Quantum Electronic Conductance of a Terminal Junction

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We rigorously treat the quantum-mechanical propagation of a two-dimensional electron gas through multithermal junctions. The elements $R_{mn,kl}$ of Büttiker's global resistance tensor are calculated for ballistic motion. Our results confirm the occurrence of negative resistance observed in recent experiments and predict oscillations of the resistance as a function of ka, where k is the electron Fermi momentum and a is the geometrical dimension of the junction leads.

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The quantum-mechanical propagation of particles through small confined regions, and terminal junctions connected to these regions, is of fundamental interest from both conceptual and technological points of view. In the context of electrical conductance, two-terminal junctions are quite common; for example, they were used in the recent beautiful experiments by van Wees *et al.*¹ and Wharam *et al.*² on ballistic motion of electrons through a narrow constriction which revealed conductance quantization in units of $2e^2/h$. Three-terminal junctions occur when a wire is connected to a ring; in the experiments on the Aharonov-Bohm effect in normal metal rings,³ two junctions of this kind occur (the configuration looks like -O- with the current entering the ring in one wire and leaving it in the second wire).

Four-terminal measurement of resistance for flat arbitrarily shaped samples was described by van der Pauw,⁴ and allows extraction of unwanted geometrical information in the determination of the resistivity of a sample.

The importance of four-terminal junctions in conductance measurements, and their relation to the measurement of the Hall conductance, has been stressed in fundamental papers by Büttiker^{5,6} which are the impetus for the present work. Büttiker described how to relate the resistance tensor of a system with several leads, or terminals, to the quantum-mechanical transmission and reflection coefficients describing the probability for carriers incident on one lead to reach another lead or to be reflected back into the initial lead. Quantum calculations of reflection and transmission coefficients for sam-



FIG. 1. Resistance $R_{12,34}$ (in units h/e^2) as a function of ka/π for the empty cross configuration (see inset). Integer values of ka/π mark the opening of a new physical channel.

ples with the topological structure of multiterminal junctions have been recently performed in order to study resistance fluctuations in multiprobe geometries.^{7,8} Here we develop an algorithm, based on rigorous quantum scattering theory, for the evaluation of transmission and reflection amplitudes of a system connected to multiterminal leads, thereby making possible calculation of the macroscopic global resistance tensor.

We consider a two-dimensional electron gas where particle motion is free except for its interaction with the boundaries of a cross-shaped four-terminal junction (see the inset of Fig. 1). A charged particle of mass m^* and energy E propagates through a fourfold-symmetric twodimensional cross with each of the arms of width a. For convenience we put the coordinate system origin at the bottom left corner of the cross. The energy $E = \hbar^2 k^2 / 2m^*$ and the width *a* of the cross determine the number of physical channels, $N = [ka/\pi]$, for which the squares of the channel momenta are positive, $k_n^2 = k^2 - n^2 \pi^2 / a^2 > 0$. The particle approaches the cross from the left (region 1) in a definite channel n, and is reflected back to region 1 (reflection amplitude matrix R_{mn}) and transmitted into regions 2, 3, and 4 (transmission matrix amplitudes $T_{mn}^{(2)}$, $T_{mn}^{(3)}$, and $T_{mn}^{(4)}$), where $m = 1, 2, \ldots, M > N$ contains also evanescent waves, i.e., closed channels. M, the number of channels retained in the calculation, is of course finite, but taking M = N may not be enough to achieve convergence. Our first task is to evaluate the transmission and reflection amplitudes. The electron wave function $\psi_n(x,y)$ has the following form in each of the four regions:

$$\psi_{n}(x,y) = \left(\frac{2}{a}\right)^{1/2} \left[e^{ik_{n}x} \sin\left(\frac{n\pi y}{a}\right) + \sum_{m=1}^{M} R_{mn}e^{-ik_{m}x} \sin\left(\frac{m\pi y}{a}\right)\right], \quad (x,y) \in \text{ region } 1,$$

$$\psi_{n}(x,y) = \left(\frac{2}{a}\right)^{1/2} \sum_{m=1}^{M} T_{mn}^{(2)}e^{-ik_{m}y} \sin\left(\frac{m\pi x}{a}\right), \quad (x,y) \in \text{ region } 2,$$

$$\psi_{n}(x,y) = \left(\frac{2}{a}\right)^{1/2} \sum_{m=1}^{M} T_{mn}^{(3)}e^{ik_{m}(x-a)} \sin\left(\frac{m\pi y}{a}\right), \quad (x,y) \in \text{ region } 3,$$

$$\psi_{n}(x,y) = \left(\frac{2}{a}\right)^{1/2} \sum_{m=1}^{M} T_{mn}^{(4)}e^{ik_{m}(y-a)} \sin\left(\frac{m\pi x}{a}\right), \quad (x,y) \in \text{ region } 4.$$
(1)

