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## Rapid Communications

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# Quantum bound states in a classically unbound system of crossed wires

R. L. Schult, D. G. Ravenhall, and H. W. Wyld
*Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801*
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We have computed the energy and the wave function for an electron caught at the intersection of two narrow channels. There are two bound energies for the case with fourfold rotational symmetry. For impenetrable walls the energies are $E_1=0.66E_t$ and $E_2=3.72E_t$, where the threshold for propagation of electrons in one channel is $E_t=\hbar^2\pi^2/2m^*w^2$ and $w$ is the width of the channel. The state at $E_2$ is bound only because it has odd parity and thus cannot decay into the even-parity propagating wave at the same energy. (The odd-parity propagation threshold is at $4E_t$.) We have also computed the transmission and reflection probabilities in the propagating case for a range of energies up to slightly above the odd-parity threshold.

With the advance of fine-line lithography, devices can now be made which conduct along two-dimensional surfaces shaped into channels the width of which can be as narrow as 75 nm. Configured in four terminal junctions, such quantum wires are used to investigate quantum interference effects.[1-4] In this paper we report calculations designed to determine whether quantum effects can cause the trapping of an electron at the intersection of such wires. The presence of such trapped electrons could modify considerably the operation of devices made of these wires.

Since for the configurations we consider there is no trapping classically, the presence of a localized quantum-mechanical state is not an obvious phenomenon. It shows the quantum binding of a classically unbound system, and thus complements the phenomenon of the decay of a classically bound state by quantum tunneling. The problem is distinct from open geometries explored previously, such as that where the conducting region is contained by hyperbolas $x^2y^2=$const.[5] Because of the "pinched-off" arms of that shape, there are an infinity of classical periodic orbits, so that the presence there of quantum bound states is not surprising. We return to this point later.

We believe that the detailed shape of the potential which confines the electron to the channel is not important in determining the qualitative fact of the presence of a bound state at the intersection. We take a potential which is zero inside the channels and infinite outside, so that the Hamiltonian is just $H=\mathbf{p}^2/2m$ inside the well, with the boundary condition that the electron's wave function goes to zero on the sides of the channel (see Fig. 1). We have used two methods to calculate the bound-state energy and wave function and describe them in the following paragraphs. One of these methods is also suitable for extension to the propagating case, and we show results from such calculations. We conclude with some remarks on other configurations, and on the two-electron case.

Our first model is a mesh point method in which we replace the Schrödinger equation $H\Psi=E\Psi$ by a difference equation for the wave function evaluated on a rectangular mesh of points in the $x$-$y$ plane with discrete evolution in a "pseudotime" variable, $t$.[6] This equation is the discretized version of the differential equation $\delta\Psi/\delta t=\Delta\Psi$ where $\Delta$ is

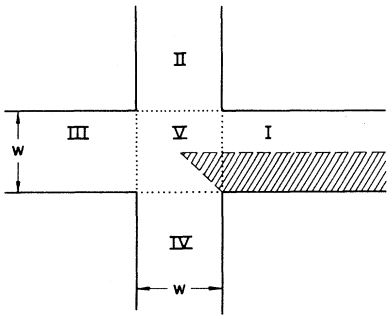


FIG. 1. Schematic diagram of the potential formed by the crossed wires. The hatched area, together with symmetry statements, is sufficient to display information about the bound-state wave functions and is the area shown in Fig. 2. The regions I through V are used in our function expansion method. The origin of the $x$ and $y$ axes is taken to be located at the lower left corner of region V.

 

the Laplacian operator. Solutions of this equation should be of the general form

$$\Psi = \sum_n a_n \exp(-k_n^2 t)\Psi_n ,$$

where $\Psi_n$ is an eigenfunction of $\Delta$ with eigenvalue $(-k_n^2)$. As pseudotime increases, the terms with larger values of $k_n^2$ die away, leaving the $\Psi_n$ with the lowest value of $k_n^2$. The explicit difference equation at time step $t = n(\delta t)$ is

$$\Psi_{i,j,n+1} = \Psi_{i,j,n} + (\delta t)[(\Psi_{i+1,j,n} + \Psi_{i-1,j,n} - 2\Psi_{i,j,n})/(\delta x)^2 + (\Psi_{i,j+1,n} + \Psi_{i,j-1,n} - 2\Psi_{i,j,n})/(\delta y)^2] .$$

(To keep $\Psi$ from becoming too small as pseudotime increases one renormalizes $\Psi$ at each pseudotime step by multiplying $\Psi$ by a constant to bring it up to a reasonable size.) We then iterate this difference equation until $\Psi$ becomes an eigenfunction of the discretized $\Delta$ operator.

