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Theory of nonlinear transport in narrow ballistic constrictions

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We present quantum-mechanical model calculations of nonlinear transport in narrow ballistic constrictions. We calculate the current and differential conductance g as functions of the applied voltage V_0 and the electron Fermi energy E_F. Nonlinear effects in g smooth out transmission resonances and shift and degrade the quantized ballistic conductance plateaus. Contrary to previous claims, we find that g does not develop additional plateaus between those quantized at $2ne^2/h$. At high V_0 the current saturates at values strongly dependent on E_F.

The experimental study of electronic transport through narrow ballistic constrictions in two-dimensional electron gases (2D EG), made possible by the remarkable recent advances in microfabrication,[1] has opened up a novel and active field where many fascinating phenomena are being observed. At low temperatures, the electronic motion in these nanostructures is ballistic since the electron mean free path is comparable with their spatial dimensions, and boundary scattering is the main collision process. Because of the small size of the constrictions, the quantization of the electron energy levels dominates the transport properties and, in linear response (LR), the conductance is sharply quantized in units of $2e^2/h$.[2-11]

Recently, some interesting work has begun to appear on ballistic constrictions in the high-field (HF) regime, where nonlinear effects are expected. The first experimental study was reported by Kouwenhoven *et al.*[12] who obtained highly nonlinear *I-V* characteristics, and a breakdown of conductance quantization ascribed to an unequal population of transverse subbands in the two velocity directions. Glazman and Khaetskii[13] proposed a theoretical model predicting the possible existence of half-plateaus (HP's), i.e., quantized conductance plateaus at values intermediate between those observed in LR; however, experiments have not supported the existence of the HP's. The theoretical work of Lent, Sivaprakasam, and Kirkner[14] has focused on the related problem of wide-narrow-wide configurations of 1D conductors at high temperatures and HF's showing, among other things, that the behavior of a narrow constriction is qualitatively different from that of a potential barrier (in contrast with the situation occurring in LR), and that the current saturates for high voltages.

In this paper we also study the transport properties of narrow ballistic constrictions in the HF regime. However, we consider constrictions between two infinite 2D EG's, a model more appropriate for the experimental systems in Refs. 2, 3, 10, and 12. Our model is shown schematically in Fig. 1(a). A narrow constriction C of width W and length D connects two semi-infinite 2D EG's, L and R. The shaded areas are inaccessible to the electrons and are modeled by a hard-wall potential. The levels are occupied up to E_F in L and up to $E_F-|eV_0|$ in R, where V_0 is the total potential drop along C as shown in Fig. 1(b). The electronic current through the constriction is due to electrons incident on C from L with energies in a window between $E_F-|eV_0|$ and E_F. We assume a linear potential drop in C but our method can be readily generalized to other situations. At present there is no precise knowledge of the potential variation in these systems; our choice is the simplest one and allows the prediction of the main features expected in the HF regime.

We perform quantum-mechanical model calculations of the wave function, the current $I(E_F,eV_0)$, and the differential conductance $g(E_F,eV_0)$ in the effective-mass approximation. The model Hamiltonian is

$$H=-\hbar^2(\partial^2/\partial x^2+\partial^2/\partial y^2)/2m^*+U(x,y)\,,$$

where m^* is the electron effective mass and $U(x,y)$ is the potential describing the system shown in Fig. 1; $U(x,y)$ is zero for $y<0$, $-|eV_0|$ for $y>D$, $-y|eV_0|/D$ for $|x|\leq W/2, 0\leq y\leq D$, and ∞ elsewhere.

