Conduction in Curvilinear Constrictions: Generalization of the Landauer Formula

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We have generalized the multichannel Landauer formula to the case of leads with a variable cross section. Local equilibrium is achieved as a result of widening the constriction, rather than by the usual introduction of reservoirs and inelastic scattering. The generalized formula provides an explicit dependence of the conductance on the position of the voltage probes. We show that the previous Landauer formulas are obtained as limiting cases. Application of this formula to ballistic transport predicts new structure for the conductance.

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The scattering approach to electric transport in mesoscopic systems, which was pioneered by Landauer,[1] has been very successful, most notably in the treatment of strictly one-dimensional conductance. However, generalizations of the Landauer formula to the multichannel case have been the subject of significant controversy,[2] and several different formulas have been proposed. The diverse treatments[3] of the multichannel conductance have all employed the same geometry which seemed to be inherent to the scattering approach. The scattering region was always embedded between long perfect leads of constant cross section, the purpose of the introduction of the leads being the definition of the conductance channels. Once the channels are specified, the scattering matrix can be given in terms of transmission and reflection probabilities of various channels.

In addition to the scattering matrix, it is also necessary to specify the channel population. The most natural population is achieved[4] by means of reservoirs attached to the ends of the leads, which are kept at different chemical potentials. Equilibrium population in the reservoirs is maintained by the introduction (only inside the reservoirs) of some inelastic process. Two different conductance formulas can thus be obtained:

$$G=\frac{e^2}{\pi\hbar}\,\mathrm{tr}(tt^{\dagger}) \tag{1}$$

which is valid[3] if the voltage probes are located deep inside the reservoirs, and the formula of Büttiker *et al.*,[4,5]

$$G=\frac{e^2}{\pi\hbar}\,\mathrm{tr}(tt^{\dagger})\frac{2\sum v_m^{-1}}{\sum(1+R_m-T_m)v_m^{-1}} \tag{2}$$

which is valid if the voltage is measured inside the leads.

Since the reservoirs and the leads have very different properties, the matching between them is highly nontrivial and a contact resistance is expected[3,6] to arise. This additional resistance is not included in either of the two above conductance formulas and must be treated separately.

The shape of the constrictions used in recent experiments[7,8] studying electron transport through a narrow aperture is very different from the geometry assumed in the derivation of the standard conductance formulas. The walls of the conducting regions are far from being straight. Moreover, the quality of conductance quantization actually improves at low temperatures when the inelastic mean free path exceeds the size of the sample, suggesting that the importance of the process of equilibration has been somewhat overestimated.[9]

In this Letter, we apply the Landauer approach to electron transport in wires with a variable cross section. We derive a generalized conductance formula which contains both (1) and (2) as limiting cases and permits a smooth crossover between them when the voltage probes are moved from the narrow to the wide parts of the leads. We show that the wide regions serve as effective reservoirs even in the absence of inelastic scattering. Furthermore, we show that there is no need for separate treatment of the contact resistance.

We start with a simple observation that the free Schrödinger equation can be separated in several coordinate systems[10] in addition to the usual rectangular coordinates. If the boundaries of the leads coincide with lines (surfaces) $q_1=$const, in one of these systems, quasi-one-dimensional conduction channels can be defined. A wave incident from the mth left-hand-side channel has the following form:

$$\phi_m(\xi)\chi_m(\theta)+\sum_{m'} r_{m'm}\phi^*_{m'}(\xi)\chi_{m'}(\theta) \tag{3a}$$

in the left-hand-side lead, and

$$\sum_{m'} t_{m'm}\phi_{m'}(\xi)\chi_{m'}(\theta) \tag{3b}$$

in the right-hand-side lead. We have denoted the longitudinal coordinate by ξ and the transverse coordinate by θ. In three-dimensional systems θ denotes a pair of transverse coordinates.

To derive the conductance, we follow the same approach that led Büttiker *et al.*[4] to Eq. (2). We assume that all the states incident from the right are filled up to energy E_2, whereas the states incident from the left are filled up to $E_1=E_2+\Delta E$. The total current is then given

by

$$I=\frac{e}{\pi\hbar}\Delta E\,\mathrm{tr}(tt^{\dagger}), \tag{4}$$

where we have allowed spin degeneracy.