When the initial wave function is taken to be symmetric about the center lines in the $x$ and $y$ directions (referred to as an even-parity state) and about the diagonal line $x = y$ (the symmetry expected for the nodeless ground-state wave function), we find the eigenvalue to be $kw = 0.812\pi$. This is below the propagation threshold at $kw = \pi$. The corresponding energy is $E_1 = \hbar^2 k^2/(2m^*) = 0.66E_t$, where the threshold energy is at $E_t = \hbar^2(\pi/w)^2/(2m^*)$. For an effective mass, $m^*$, of 0.067 times the free-electron mass, and a channel width of 75 nm, this bound-state energy is 0.66 meV, compared with the propagation threshold energy of 1.00 meV. The wave function is shown in contour plots in Fig. 2(a).

Some physical remarks concerning the shape of the wave function may give insight into the reason for its existence. Analysis of the wave function near the corners of the intersection (analysis similar to the conformal mapping argument for solutions of Laplace's equation near a corner) show that the wave function goes to zero as $r^{2/3}$, where $r$ is the distance form the corner. Thus it has a very steep slope near the corner. In a channel, well away from the intersection, the wave function is convex upwards across the channel and concave along it. The wave number across the channel is $\pi/w$, and the exponential decay wave number along the channel, $\kappa$, is related to the eigenvalue $k$ by $k^2 = (\pi/w)^2 - \kappa^2$. Thus $k^2$ is less than $(\pi/w)^2$. Near the center of the intersection, however, the wave function is convex upwards in all directions. Along the diagonals between the corners, which are $\sqrt{2}w$ apart, the steepening of the wave functions near the corners, mentioned earlier, results in a flattening near the center. Thus the effective diagonal wave number near the center, $k_d$, must have the property $k_d < \pi/\sqrt{2}w$, so that $k^2 = 2k_d^2 < \pi^2/w^2$. Thus the physically necessary behavior of the wave function there is consistent with that in the arms, and characteristic of a bound state. Figuratively speaking, the bound state is held in place by the corners.

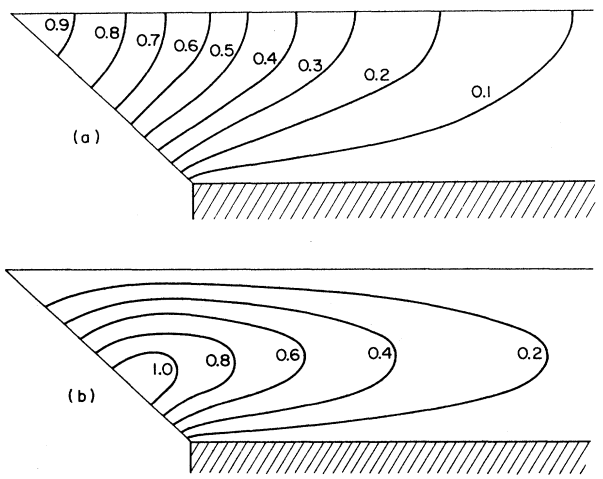


FIG. 2. Contour plots of the bound-state wave functions, covering the hatched region shown in Fig. 1. (a) The lowest-energy state. (b) The lowest odd-parity state. In each case the complete wave function consists of eight versions of the pattern shown, repeated in the other octants with appropriate reflections.