Consider an electron with a wave vector $\mathbf{k}=(K,k)$ and energy $\varepsilon_{\mathbf{k}}$ incident on C from L. In each region (L, C, or R) the wave function is written as a linear superposition of a complete set of appropriate eigenfunctions. For L ($y<0$) we have

$$\psi_{\mathbf{k}}^L(\mathbf{r})=e^{ik_Ly}\phi_K^{2D}(x)+\sum_K a_K^- e^{-ik_Ly}\phi_K^{2D}(x) \qquad (1)$$

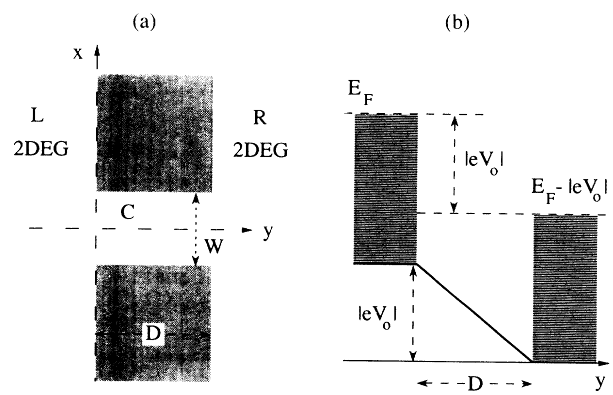

FIG. 1. (a) Schematic representation of the system, and (b) of the potential drop across the constriction and the energy levels in L and R.

and for R $(y > D)$ the wave function is

$$\psi^R_{\mathbf{k}}(\mathbf{r}) = \sum_Q a_Q^+ e^{ik_R y}\phi_Q^{2D}(x)\,, \qquad (2)$$

where the transverse wave functions are $\phi_K^{2D}(x)=e^{iKx}$, $k_L=(2m^*\varepsilon_{\mathbf{k}}/\hbar^2-K)^{1/2}$, and $k_R=[2m^*(\varepsilon_{\mathbf{k}}+|eV_0|)/\hbar^2-Q^2]^{1/2}$. We sum over all K and Q in (1) and (2) thus including every current transporting state, and also every evanescent state.

We approximate the linear potential in C by a staircase potential with a number of steps, N, large enough to ensure a converged approximation for the current. Then

$$\psi^C_{\mathbf{k}}[x,(j-1)D/N \le y < jD/N] = \sum_n \phi^C_{nj}(x)(a^-_{nj}e^{-iq_{nj}y}+a^+_{nj}e^{iq_{nj}y})\,, \qquad (3)$$

where $\phi^C_{nj}(x)$ is the nth transverse eigenstate of the jth step in C, $j=1,2,\ldots,N$. For a square-well confining potential, at each step, the transverse-level eigenenergies are given by $E_{nj}=\hbar^2/2m[(n\pi/W)^2-(j-1)|eV_0|/N]$, where W is the width of the constriction and $\phi^C_{nj}(x)$ are the usual square-well eigenstates.

These wave functions (1)-(3) are matched at the different boundaries using the conditions of continuity on $\psi(x,y)$ and $\partial\psi(x,y)/\partial y$. We find a set of linear equations for the expansion coefficients in (1)-(3) which we solve numerically, using a mode-truncation procedure. We keep enough modes to assure convergence. Next, we calculate the total transmission coefficient $T(E,eV_0)$ for electrons incident on the constriction with energy E, by a straightforward generalization of the procedure described in Refs. 4 and 11. At zero temperature, the current and

