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Conductance oscillations in two-dimensional Sharvin point contacts

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The conductance of quantum-mechanical particles through two-dimensional point contacts, with and without impurities, is calculated. It is shown that, even for a zero-length constriction, steplike structures occur at integer multiples of $2e^2/h$ as a function of the constriction width. These step precursors evolve rapidly into horizontal plateaus on increasing the length of the constriction. It is also shown that the effect of impurities is to modify the structures and to shift the value of the conductance at the steps away from the quantized values.

Recently van Wees *et al.* published experiments on the conduction of ultranarrow constrictions in a two-dimensional electron gas (2D EG) based on a GaAs heterostructure.[1] In their experimental setup a split gate defines a short constriction connecting two larger areas of 2D EG. The constriction width is varied by tuning the gate voltage, which results in a surprising feature: The conductance increases in a sequence of steps of height $2e^2/h$. Shortly afterwards, similar results were independently reported by a second group.[2] Immediately the question came up as to what extent this type of conductance quantization is a universal property, insensitive to the details of sample geometry.

Imry,[3] Büttiker,[4] and Landauer[5] already anticipated quantized conductance between a reservoir and a quasi-one-dimensional lead, based on the quantization of transverse momentum in the lead. In the Letter by van Wees *et al.* an explanation was given based on similar considerations, which require a constriction that is much longer than it is wide. Assuming ballistic transport through the narrow region, it was shown that the conductance can indeed be quantized: On increasing the constriction width the Fermi level crosses a sequence of spin-degenerate one-dimensional subbands, each of which contributes precisely $2e^2/h$ to the conductance.

An obvious limitation of the above explanation is the assumption of virtually infinite length of the constriction, and the important question remains open as to whether quantized steps can also occur in the case of a constriction of finite or even zero length. The latter case corresponds to a two-dimensional Sharvin point contact[6] and the corresponding geometry is pictured in Fig. 1(a). In this paper we show that even in the zero-length limit conductance steps occur at integer multiples of $2e^2/h$. The steps are not very pronounced and decay rapidly on increasing the constriction width. Our theoretical method can also be used to predict the behavior of other geometries, in particular, constrictions with finite length and impurities in addition to a constriction.

We will now give a general outline of the formalism. A detailed description is given elsewhere.[7,8] Suppose that we can create a quasiequilibrium situation where the electrochemical potential μ on the left-hand side of the constriction region is given a small energy difference eV relative to μ on the right-hand side by applying an external voltage. In this way we create an imbalance between electrons moving from left to right and vice versa, which results in a net particle current. At zero temperature the number of ballistic electrons passing the constriction per unit of time equals the product of two terms:[6] (1) the number of particles per unit area in the energy interval eV at the Fermi level and in the angular interval $d\alpha$ around the angle of incidence α: $(\partial^2 n/\partial E\,\partial\alpha)eVd\alpha$; (2) the flux $\Phi(E_F,\alpha)$, which is the rate at which a unit area of these particles crosses the constriction region. The conductance G at zero temperature is now obtained by multiplying the angle-integrated particle current with the elementary charge and dividing by V, which results in

$$G=e^2\int_{-\pi/2}^{\pi/2}\Phi(E_F,\alpha)\frac{\partial^2 n}{\partial E\,\partial\alpha}d\alpha\,. \tag{1}$$

The problem of quantum transport of electrons through a Sharvin constriction can be mapped on an almost archetypal topic of wave mechanics: The diffraction of scalar waves by a slit in a perfectly soft screen[9] ($\phi=0$ on the screen). In spite of the apparent simplicity of this problem, no solutions in closed form have been found. There

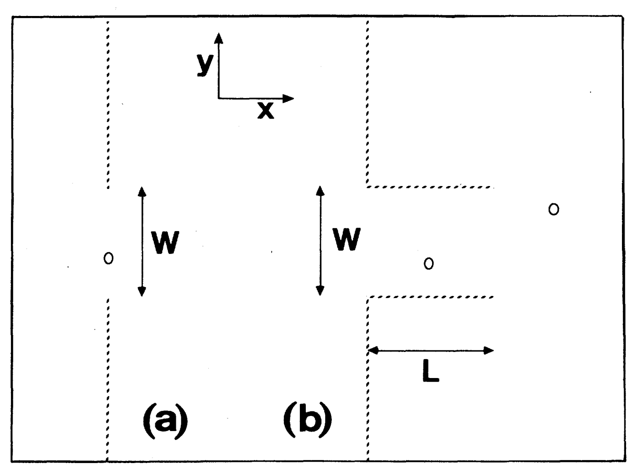

FIG. 1. Geometry for a constriction of (a) zero length and for a constriction of (b) finite length L. Impurities can be incorporated in the constriction on positions such as those indicated by the circles.