For an initial wave function which is odd about the $x$ and $y$ center lines and even about the $x = y$ line, the eigenvalue is given by $kw = 1.93\pi$, and the energy is $E_2 = 3.72E_t$. For states of this parity, the propagation threshold is at $kw = 2\pi$. Contour plots of the wave function are shown in Fig. 2(b). No bound states are found which are odd about the $x = y$ line. Unfortunately, this mesh-point method gives only the lowest state of each symmetry class. Possible higher-energy bound states would be inaccessible. For these we report our second method.

Our second method uses an expansion in a complete set of solutions of the differential equation $\Delta\Psi = -k^2\Psi$ (for a trial value of $k^2$) in each of the five large rectangular regions shown in Fig. 1, with the labels I,II,...,V. The coefficients in this expansion should then be chosen to match $\Psi$ and its derivatives at the boundaries between the five regions. This leads to a set of coupled linear equations for these expansion coefficients which can be treated as a single matrix equation. Specifically, in region I the expansion is

$$\Psi_{\mathrm{I}} = \sum_n a_n \sin(n\pi y/w)\exp(-K_n x)$$

with $(n\pi/w)^2 - K_n^2 = 2mE/\hbar^2 = k^2$. In region II the coefficients $a_n$ are replaced by $b_n$, and the variables $x$ and $y$ are interchanged:

$$\Psi_{\mathrm{II}} = \sum_n b_n \sin(n\pi x/w)\exp(-K_n y) .$$

Regions III and IV are similar using coefficients $c_n$ and $d_n$. In region V, the expansion is

$$\Psi_{\mathrm{V}} = \sum_n \{\sin(n\pi y/w)[e_n \exp(-K_n x) + f_n \exp(K_n x)] + \sin(n\pi x/w)[g_n \exp(-K_n y) + h_n \exp(K_n y)]\} .$$

When each sum is truncated at $N$ terms, we have a vector, $V_i$, made up of the $N$ sets of eight coefficients $(a_n, b_n, \ldots, g_n, h_n)$. There are eight boundary conditions (i.e., we must match the function $\Psi$ and its normal derivative on each of the four boundaries where regions meet). The orthogonality of the sine functions on these boundaries, together with these eight conditions, gives us an $8N \times 8N$ matrix, $M_{ij}$, and $8N$ coupled equations relating the $8N$ coefficients. (The coupling between coefficients having different $n$ values comes from the boundary conditions involving derivatives of the wave function.) Since there is no inhomogeneous term in this matrix equation, $M_{ij}V_j = 0$, the only nontrivial solutions will occur when the determinant of the matrix is zero. We find that the only zeros of the determinant occur at the energies found with our first method. There are no other bound states.

This second method has the further advantage that it can be extended to energies above the propagation threshold, where one or more of the $K_n$'s becomes imaginary, and the decaying potential $\exp(-K_n x)$ becomes the outgoing wave $\exp(i|K_n|x)$. The inverse of the matrix $M_{ij}$ becomes the scattering matrix describing reflection, direct transmission, and side transmission. (Outgoing wave amplitudes are obtained by applying $M^{-1}$ to a column vector of incoming wave amplitudes.) In Fig. 3 we show the various scattering probabilities in the energy range up past the opening of the $n=2$ channel. We note the appearance of the expected cusps at the energy corresponding to the opening of the new channel.

We turn now to a comparison with previous work. As extended by Simon,[5] Rellich's criterion (see the note added in proof to Simon[5]) refers to the lowest band edge (i.e., lowest transverse energy) at an infinite distance along the channels. In the case examined in Ref. 5, where the effective width of the channel tends to zero as one moves out to infinity along the channel, the lowest band edge also tends to infinity. By Rellich's criterion, that Hamiltonian has therefore only a discrete spectrum. In our case, however, the lowest band edge is the finite quantity $E_t$ in this limit, so that there can be a continuous spectrum, a not surprising result. That there are also bound states, our result, is a question not addressed by that criterion.

Finally we turn to some remarks about the generality of these results and observations on other phenomena which are related to this problem.

(1) The odd-parity bound state lies in the continuum of the even-parity channel, so if parity symmetry were not exact, as would be true of most physical devices, the odd-parity bound state should show up as a resonance in the scattering just below the opening of the $n=2$ channel, i.e., as a long-lived intermediate state of the scattering process. Such a resonance should be observable.