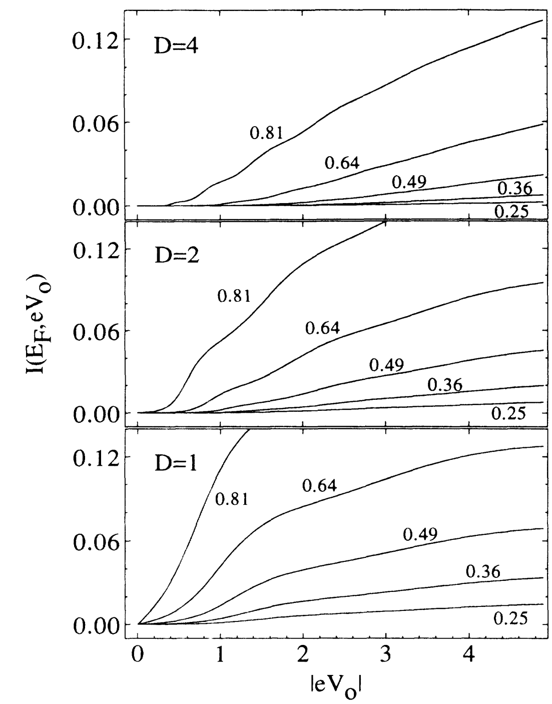

FIG. 3. $I(E_F,V_0)$ vs $|eV_0|$ for $0\le E_F\le 1$. For each curve, the value of E_F is written next to its corresponding curve. $D=4$, 2, and 1.

the differential conductance can then be readily calculated since

$$I(E_F,eV_0)=2e/h\int_{v(E_F-|eV_0|)}^{E_F}T(E,eV_0)dE \qquad (4)$$

and $g(E_F,eV_0)=\partial I(E_F,eV_0)/\partial V_0$, where $v(z)=z$ for $z>0$ and $v(z)=0$ for $z\le 0$. If $E_F\le |eV_0|$, all of the incoming energy levels in L contribute to the conduction and the lower limit of integration in Eq. (4) is zero.

Some of our results are summarized in Figs. 2-4. In what follows we use normalized units. The unit of length

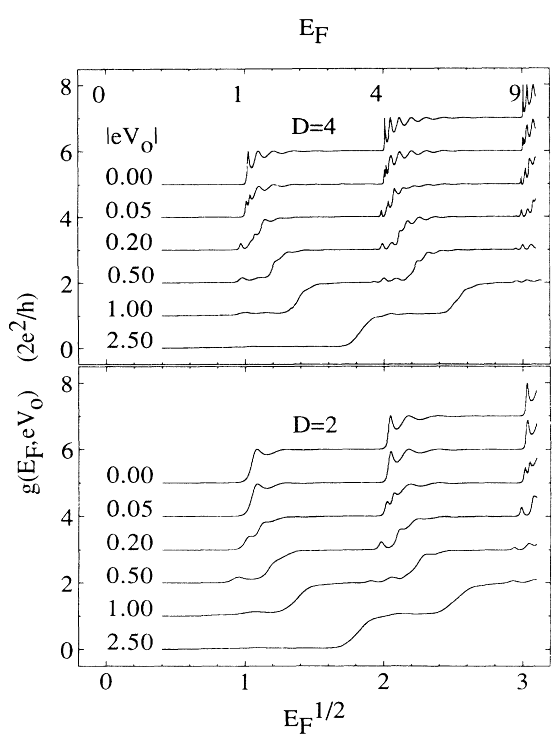

FIG. 2. $g(E_F,V_0)$ vs $(E_F)^{1/2}$ for various $|eV_0|$. $D=4$ and 2. The top (nonlinear) horizontal scale is for E_F.

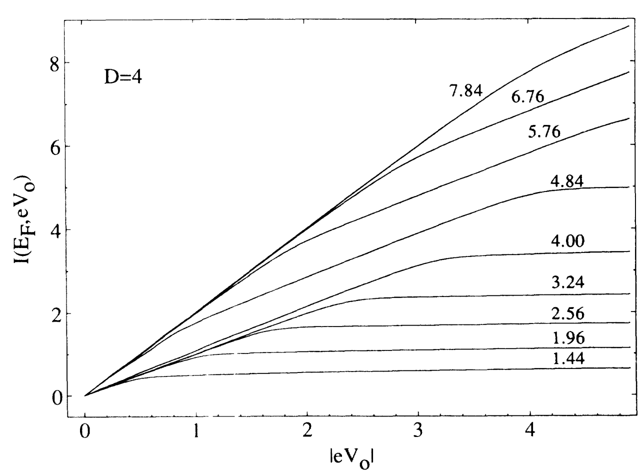

FIG. 4. $I(E_F,V_0)$ vs $|eV_0|$ for E_F's in the first $(1\le E_F\le 4)$ and second $(4\le E_F\le 9)$ zero-voltage subbands. For each curve, the value of E_F is written next to its corresponding curve. $D=4$.

is the width of the constriction and the unit of energy is the lowest transverse level inside the constriction when there is no applied voltage, $E_1 \equiv \hbar^2/2m(\pi/W)^2$. The unit of conductance is $2e^2/h$ and the unit of current is $i_0 \equiv 2e^2/h(E_1/e)$.

