveguide. In our calculation, the length of the arms of the waveguide were six times their width, and the mesh size was taken to be 1/40 of the width. On this mesh we approximate the Hamiltonian with a discrete Laplacian. We then numerically solve Eq. (2), normalizing after each time step, until the energy approaches its asymptotic value. The great advantage of this approach is that we never need to invert or diagonalize the matrix representation of the Hamiltonian. It is possible to generalize the method to find arbitrary eigenvalues.[14]

We also used a variational method to estimate bound-state energies. Our method is that of Avishai *et al.*,[13] who applied it to waveguides that were almost straight. Consider a bent waveguide of Fig. 1(b), with bend angle θ. In the right-half waveguide, define a variational wave function

$$\psi(x,y)=\sum_{n=1} A_n\sin(n\pi y)\exp(-a_n x)\ ,$$

$$x\geq yt,\quad 0\leq y\leq 1\ , \tag{3}$$

where $t=\tan(\theta/2)$, and the A_n are variational parameters determined from the stationary conditions

$$\frac{\partial}{\partial A_n}\left[\frac{\int(\nabla\psi)^2}{\int\psi^2}\right]=0\ . \tag{4}$$

The variational condition can then be expressed as a determinant equation of the form[13] $\mathrm{Det}[\mathcal{H}(k^2)-k^2\mathcal{N}(k^2)]=0$. We truncated the matrices in this determinant to a finite basis, solved the determinant equations, and obtained the ratio k^2/π^2 of the eigenvalues to the continuum, as a function of the basis size N.

The dashed curve in Fig. 3 shows variational eigenvalues (for $N=16$) as a function of the bend angle θ; these are compared with experimental values for the bent waveguides (solid circles), and with numerical eigenvalues obtained by the relaxation method (solid curve). The experimental values agree with the numerical predictions to within experimental error. The variational results give higher energies than the experiment and relaxation method results (since they give an upper limit to the true energy). For small bend angles, our variational calculations are quite good but they overestimate the exact results by an increasing amount for larger bend angles; for sufficiently large bend angles, this variational method becomes numerically unstable.

Our results clearly demonstrate the existence of bound states in these systems, and the variation of bound-state

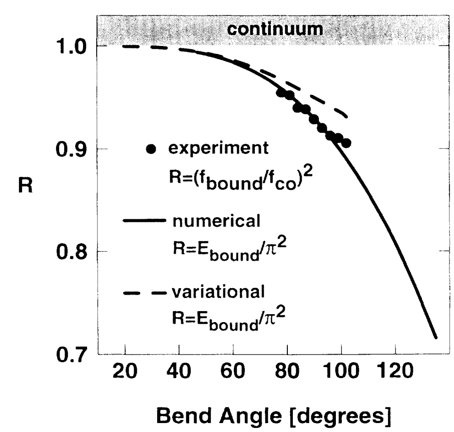

FIG. 3. Bound-state eigenvalue for bound state of bent waveguide vs bend angle θ. R denotes the ratio of the bound-state energy to the beginning of the continuum for a quantum wire ($E_{\rm bound}/\pi^2$) [or, for a waveguide, the square of the resonant frequency over the cutoff frequency ($(f_{\rm res}/f_{\rm co})^2$]. Solid circles, experimental measurements; solid curve, energy eigenvalues numerically calculated by relaxation method; dashed curve, variational estimate for energy eigenvalues.

energy with bend angle. For real waveguides, the presence of a resonance below cutoff frequency will affect the propagation of waves above cutoff frequency. For quantum wires, the presence of a bound electron at the bend could seriously affect the conductance properties of such systems.

One of the authors (J.T.L.) wishes to thank R. L. Jaffe for conversations which stimulated our interest in these systems, and for communicating to us his results with J. Goldstone prior to publication. The authors thank E. Davidson for making them aware of the relevant literature in quantum chemistry. Two of the authors (J.T.L. and D.P.M.) thank R. E. Kumon for assistance with preliminary calculations of bound-state energies. The work in this paper was supported in part by the NSF under Contracts Nos. NSF-PHY91-08036, NSF-DMR-9020816, and NSF-DMR-9113911. One of the authors (J.P.C.) acknowledges support from the Alfred P. Sloan Foundation.

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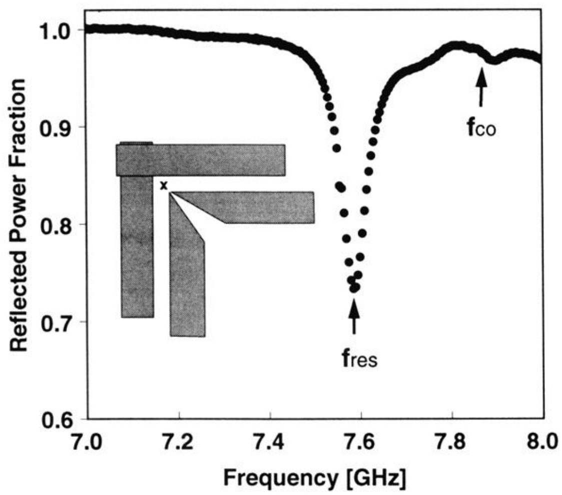

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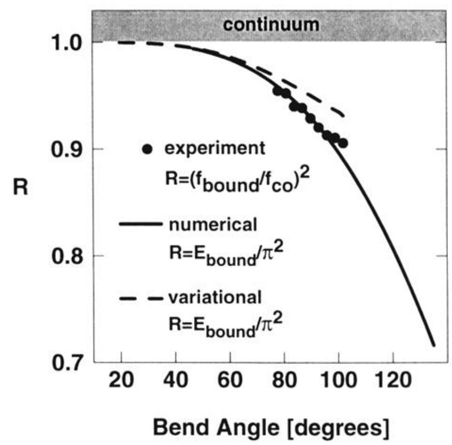

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