Ballistic electronic conductance of an orifice

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(Received 1 September 1988; revised manuscript received 15 May 1989)

We rigorously treat the quantum-mechanical ballistic propagation of a two-dimensional noninteracting-electron gas in a region where the electrons are free except for their interaction with the boundaries of the region. We compute the conductance of an orifice as a function of its width and length. The basic global structure of the conductance when the length is large reveals nearly quantized jumps of $2e^2/h$ as the width varies. A closer inspection shows oscillatory behavior between the plateaus. Both quantization and oscillations are explained in terms of a simple description based on barrier penetration, longitudinal wave resonances, and impedance matching.

Recent experiments by van Wees *et al.*[1] and by Wharam *et al.*[2] on ballistic motion of electrons through a narrow two-dimensional constriction revealed the phenomenon of conductance quantization, i.e., the conductance increases as a function of the constriction width by integer values in units of the fundamental conductance unit. A qualitative explanation of this phenomenon was advanced in Refs. 1 and 2, and additional theoretical studies have been performed.[3] The purpose of this paper is to present the results of our exact quantum-mechanical calculations of the conductance of an orifice of varying width a and length L, and to suggest a simple explanation of the structure of the conductance and its dependence on geometry. The basic quantities we calculate are the transmission amplitude matrix **t**, from which the conductance is evaluated using the linear conductance formula, $G=(2e^2/h)\mathrm{Tr}(\mathbf{t}\mathbf{t}^\dagger)$.[4] For the case of ballistic motion through the orifice we show that the calculated conductance of an orifice indeed approaches quantized values $n(2e^2/h)$ as $L\to\infty$, where the integer n varies with width a, and we describe the L dependence of this quantization. For finite L, the transition from the n to the $n+1$ plateau is not abrupt but oscillatory; these oscillations are longitudinal wave resonances. A semianalytic formula is suggested for the conductance based on concepts of barrier penetration and impedance matching. This simple formula reproduces the plateaus and the oscillations of the conductance remarkably well although the locations of the maxima are slightly shifted. Our methods can be easily extended to study samples containing impurities and the effect of a perpendicular magnetic field.

We study the conductance of an orifice shown in the inset of Fig. 1. Consider the quantum-mechanical motion of a particle with mass m and (Fermi) energy E in a planar region composed of two semi-infinite strips defined by $(-\infty<x\le 0,\ 0\le y\le b)$ and $(L\le x<\infty,\ 0\le y\le b)$ and a finite narrower strip separating them, defined by $(0<x\le L,\ 0\le y\le a)$ with $a<b$. We look for a solution of the Schrödinger equation, $-\Delta\psi_n=(2mE/\hbar^2)\psi_n$, corresponding to an incoming initial wave moving from left to right in a definite channel n, and which vanishes on the boundaries of the orifice. In the left region the wave function has the form

$$\psi_n(x,y)=\left[\frac{2}{b}\right]^{1/2}\left[e^{ik_nx}\sin\left[\frac{n\pi y}{b}\right]+\sum_{m=1}^{N}R_{mn}e^{-ik_mx}\sin\left[\frac{m\pi y}{b}\right]\right], \tag{1a}$$

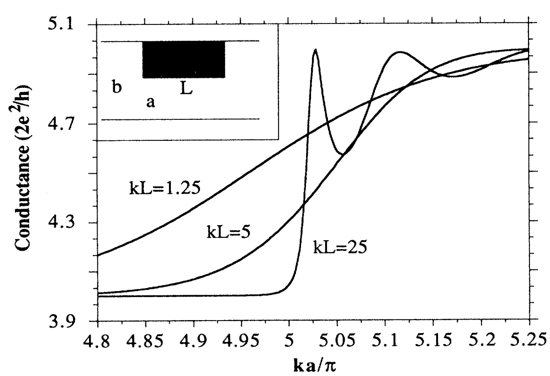

FIG. 1. Conductance (in units of $2e^2/h$) of an orifice of length L and width a situated between two regions of width b, $b>a$, for a two-dimensional electron gas with Fermi momentum k. The conductance is plotted as a function of ka/π between 4.75 and 5.25, for $kL=1.25$, 5, and 25.

while in the right region it reads

$$\psi_n(x,y)=\left[\frac{2}{b}\right]^{1/2}\sum_{m=1}^{N}T_{mn}e^{ik_m(x-a)}\sin\left[\frac{m\pi y}{b}\right] . \quad (1b)$$

Inside the orifice the wave function is

$$\psi_n(x,y)=\left[\frac{2}{a}\right]^{1/2}\sum_{j=1}^{J}(u_{jn}e^{iq_jx}+y_{jn}e^{-iq_jx})\times\sin\left[\frac{j\pi y}{a}\right] . \quad (2)$$

Here, $k^2=2mE/\hbar^2$, and the wave numbers k_n and q_j are given by

$$k_n=\left[k^2-\frac{n^2\pi^2}{b^2}\right]^{1/2}, \quad q_j=\left[k^2-\frac{j^2\pi^2}{a^2}\right]^{1/2} . \quad (3)$$

Thus, the reflection and transmission amplitudes R_{mn} and T_{mn} $(m,n=1,2,\ldots,N)$ are finite-dimensional matrices, the number N contains all channels for which the momenta k_n of Eq. (3) are real (namely $n<[kb/\pi]$) plus a finite number of evanescent waves for which the momenta k_n are imaginary which is sufficient to guarantee convergence with desired accuracy. The role of the evanescent waves within the orifice is even more crucial as we shall see below. Therefore, we set $J>[ka/\pi]$ in Eq. (2) and fix J so that convergence is assured.