In the center of the cross (region 5) we write the wave function as the most general solution of the free-particle Schrödinger equation in two dimensions (an integral on the energy circle),

$$\psi_n(x,y) = \int_0^{2\pi} C_n(\theta) e^{ik(x\cos\theta + y\sin\theta)} d\theta, \quad (x,y) \in \text{ region 5},$$
(2)

where the functions $C_n(\theta)$ (together with the reflection and transmission matrices) are determined by matching the wave function and its derivatives on the boundaries between region 5 and regions 1-4. Since the sine functions are complete on each domain, the matching equations can easily be written in terms of the overlap integrals,

$$f_m(t) = \left(\frac{2}{a}\right)^{1/2} \int_0^a \sin\left(\frac{m\pi y}{a}\right) e^{ikty} dy = (2a)^{1/2} m\pi \frac{(-1)^m e^{ikta} - 1}{(kta)^2 - (m\pi)^2},$$
(3)

which decrease in magnitude (albeit slowly) with m. Thus, we obtain the matching equations

$$\int_{0}^{2\pi} f_m(\sin\theta)C_n(\theta)d\theta = \delta_{mn} + R_{mn}, \quad k \int_{0}^{2\pi} \cos\theta f_m(\sin\theta)C_n(\theta)d\theta = k_m(\delta_{mn} - R_{mn}), \quad (4a)$$

$$\int_0^{2\pi} f_m(\cos\theta) C_n(\theta) d\theta = T_{min}^{(2)}, \quad k \int_0^{2\pi} \sin\theta f_m(\cos\theta) C_n(\theta) d\theta = -k_m T_{min}^{(2)}, \tag{4b}$$

$$\int_{0}^{2\pi} e^{ika\cos\theta} f_m(\sin\theta) C_n(\theta) d\theta = T_{mn}^{(3)}, \quad k \int_{0}^{2\pi} \cos\theta e^{ika\cos\theta} f_m(\sin\theta) C_n(\theta) d\theta = k_m T_{mn}^{(3)}, \tag{4c}$$

$$\int_{0}^{2\pi} e^{ika\sin\theta} f_m(\cos\theta) C_n(\theta) d\theta = T_{mn}^{(4)}, \quad k \int_{0}^{2\pi} \sin\theta e^{ika\sin\theta} f_m(\cos\theta) C_n(\theta) d\theta = k_m T_{mn}^{(4)}.$$
(4d)

Here, m = 1, 2, ..., M and n = 1, 2, ..., N. For each physical channel *n* we have 8*M* equations for the 4*M* unknowns $R_{mn}, T_{mn}^{(2)}, T_{mn}^{(3)}$, and $T_{mn}^{(4)}$ and for the unknown function $C_n(\theta)$. If we replace the integration over θ by a quadrature sum with *K* mesh points, we must require the equality K=4M to obtain a system of equations whose solution can be determined. Therefore, *M* must be chosen sufficiently large to allow enough integration points for the integrals to be accurately determined (remembering that we need M > N anyhow, to allow for evanescent waves). A simple elimination procedure for each pair of matching equations in Eq. (4) leads to a system of 4*M* equations in the 4*M* unknowns

 $C_n(\theta_i)$, where θ_i , $i=1,2,\ldots,K=4M$, are the mesh points for the angular integrations. With $C_n(\theta_i)$ in hand, the transmission and reflection matrices are obtained using Eqs. (4) by quadrature. We check the numerical stability of the algebraic equations by monitoring the unitarity constraint,

$$\sum_{m=1}^{M} k_m \{ |R_{mn}|^2 + |T_{mn}^{(2)}|^2 + |T_{mn}^{(3)}|^2 + |T_{mn}^{(4)}|^2 \} = k_n$$

$$(n = 1, 2, \dots, N). \quad (5)$$

Thus, Eqs. (4) constitute a solution for the reflection and transmission amplitudes for the four-terminal ballistic motion case.

The elements of Büttiker's resistance tensor, $R_{mn,kl}$, where the first pair of indices indicate the contacts used to feed and draw current from the system while the second pair of indices indicate the probes measuring the potential difference, can now be calculated in terms of the reflection and transmission amplitudes. For ballistic motion, two elements of $R_{mn,kl}$ are identically zero due to symmetry (those for which the two terminals in a pair are not adjacent, e.g., $R_{13,24}$). This is easily understood since with this symmetry a current from, say, 1 to 3 cannot lead to a potential drop between 2 and 4. The remaining elements with m,n,k,l all different are equal up to a sign change (occurring when two indices in one of the pairs are permuted). We calculated $R_{12,34}$ based on Eq. (12) of Ref. 6, using the coefficients

$$T_{13} = \sum_{mn} \frac{k_m}{k_n} |T_{mn}^{(3)}|^2, \quad T_{12} = \sum_{mn} \frac{k_m}{k_n} |T_{mn}^{(2)}|^2,$$
$$R_{11} = \sum_{mn} \frac{k_m}{k_n} |R_{mn}|^2,$$

and the symmetry relations $T_{13} = T_{42}$ and $T_{12} = T_{34}$ valid for the ballistic configuration under consideration:

$$R_{12,34} = \frac{h}{e^2} \frac{T_{13}^2 - T_{12}^2}{4T_{12}(N - R_{11} - T_{12})^2}.$$
 (6)