exists, however, a vast literature on these and related issues. Various approximations and series expansions have been derived.[10] The main difficulty is that the boundary conditions at the screen are of mixed von Neumann–Dirichlet character. The resulting integral equation contains singularities that are related to the ultraviolet divergencies of quantum electrodynamics.

In order to avoid these difficulties, we decided to treat the problem using a tight-binding scheme which, in the way we implemented it, has several advantages over the methods based on the above-mentioned integral equation: (1) The bulk of the numerical calculation involves the inversion of a complex valued matrix. The rank of this matrix equals the number of lattice points inside the aperture, which in our case could be kept below one hundred. Therefore, computational cost can be kept low. (2) No ultraviolet divergencies occur in the theory due to the high-energy cutoff that is automatically provided by tight-binding theory. Tight-binding schemes have been applied before to topics in weak electron localization,[11–13] which are intimately related to the present problem. In these approaches the transmission matrix is related to the conductance in a similar way as in Landauer's one-dimensional transport theory.[14] We will see that the T matrix is a useful tool in this particular problem. The Hamiltonian is

$$\begin{aligned} H &= H_0(t,V)+H_A(V)\,, \\ H_0(t,V) &= 4t\left(1-\tfrac{1}{4}\sum_{m,n}|m,n\rangle\langle m\pm 1,n\pm 1|\right) \\ &\quad + V\sum_{n=-\infty}^{\infty}|0,n\rangle\langle 0,n|\,, \\ H_A(V) &= -V\sum_{n=1}^{w/a}|0,n\rangle\langle 0,n|\,. \end{aligned} \tag{2}$$

Here $|m,n\rangle$ refers to a site with x coordinate ma and y coordinate na, where a is the lattice parameter on a square lattice. Note that the aperture potential H_A is proportional to V, which we will take in the limit $V\to\infty$. This means that H_A cannot be treated with Rayleigh-Schrödinger or Brillouin-Wigner perturbation theory. We will expand our expressions in a Taylor series of $1/V$ and take $V\to\infty$ in the final expressions.

Employing the time-dependent Schrödinger equation, one can easily derive that for a tight-binding Hamiltonian with only nearest-neighbor hopping the flux from left to right carried by an eigenstate $|\psi\rangle$ is given by

$$\Phi(\psi)=\frac{2ta^2}{\hbar}\,\mathrm{Im}\sum_{n=-\infty}^{\infty}\langle\psi|m,n\rangle\langle m+1,n|\psi\rangle\,. \tag{3}$$

As the total flux is conserved in an eigenstate, the coordinate m can be taken at any position. In our case a convenient choice is $m=0$ as the summation over n will now be constrained to the interval $[1,w/a]$. Using $|\psi\rangle=(1+gT)|\phi\rangle$, we can express the eigenstates $|\psi\rangle$ of the total Hamiltonian in terms of their parent states $|\phi_{E,\alpha}\rangle$, which are the solutions of H_0 with kinetic energy E and angle of incidence α.[15] In Refs. 7 and 8 we solve the Green's function g for H_0. We give the result in leading orders of V^{-1}:

$$\begin{aligned} \langle 0,n|g|0,n'\rangle &= -V^{-1}\delta_{n,n'}-2tV^{-2}\Gamma_{n,n'}\,, \\ \langle 1,n|g|0,n'\rangle &= -V^{-1}[\Gamma_{n,n'}-(E/2t-2)\delta_{n,n'} \\ &\qquad -\tfrac{1}{2}\delta_{1,|n-n'|}]\,, \end{aligned} \tag{4}$$

$$\Gamma_{n,n'}\equiv\pi^{-1}\int_0^{\pi}[\cos(n-n')\phi][(E/2t-2+\cos\phi)^2-1]^{1/2}d\phi\,.$$