In Fig. 2 we have plotted $g(E_F,eV_0)$ vs $(E_F)^{1/2}$ for several values of $|eV_0|$, and constriction lengths $D=4$ and 2. At $V_0=0$ the differential conductance shows modulation due to transmission resonances.[4-11] At low $|eV_0|$ the resonant structure is still present, albeit in a weaker form, with plateaus quantized roughly at $2ne^2/h$, $n=1,2,\ldots$, preceded by a few undeveloped resonances. However, we find that g does not develop the HP's predicted by Glazman and Khaetskii.[13] These authors work in the adiabatic limit and consequently no resonances are predicted by their method. However, this is *not* the essential difference between their treatment and ours: In their approach, $T(E,eV_0)$ is approximated by its zero-voltage value, a simplification valid only in linear response. Also, the limits of integration for the energy window in their Eq. (1) (Ref. 13) are at variance with the physically correct values given in Eq. (4) of this work;[15] this appears to be the source of the HP's predicted in Ref. 13. Note that the feature at $(E_F)^{1/2} \approx 1$ in the $|eV_0|=0.2$, $D=2$ curve of Fig. 2 is not a rudimentary HP. It is a remnant of the resonance clearly visible for $|eV_0|=0$ and 0.05.

In (4) we have that the current is proportional to an energy-averaged total transmission probability, meaning that the quantization of energy levels becomes less important as the voltage is increased and that resonant features tend to be averaged out. The differential conductance can be written as

$$g(E_F,eV_0)=2e^2/h\left[T(E_F-|eV_0|,eV_0)+\int_{v(E_F-|eV_0|)}^{E_F}\partial T(E,eV_0)/\partial(eV_0)dE\right], \tag{5}$$

where the first term on the right-hand side is the total transmission probability $T(E,eV_0)$ evaluated at $E=E_F-|eV_0|$. Note that $T(E,eV_0)\equiv 0$ for $E\leq 0$. At low voltages this is the dominating term and the main effect of V_0 is to shift g towards higher energies, thus increasing the threshold of each quantized plateau by $|eV_0|$ while preserving the main features observed in LR. For a finite voltage the transverse levels at the C-R boundary have been pulled down with respect to the levels at the C-L boundary, making resonant transmission more difficult. For higher voltages the second term on the right-hand side of (5) becomes important, producing a smeared contribution from (several) consecutive zero-voltage plateaus, averaging out the conductance quantization and the resonant transmission. This also affects the rigid shift towards higher energies produced by the first term in (5).

In Figs. 3 and 4 we plot $I(E_F,eV_0)$ vs $|eV_0|$ for several different E_F's. For $0\leq E_F\leq E_1$ (Fig. 3) we observe that $I(E_F,eV_0)$ increases rapidly with $|eV_0|$, and more quickly as E_F approaches the lower edge of the first plateau E_1 or the length of the constriction is reduced. At zero voltage, the electrons with energies lower than E_1 must tunnel all the way through C and the current is very low. For nonzero voltages the electrons tunnel only over lengths shorter than the length of C, from $y=0$ up to the point $y_c<D$ where the effective potential equals the energy of the electron. Multiple reflections between y_c and the end of the channel (in our model there is an impedance mismatch between C and R) produce resonances even for E_F below E_1 as shown in Figs. 2 and 3. This effect is stronger for longer C's.