(2) The odd-parity case is equivalent to the case of a single wire, with half the width, bent at a right angle to look like an "L." We find, therefore, a bound state at such a bend, with wave number $kw = 0.96\pi$. We expect bound states to occur in other geometries as well. The "T" is one obvious candidate which arises in practical situations; for all three arms open and of equal width, it has just one bound state, at $kw = 0.90\pi$. Our second method is easily extended to any geometry composed of rectangles, open or closed, with equal or different widths.[7]

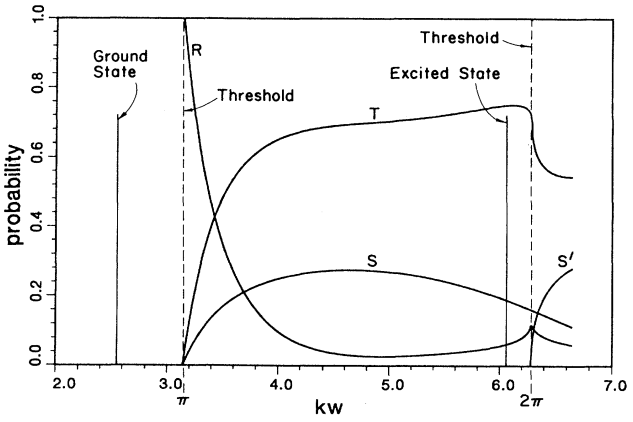


FIG. 3. Properties of the crossed-wire system, as a function of $kw$, with $w$ being the width of the wire and energy given by $E = \hbar^2 k^2/2m^*$. The bound states are shown as vertical lines. The functions are $R$, the reflection probability in the incident wire; $T$, the straight-through transmission probability; $S$, the probability of sideways transmission into the side wires; and $S'$, the probability of sideways scattering into the second transverse band, $n=2$.

(3) If one electron can be bound, can a second electron of opposite spin also be captured at the intersection? We have estimated the binding energy of the second electron using a product wave function with the results of our one-electron calculation as described above for each electron. The estimated energy of the two-electron system is

$$E_{2e} = 2E_1 + 2.56e^2/(\epsilon w),$$

where $\epsilon/\epsilon_0$ is the dielectric constant. Stability of the two-electron bound state depends on the sign of the energy difference $E_{2e} - (E_1 + E_t)$. We find that with $w = 75$ nm, dielectric constant $\epsilon/\epsilon_0 = 13$, and effective mass $m^* = 0.067 m_0$, the Coulomb repulsion energy is about 10 times the one-particle binding energy, so that two electrons are not likely to be bound in that case.

(4) Other multielectron effects can be investigated, such as the influence of the bound electron on the transmission of other electrons past the crossing.

(5) We have not yet investigated the effect a magnetic field would have on the bound state or on the scattering process, and thus on the Hall effect, but intend to do so. Our method may be used to investigate the importance of the sharp corners in forming the bound state, and the amount of bend required to form a bound state of the bent wire.

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[1]M. L. Roukes, A. Scherer, S. J. Allen, Jr., H. G. Craighead, R. M. Ruthern, E. D. Beebe, and J. P. Harbison, Phys. Rev. Lett. **59**, 3011 (1988).

[2]G. Timp, H. U. Baranger, P. deVegvar, J. E. Cunningham, R. E. Howard, R. Behringer, and P. M. Mankiewich, Phys. Rev. Lett. **60**, 2081 (1988).

[3]F. M. Peeters, Phys. Rev. Lett. **61**, 589 (1988).

[4]H. V. Baranger, A. D. Stone, and D. P. Di Vicenzo, Phys. Rev. B **37**, 6521 (1988).

[5]B. Simon, Ann. Phys. (N.Y.) **146**, 209 (1983). See also, S. J. Chang, Phys. Rev. D **29**, 259 (1984).

[6]W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge Univ. Press, Cambridge, 1986), p. 652ff.

[7]For a tight-binding approach to such problems, see F. Sols, M. Macucci, U. Ravaioli, and K. Hess, Appl. Phys. Lett. **54**, 350 (1989).