In order to evaluate the transmission and reflection matrices $\mathbf{T}$ $(N\times N)$ and $\mathbf{R}$ $(N\times N)$ and the unknown matrices $\mathbf{u}$ $(J\times N)$ and $\mathbf{v}$ $(J\times N)$, we match the wave function and its derivatives with respect to x at $x=0$ and L. To this end it is useful to define the matrices

$$\mathbf{I}_{(N\times N)}=\{\delta_{mn}\},\quad \mathbf{K}_{(N\times N)}=\{k_m\delta_{mn}\} ,\quad \mathbf{Q}_{(J\times J)}=\{q_i\delta_{ij}\} , \quad (4)$$

and the matrix $\mathbf{A}_{(N\times J)}$ of overlap integrals

$$A_{nj}=\frac{2}{\sqrt{ab}}\int_0^a\sin\left[\frac{n\pi y}{b}\right]\sin\left[\frac{j\pi y}{a}\right]dy . \quad (5)$$

Using the completeness and orthogonality properties of the sine functions, we obtain the following set of matrix equations for the matrices $\mathbf{u}$ and $\mathbf{v}$,

$$\begin{bmatrix}\mathbf{A}^T\mathbf{K}\,\mathbf{A}+\mathbf{Q} & \mathbf{A}^T\mathbf{K}\,\mathbf{A}-\mathbf{Q}\\ (\mathbf{Q}-\mathbf{A}^T\mathbf{K}\,\mathbf{A})e^{iL\mathbf{Q}} & -(\mathbf{Q}+\mathbf{A}^T\mathbf{K}\,\mathbf{A})e^{-iL\mathbf{Q}}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix}=\begin{bmatrix}2\,\mathbf{A}^T\mathbf{K}\\ 0\end{bmatrix} , \quad (6)$$

where $\mathbf{A}^T$ is the transpose of $\mathbf{A}$. The matrices $\mathbf{T}$ and $\mathbf{R}$ are given in terms of $\mathbf{u}$ and $\mathbf{v}$ by the equations

$$\mathbf{T}=\mathbf{A}(e^{iL\mathbf{Q}}\mathbf{u}+e^{-iL\mathbf{Q}}\mathbf{v}),\quad \mathbf{R}=\mathbf{A}(\mathbf{u}+\mathbf{v})-\mathbf{I} . \quad (7)$$

Unitarity relations for the reflection and transmission amplitudes are easily written in terms of the flux normalized amplitudes $r_{mn}=(k_m/k_n)^{1/2}R_{mn}$ and $t_{mn}=(k_m/k_n)^{1/2}T_{mn}$:

$$\sum_{m=1}^{N}(|r_{mn}|^2+|t_{mn}|^2)=1 \quad \text{for } n=1,2,\ldots,N . \quad (8)$$

We evaluated $\mathrm{Tr}(\mathbf{tt}^\dagger)$ as a function of orifice (dimensionless) length kL and width ka, for $kb=50$, where $k=k_F$, the Fermi momentum (for the experiment reported in Ref. 1, the electron density was 3.56×10^{15} m^{-2} which yields $k_F=0.015$ Å^{-1}). In the numerical calculations, it was tempting to consider using only open channels in the orifice (i.e., $J=[ka/\pi]$). We tried the former and found, that the nearly exact quantization occurs also for very small L.[5] This indicates that the inclusion of evanescent waves is crucial to obtaining the correct result. We checked for convergence in the number of basis states used, i.e., adding additional evanescent waves in the wide regions and in the orifice did not significantly affect the results. In all calculations, unitarity was maintained to 13 digits.

In analyzing our results, we address the following points. (1) Does the simple model proposed above reproduce the observed conductance? (2) Is there a simple explanation for the quantization? (3) What is the role of the geometry of the constriction?

In Fig. 1 we plot the conductance as a function of the dimensionless parameter ka/π (which counts the number of channels with real momenta in the orifice) in the range $4.75<ka/\pi<5.25$ for $kL=1.25$, 5, and 25. For small orifice length, the conductance is monotonic and the step structure is very weak. In the limit of zero length (a Sharvin point contact,[6] studied by Haanappel and van Der Marel[3]) there is hardly any quantization. As the length increases, two interesting features appear. To the left of the step, as ka/π approaches an integer from below, the conductance is nearly quantized at 4 units, to within four digits. When ka/π exceeds an integer value (5 in this case), an oscillatory structure is observed with several well-defined resonances (justification for identifying these oscillations as resonances is presented below). These resonances initially have large amplitudes and small widths, but as ka/π increases towards the next integer, they become broader and their amplitudes diminish such that the near quantization at 5 units dominates. To the best of our knowledge, these resonances have not been observed experimentally. This may be due to experimental resolution and to thermal averaging. Experimental observation of these resonances would help confirm the validity of the model.