Since our boundary conditions are asymmetric, the carrier distribution cannot be described by a simple chemical potential. We can, however, introduce an effective chemical potential $\mu(\xi)$, defined by the condition that the equilibrium carrier density implied by $\mu(\xi)$ is equal to the actual density $\rho(\xi)$. The potential difference eV between voltage probes located at ξ_p and $\xi_{p'}$ is given by[4] $eV=\mu(\xi_{p'})-\mu(\xi_p)$. The total carrier density can be decomposed into a density of particles that came from the right and the density that came from the left, $\rho(\xi)=\rho_R(\xi)+\rho_L(\xi)$. Expressing the voltage in terms of $\rho_L(\xi)$, we find

$$eV=\frac{\partial\rho_L(\xi_{p'})/\partial E-\partial\rho_L(\xi_p)/\partial E}{\partial\rho(\xi_p)/\partial E}\Delta E, \tag{5}$$

where we have assumed for simplicity that $\partial\rho(\xi_p)/\partial E=\partial\rho(\xi_{p'})/\partial E$. Combining (4) and (5) we finally obtain our central result

$$G=\frac{e^2}{\pi\hbar}\mathrm{tr}(tt^{\dagger})\frac{\partial\rho(\xi_p)/\partial E}{\partial\rho_L(\xi_{p'})/\partial E-\partial\rho_L(\xi_p)/\partial E}. \tag{6}$$

In the case of rectangular leads, this result reduces to Eq. (2). Much more interesting, however, is the case of leads with variable cross section—wide in the asymptotic regions and narrow in the middle. We will discuss in detail two-dimensional leads bounded by a pair of confocal hyperbolas [Fig. 1(a)]. This geometry is of particular importance since it closely approximates the shape of constrictions used in actual experiments.[7,8] Elliptic coordinates [Fig. 1(b)] are defined by

$$\begin{aligned} x&=a\sinh\xi\cos\theta, \quad -\infty<\xi<\infty,\\ y&=a\cosh\xi\sin\theta, \quad \tfrac{1}{2}\pi\le\theta\le\tfrac{1}{2}\pi, \end{aligned} \tag{7}$$

where $2a$ is the distance between the foci. In these coordinates, the Schrödinger equation inside the leads separates into

$$\frac{d^2\chi}{d\theta^2}+(b^2-h^2\sin^2\theta)\chi(\theta)=0, \tag{8a}$$

$$\frac{d^2\phi}{d\phi^2}+(h^2-b^2+h^2\sinh^2\xi)\phi(\xi)=0, \tag{8b}$$

where $h=k_Fa$. Using the transverse equation (8a) and the boundary conditions $\chi(\theta_1)=\chi(\theta_2)=0$ one can determine the set of transverse functions $\chi_m(\theta)$ together with the corresponding values b_m of the separation constant. The asymptotic form of the longitudinal wave function $\phi_m(\xi)$ in the mth channel is given by

$$\phi_m(\xi)\sim\frac{1}{\sqrt{h_m(\xi)}}\exp\left(\pm\int^{\xi}h_m(\xi)d\xi\right), \tag{9}$$

where $h_m^2(\xi)=h^2-b_m^2+h^2\sinh^2\xi$. The classical turning point ξ_m of the mth channel is determined by the condition $h_m(\xi_m)=0$. Although the total number of channels is infinite, only a finite number of channels can have a nonzero transmission probability. According to Eq. (6), the measured conductance depends on ξ_p and $\xi_{p'}$—the position of the voltage probes. Consider first the case of $0<-\xi_{p'},\xi_p\ll1$, i.e., voltage probes located in the narrow region where we have N propagating channels. If we also assume that $|\theta_1-\theta_2|\ll1$, the narrow region will be long enough so that evanescent modes can be neglected. The wave functions of the propagating channels are given by (9), where we can set $h_m^2=h^2-b_m^2$, $m=1,\ldots,N$. The wave functions are then just plane waves and Eq. (6) coincides with Eq. (2).