From the T-matrix Dyson equation $T=H_A+TgH_A$, we immediately find that $\theta_{n,m}$, which we define as $(2t/V^2)\langle 0,n|T|0,m\rangle$, is the inverse matrix of Γ, where n and m are in the interval $[1,w/a]$. All other matrix elements of T are zero. The inversion of Γ forms the core of our numerical procedure. Inversions of large matrices are easily accomplished on most computers nowadays, so that the calculation for an aperture containing a hundred lattice points takes only a few seconds on a main frame. We now insert Eq. (4) in Eq. (3). After some algebra we obtain

$$\Phi(\phi_{E,\alpha})=\frac{V^2a^2}{2\hbar t}\,\mathrm{Im}\sum_{n,m}\langle\phi_{E,\alpha}|0,n\rangle\theta_{n,m}\langle 0,m|\phi_{E,\alpha}\rangle\,, \tag{5}$$

where $\langle\phi_{e,\alpha}|0,n\rangle=2itV^{-1}\sin(k_xa)\exp(ik_yan)$ is an eigenstate of H_0 projected on a site in the aperture. If we insert this in Eq. (5), we obtain a finite value for Φ in the limit $V\to\infty$.

The only other ingredient that we need in Eq. (1) is the expression $\partial^2n/\partial E\,\partial\alpha=k^2/4\pi t(x\sin x+y\sin y)$, where $x=k_xa$ and $y=k_ya$ for the density of states. Here we take into account the noncircular shape of the Fermi surface of our tight-binding band. After carrying out the angular integration in Eq. (1) we arrive at the simple expression

$$G=-\left(\frac{2e^2}{h}\right)\sum_{n,m}(\mathrm{Im}\theta_{n,m})(\mathrm{Im}\Gamma_{n,m})\,, \tag{6}$$

which is exact for all values of E_F including the long-wavelength limit. In the latter case, to which we will restrict our discussion, we have $E_F=ta^2k_F^2$, where k_F is the Fermi wave vector. A straightforward extension of Eq. (6) allows the study of more complicated structures, in particular, of finite-length constrictions. The resulting expressions are slightly more complicated and are treated in a forthcoming article.[8]

In Fig. 2 we present a graph of the conductance versus constriction width calculated with Eq. (6). This result is practically independent of k_Fa for $k_Fa<0.2$. We conclude from Fig. 2 that even for an ideal Sharvin point contact steplike structures are present. Also indicated in this figure are the conductance traces for finite-length constrictions of the type depicted in Fig. 1(b) with $L=0.48\lambda_F$ and $L=0.99\lambda_F$. We observe that the steps become more pronounced on increasing L and that there is an oscillatory structure on the plateaus for the longest constriction. To analyze these graphs in more detail, we present in Fig.

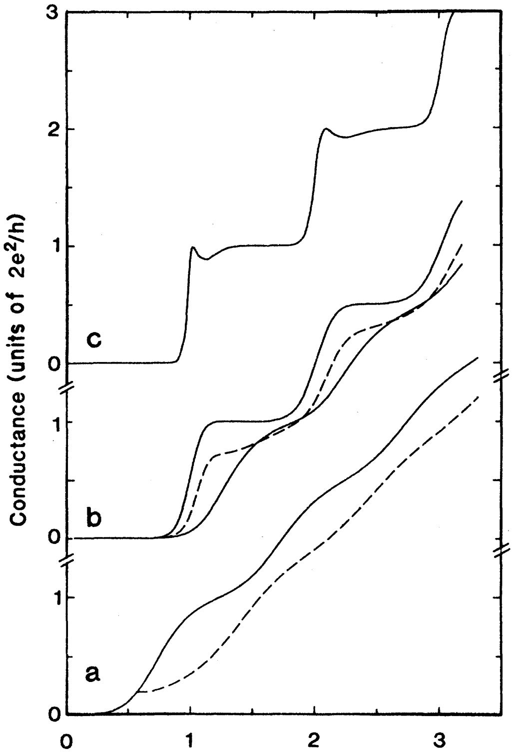

FIG. 2. Conductance vs constriction width. (a) $L=0$. Solid and dashed curve: constriction without and with impurity. (b) $L=0.48\lambda_F$. Upper solid curve: channel without impurity; lower solid curve: impurity inside the constriction ($x=0.32\lambda_F$, $y=0.32\lambda_F$); dashed curve: impurity outside the constriction ($x=0.57\lambda_F, y=0.32\lambda_F$). (c) $L=0.99\lambda_F$.