We propose the following simple explanation for the quantization and the resonances. For each mode j in the orifice ($j=1,2,\ldots,J$) with wave number q_j there is a mode $m(j)$, $m(j)=[j(b/a)]$, in the wide domains whose wave number $k_{m(j)}$ is closest to q_j. Mode $m(j)$ on the left excites mode j with a degree of excitation determined by the impedance matching between the two waves. Similarly, to the right of the orifice, mode j excites the mode $m(j)$. What we have then is transmission through a barrier of length L such that the wave number outside the barrier is $k_{m(j)}$ and inside the barrier it is q_j (i.e., a plane wave having wave number $k_{m(j)}$ penetrates through a "potential" barrier having height V_j given by $2mV_j/\hbar^2=k_{m(j)}^2-q_j^2$). The transmission coefficient for this penetration is

$$T_{m(j)}=\left[1+\frac{(k_{m(j)}^2-q_j^2)^2\sin^2(q_jL)}{4k_{m(j)}^2q_j^2}\right]^{-1} . \tag{9}$$

For $q_j^2<0$ replace q_j by $|q_j|$ and sin by sinh to obtain the tunneling transmission coefficient. The expression for the conductance just incoherently sums the contributions from all modes in the orifice. Therefore, we suggest the following approximate formula for the conductance:

$$G\approx G(\text{approx.})=\sum_{j=1}^{J}T_{m(j)} . \tag{10}$$

Figure 2 compares this expression with the exact solution for $kL=100$ in the range $4.99<ka/\pi<5.1$. The resonance structures obtained using this expression is very similar to that of the exact solution both in amplitude and in width, but are shifted somewhat in position. This shift is due to the imperfect matching implied by the approximate formula (10). The exact solution seems to have an effective length slightly larger than that of the approximate solution. If the later is increased, the peaks move to the left [$q_jL=(n+\frac{1}{2})\pi$ implies that a is a decreasing function of L] and the comparison improves substantially. This technique is known in reactor physics as the "extrapolated length" method,[7] in which one solves the Helmholtz equation in a box, but due to neutron leakage from the walls the wave function not strictly zero on the walls. One then identifies the solution in the actual box with the solution in a somewhat larger box whose wave

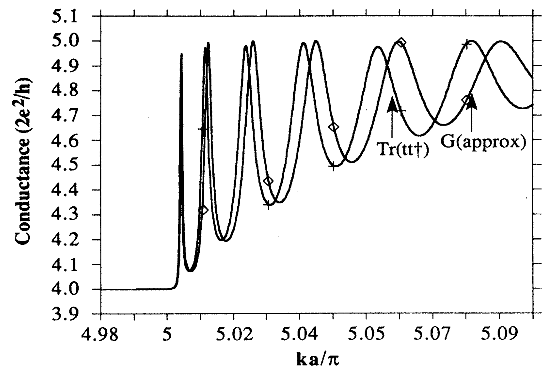

FIG. 2. Conductance (in units of $2e^2/h$) of an orifice of length L and width a situated between two regions of width b, $b>a$, for a two-dimensional electron gas with Fermi momentum k. The conductance is plotted as a function of ka/π between 4.99 and 5.1 for $kL=100$. The exact solution (squares) is compared with the approximation Eq. (10) (circles).

function does vanish on its walls; the extrapolated length is therefore always slightly larger than the original length. Since the exponents in the exact solution [see Eq. (6)] appear with the actual length L, the shift of the position of the resonances is hidden in the complex coefficients u_j and v_j, Eq. (2). The identification of oscillations with resonances in this context is now self-evident. When the product of the wave number and the length equals half an integer times π, the longitudinal waves in the orifice resonate.

Note added. After completion of this work a manuscript by Szafer and Stone[8] on the same topic appeared. They obtained similar results. Our explanation of the quantization and oscillations in terms of a simple description, based on barrier penetration, longitudinal wave resonances, and impedance matching, assumes that the orifice channel couples to only the channels nearest it in transverse wave number in the wide region. Reference 8 couples to a band of channels in the wide region and then obtains an effective one-dimensional problem. The present explanation works well for the wide-narrow-wide geometry considered here.

One of us (Y.A.) would like to thank Allied Signal, Inc. for the hospitality extended to him when this work was initiated. Discussions with B. J. van Wees, M. Buttiker, Ora Entin Wohlman, G. Erez, and R. Balian are highly appreciated. This work was partially supported by a grant from the U.S.-Israel Binational Science Foundation (Jerusalem, Israel).

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[5]This somewhat astonishing result can be understood as follows. The length L enters only through the matrix e^{iLQ} [see Eqs. (6) and (7)]. Each exponent $q_j L$ is numerically arbitrarily close to a rational number times 2π. Equations (6) and (7) remain numerically identical if L is replaced by $L'=pML$ where M is the common divisor of the rational numbers and $p=2,3,\ldots$. Thus, if the conductance is nearly quantized at large length L', this implies near quantization also for small L.

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