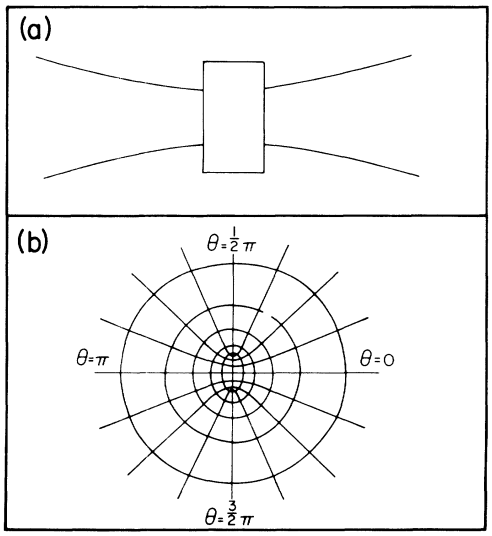

FIG. 1. (a) The geometry for leads with a variable cross section. The leads are formed by a pair of confocal hyperbolas. (b) Elliptic coordinate system.

Consider now the opposite limit of voltage probes located in the asymptotic region ($\xi_p,|\xi_{p'}|\gg1$). Here we can use for the transmitted channels the asymptotic form (9) with $h_m(\xi)=he^{|\xi|}$. In two dimensions, $\partial\rho/\partial E=m^*/2\pi h^2$ (m^* is the carrier mass), and (6) reduces to

$$G=\frac{e^2}{\pi\hbar}\mathrm{tr}(tt^{\dagger})\frac{1}{1-[2\mathrm{tr}(tt^{\dagger})/k_Fa|\theta_1-\theta_2|](e^{-\xi_p}+e^{-|\xi_{p'}|})}. \tag{10}$$

As the probes are moved closer to the wide regions, the measured conductance approaches the standard result (1) which is expected when the voltage is measured between reservoirs. In terms of the effective chemical potential, the denomi-

nator of (10) can be written as

$$1+\frac{\mu(\xi_p)-E_1}{E_2-E_1}+\frac{\mu(\xi_{p'})-E_2}{E_1-E_2}. \tag{11}$$

The carrier population in the right (left) lead can be thought of as a completely filled up to E_2 (E_1) Fermi distribution plus current-carrying excitations (electrons in the right lead, holes in the left lead). From the definitions of E_1, E_2 and $\mu(\xi)$, it follows that the difference between $\mu(\xi)$ and E_1 (E_2) is proportional to the density of excitations. Comparing (10) and (11), we see that as a result of the spreading of the current flow, this density decreases as the leads widen. If the voltage probes are located in sufficiently wide regions, the influence of nonequilibrium electrons on the measured voltage is negligible and Eq. (1) is recovered.[11]

In our treatment, we have assumed a certain population of the incoming channels. Accumulating excitations can change this population and affect the conductance. This problem can be avoided by making the measurement during a sufficiently short period of time, before the population is changed significantly.

Alternatively, this extra energy can be dissipated by some inelastic process. The corrections to the conductance due to scattering (elastic or inelastic) in the leads becomes smaller as the mean free path (mfp) increases. In the particular geometry we are considering, $\Delta G \sim l^{-1}$, and by increasing the mfp, the influence of the additional scattering in the leads can be made arbitrarily small. The fact that the scattering in the leads weakly affects the conductance is only correct for leads which widen asymptotically. Previous derivations of the conductance formula were all restricted to the case of leads with a constant cross section, in which scattering in the leads usually modifies the conductance. In order to overcome this problem, the concept of reservoirs was introduced.[1-4] The most important property of widening the leads is that they serve as natural reservoirs.

Dissipation of the energy of the external electric field proceeds in two steps. First, the energy is transferred from the field to the carriers. This process is, in principle, reversible and does not involve an increase in entropy. In our treatment, we have discussed only this first step. The generalized Landauer formula (6) gives therefore the amount of energy absorbed by the carriers between $\xi_{p'}$ and ξ_p, that is, $P=I^2/G(\xi_p,\xi_{p'})$.