We plot $R_{12,34}$ as a function of the dimensionless parameter ka/π in Fig. 1, letting ka/π vary between 4 and 16. The first remarkable point to be noticed is that $R_{12,34}$ is positive. Naively, one would expect $R_{12,34}$ to be negative since if a constant current is maintained between leads 1 and 2, a potential drop is expected between leads 4 and 3. This is schematically represented in Fig. 2, which shows a current source between 1 and 2, the resultant potential drop generated between 4 and 3, and a voltmeter which measures this voltage drop. Thus, from the definition of $R_{12,43}$ as the voltage drop between leads 4 and 3 divided by the current between leads 1 and 2, it should be positive (i.e., $R_{12,34}$ should be negative). From a quantum-mechanical point of view, however, the fact that $R_{12,34}$ is positive is not surprising. Indeed, T_{13} , the transmission coefficient for the straight-through motion, is larger than T_{12} , the transmission coefficient for the curved motion; hence the numerator in Eq. (6) is posi-



FIG. 2. Schematic diagram of current source between leads 1 and 2, the resultant potential drop generated between leads 4 and 3, indicated with signs across an effective resistor, and a voltmeter which measures this voltage drop.

tive. A classical explanation of the negative resistance $R_{12,34}$ is as follows (for convenience, let us consider positively charged carriers). Büttiker's derivation^{5,6} of the relationship between currents and voltage differences assumes that the currents in terminals 3 and 4 vanish. However, from the geometry of the cross, it is clear that when carriers are ejected into the cross from terminal 1, most of the carriers enter terminal 3. Since the current in terminal 3 must be zero, the chemical potent al in this terminal must be sufficiently high so that the potential drop between terminals 3 and 4 creates a current to counterbalance this flow of carriers. Therefore, the potential drop is of opposite sign to that in Fig. 2. We point out that our calculated negative resistance $R_{12,43}$ is in accord with the recent measurements of multiterminal resistance in high-mobility GaAs-GaAlAs heterostructures by Takagaki et al.9 who observed a negative resistance in a similar geometry, and their interpretation of this measurement. Experiments on quantum transport in an electron waveguide and its dependence on magnetic field and temperature have also been reported recently.¹⁰

The second point to be emphasized is the oscillatory structure of $R_{12,34}$, which can be understood as follows. For a fixed number of channels N, the numerator of Eq. (6) is dominated by T_{13} since, in the ballistic regime it is larger than T_{12} . The coefficient T_{13} increases with energy faster than the difference $R_{11} - T_{11}$ in the denominator of $R_{12,34}$. However, as a function of N, the dominant term is $(N - R_{11} - T_{12})^2$ occurring in the denominator. Hence, $R_{12,34}$ is an increasing function of k in a region of fixed N while globally it is a decreasing function of k since N increases with k. The global decrease is of course expected since as more and more channels become available, the resistance should decrease.

In addition to $R_{12,34}$, the two-terminal resistance $R_{13,13}$ with leads 2 and 4 connected to the sample can also be measured. This two-terminal resistance is given by the expression,⁶

$$R_{13,13} = \frac{V_1 - V_3}{I_1} = \frac{h}{e^2} \frac{1}{T_{12} + T_{13}}.$$
 (7)

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FIG. 3. Two-port conductance $[R_{13,13}]^{-1}$ (in units $e^{2/h}$) as a function of ka/π for the empty cross configuration.

The two "open" terminals 2 and 4 are not completely passive but serve as a source for inelastic scattering, and lead to deviation from the approximate quantization reported in Ref. 1 for a bona fide two-port geometry. We plot the conductance $[R_{13,13}]^{-1}$ as a function of ka/π in Fig. 3. Clearly, quantization is spoiled, although the step structure is apparent. Notice also that the magnitude of the conductance lags behind the number of channels due to inelastic scattering in terminals 2 and 4.

In the present calculations, it is assumed that the transition from the leads to the electron reservoirs proceeds without any additional scattering. The possibility of scattering near the reservoirs¹¹ is not taken into account.

In conclusion, we have developed a method to evaluate the elements of the resistance tensor in a four-terminal junction in the ballistic regime. Reduction of the method to a three-terminal junction is straightforward. Calculations employing our method confirm the occurrence of a negative resistance observed in recent experiments and the interpretation of this remarkable phenomena, and predict oscillations of the resistance as a function of ka. Our formulation can be extended to treat cases in which an impurity potential V(x,y) and magnetic field are present. An impurity potential V(x,y)present in the central region 5 can be treated by using Green's-function techniques, and if a magnetic field is present, the wave function in the central region can be expanded in terms of Landau functions of real noninteger order in analogy with Eq. (2). Hopefully such a treatment will open the way for realistic calculations of the Hall resistance, $R_{13,24}$.

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