3 plots of $\pi dG/d(k_F W)$ vs G for several values of L. Here the positions of the minima along the horizontal axis represent the value of the conductance at a plateaus. A horizontal section is characterized by a minimum that touches the G axis. Clearly the positions of the minima are at integer multiples of $2e^2/h$. We observe that on increasing the channel length the minima become deeper and narrower, whereas the maxima are larger. The minima touch the G axis for a critical value of L, which depends on the plateaus index n. This critical length is approximately given by[8] $L_c \approx 0.32\sqrt{n}\lambda_F$. Beyond this value oscillations show up due to resonances between the front and back end of the constriction.

We next turn to the effect of impurities on the conductance. Delta function impurities can be incorporated either by excluding one or more points from the aperture Hamiltonian H_A or by adding extra terms $V|m,n\rangle\langle m,n|$.[8] In Fig. 2 we present the case of an impurity at a distance $y=0.32\lambda_F$ from one of the edges of the aperture of a zero-length constriction. For a constriction of length $L=0.48\lambda_F$ we give the result corresponding to a delta function impurity inside and just outside the narrow region, respectively. Clearly the conductance becomes smaller due to the presence of the impurity, and the oscillations are significantly suppressed and moved away from the quantized values. This is an important observation, as it shows that the details of the constriction environment influence both the quality of the steps and the value of the conductance at the steps. We checked many other configurations involving constrictions of various lengths and one or more impurities. The deterioration of the plateaus due to disorder turns out to be a very general phenomenon, regardless of the length of the narrow region.

We conclude that a numerically exact calculation of the

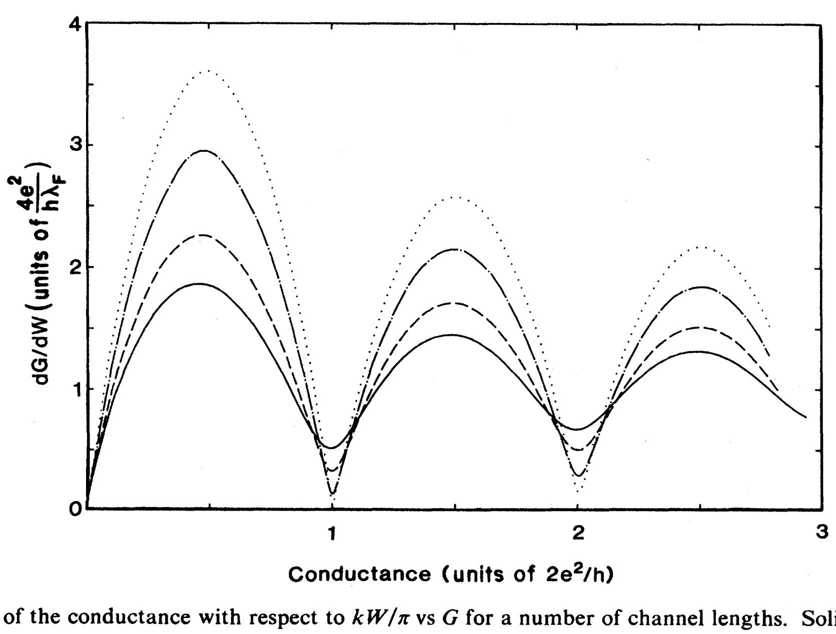

FIG. 3. First derivative of the conductance with respect to kW/π vs G for a number of channel lengths. Solid curve: $L=0$; dashed curve: $L=0.13\lambda_F$; dash-dotted curve: $L=0.25\lambda_F$; dotted curve: $L=0.35\lambda_F$.

quantum ballistic transport through an ideal two-dimensional Sharvin point contact shows that steplike structures in the conductance occur as a function of the width of the constriction, related to the steps observed by van Wees *et al.* The steps become more pronounced as the constriction acquires a finite length, which is also more representative of usual experimental conditions. Finally the presence of impurities in the constriction region modifies the value of the conductance at the plateaus.

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