To demonstrate the applicability of the generalized formula (6), we consider transport through a constriction bounded by a pair of confocal hyperbolas (inset in Fig. 2). This geometry is of particular interest from the experimental point of view since it closely approximates the shape of ballistic point contacts. It was demonstrated experimentally[7,8] that the conductance pattern consists of smoothly connected quantized plateaus. This phenomenon was treated theoretically by several workers by calculating the transmission probabilities either for sharp[12] or smoothly curved[13-16] constrictions within the framework of the formula $G=(e^2/\pi\hbar)\mathrm{tr}(tt^\dagger)$. We now calculate G for two different positions of the probes by using the generalized Landauer formula (6). In elliptic coordinates, the Schrödinger equation separates into transverse and longitudinal equations (8a) and (8b). From Eq. (8b) we calculate the transmission probabilities

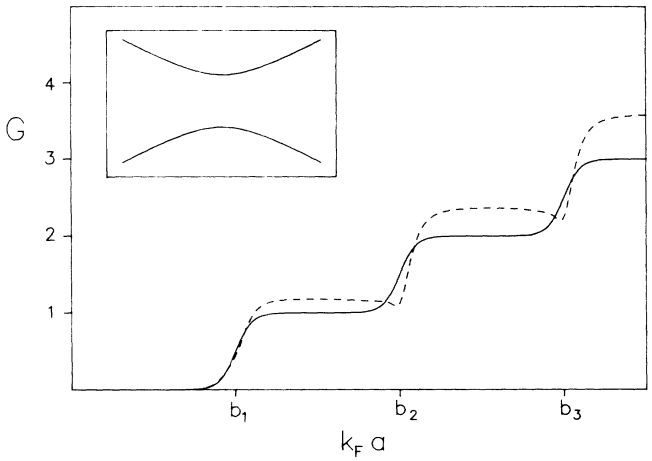

FIG. 2. G (in units of $e^2/\pi\hbar$) as a function of $k_F a$. The solid line corresponds to voltage probes in the wide regions. The dashed line corresponds to probes in the intermediate region ($\xi_p \sim 1$).

$$|t_{mm'}|^2=\delta_{mm'}\left[1+\exp\frac{\pi}{h}(b_m^2-h^2)\right]^{-1}. \tag{12}$$

In Fig. 2, we plot the conductance as a function of $k_F a$ (a is half the distance between the foci) for two different positions of the probes. When the probes are in the wide regions (solid curve), the conductance exhibits quantized plateaus. The quantization is more pronounced for a gradual opening of the constriction (small $|\theta_1-\theta_2|$). When the probes move towards the narrow region, the conductance is no longer given by Eq. (1), but rather by the generalized formula (6). The conductance for an intermediate position of the probes is shown by a dashed line in Fig. 2. The quantized pattern is preserved, but the values of the conductance on the plateaus are larger than $me^2/\pi\hbar$. The second interesting feature is the nonmonotonic behavior of the conductance due to the appearance of a dip at the end of the plateaus. Near the transition regime, the appearance of a new mode causes an increase in local voltage and a drop in the conductance.

In the derivation of Eq. (6), we assumed that the voltage probes are noninvasive. As recently discussed by Landauer,[9] this can be achieved experimentally. Nonideal probes affect the measurement in two ways: they introduce additional scattering and they extract current from the system. The second problem can be handled by the multiprobe approach of Büttiker.[17] The

scattering from the probes can affect measurements of the local voltages in the narrow region of the constriction. As the probes are moved into the wide region, the influence of scattering is diminished.

The exact solution of the Schrödinger equation in hyperbolic constrictions can be compared with the adiabatic approximation[13,14] which was recently used to explain the quantization of conductance in ballistic point contacts. For short constrictions ($L \ll \sqrt{Rd}$), the adiabatic approximation indeed gives the correct transmission probabilities.[12] For $L > \sqrt{Rd}$, the adiabatic approximation predicts strong mode mixing and a breakdown of separability of the Schrödinger equation. Since the Schrödinger equation *is* separable in elliptic coordinates, the condition $L < \sqrt{Rd}$ must be interpreted as a criterion for the validity of the adiabatic approximation.

In summary, we have derived a generalized Landauer conductance formula, which is valid also for wires with a variable cross section. We have shown that this geometry removes the need to introduce reservoirs and inelastic scattering. Moreover, the problem of contact resistance is avoided. We have applied our formula to ballistic transport and predicted new dips in the quantized plateaus.

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