For $E_F\geq E_1$ (Fig. 4) we see that the current increases with increasing voltage until it saturates when $|eV_0|\geq E_F$. For these voltages the energy window in (4) has reached its widest and every incoming level in L is a contributing current in C, so that the maximum possible current is drawn through the system. The current increases almost linearly in certain energy ranges, changing to smaller slopes whenever a transverse level saturates at $|eV_0|\approx E_F-\hbar^2/2m(n\pi/W)^2$. The change of slope around these values is gradual, reflecting the energy averaging in (4). Note also that the initial slope changes markedly as E_F moves from one zero-voltage plateau to the next one.

In conclusion, we have studied nonlinear transport through uniform narrow ballistic constrictions. We find that the conductance plateaus are displaced and the quantization is degraded by the application of a suitably large voltage, and that there are large nonlinearities in the current. The current saturates at high voltages. The earlier prediction of HP's is found to be incorrect. Finally, experimental HF studies of constrictions such as those of Hirayama *et al.*[10] would be of interest since these systems are simpler than the double-wedge geometry of Kouwenhoven *et al.*[12] and more closely approximate the situation considered in this paper.

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[1]See, e.g., M. L. Roukes *et al.*, in *Science and Engineering of 1- and 0-Dimensional Conductors,* edited by S. P. Beaumont and C. M. Sotomayor-Torres (Plenum, New York, 1989), for a survey of microfabrication techniques of nanostructures.

[2]B. J. van Wees *et al.*, Phys. Rev. Lett. **60**, 848 (1988).

[3]D. A. Wharam *et al.*, J. Phys. C **21**, L209 (1988).

[4]G. Kirczenow, Solid State Commun. **68**, 715 (1988); J. Phys. Condens. Matter **1**, 305 (1989); Phys. Rev. B **39**, 10452 (1989).

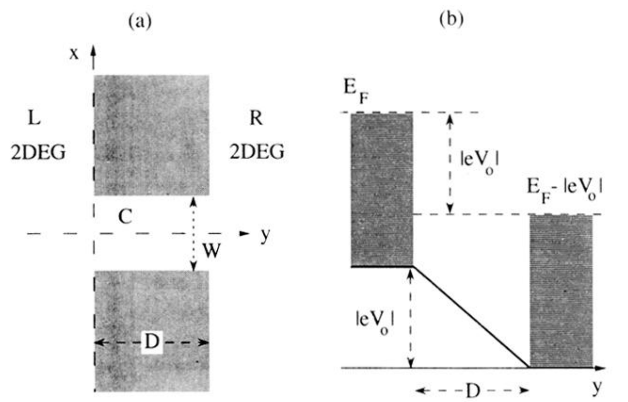
[5]A. Szafer and A. D. Stone, Phys. Rev. Lett. **62**, 300 (1989).

[6]E. Haanappel and D. van der Marel, Phys. Rev. B **39**, 5484 (1989); D. van der Marel and E. Haanappel, *ibid.* **39**, 7811 (1989).

[7]L. Escapa and N. García, J. Phys. Condens. Matter **1**, 2125 (1989).

[8]E. Tekman and S. Ciraci, Phys. Rev. B **39**, 8772 (1989).

[9]Y. Avishai and Y. B. Band, Phys. Rev. B **40**, 3429 (1989).
[10]Y. Hirayama *et al.*, Jpn. J. Appl. Phys. **28**, L701 (1989).
[11]E. Castaño and G. Kirczenow, Solid State Commun. **70**, 801 (1989).
[12]L. P. Kouwenhoven *et al.*, Phys. Rev. B **39**, 8040 (1989).
[13]L. I. Glazman and A. V. Khaetskii, Europhys. Lett. **9**, 263 (1989).
[14]C. S. Lent, S. Sivaprakasam, and D. J. Kirkner (unpublished).
[15]In the notation of our Fig. 1, Ref. 13 takes the energy window for electrons incident on C from L to be from $E_F - |eV_0/2|$ to $E_F + |eV_0/2|$.



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