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Case for nonadiabatic quantized conductance in smooth ballistic constrictions

Eleuterio Castaño
*Departamento de Física, Universidad Autónoma Metropolitana, Unidad Iztapalapa, Apdo. Postal 55-534, 09340 México, Distrito Federal, México**
and Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6

George Kirczenow
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6
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We present quantum-mechanical calculations of the conductance (G) of smooth, but not adiabatic, ballistic constrictions (BC's). Although the BC width varies smoothly with position, the effective potential for each transverse mode exhibits a *pair* of peaks that cause multiple reflections. If mode mixing is neglected, G is dominated by transmission resonances. However, the exact (nonadiabatic) G is a smooth function of E_F with quantized plateaus. This is an explicit example of the *breakdown* of adiabaticity being the *source* of conductance quantization in a smooth BC.

During the past few years there has been much interest in the study of electronic transport in mesoscopic systems in general, and most recently of quantum coherent effects in ballistic nanostructures (BN's) in two-dimensional electron gases (2DEG's). In the BN's the effective dimensionality of the electrons is reduced to one or zero, and the quantization of energy levels is very important. For example, at low temperatures, it has been observed that the conductance G of a narrow ballistic constriction (NBC) joining two 2DEG's is quantized in units of $2e^2/h$.[1,2] This result can be understood by considering the relevant length scales: the width W and length L of the constriction, the electronic Fermi wavelength λ_F, and the mean free path l. Typically, W and $L \sim 100$ nm, $\lambda_F \sim 40$ nm, and $l \sim 1$ μm. Since $W \sim \lambda_F$, the lateral confinement in the constrictions produces strongly quantized transverse subbands. Also, W and $L \sim \lambda_F < l$ so that the electrons move ballistically through the system. Thus, as the Fermi energy E_F is increased and another transverse subband becomes populated, G increases by a unit of quantum conductance, $2e^2/h$, so that

$$G \approx \frac{2e^2}{h} N(E_F) , \qquad (1)$$

where $N(E_F)$ is the number of occupied subbands for a given E_F. For E_F's between two consecutive subband minima, say between the nth and the $(n+1)$th, G has a nearly constant value equal to $2e^2 n/h$, i.e., there is a conductance plateau (CP).

Measurements of G relate the current through the constriction to the electrochemical potentials deep within the reservoirs so that G is given by[3-8]

$$G = \frac{2e^2}{h} T(E_F) , \qquad (2)$$

where $T(E_F)$ is the total transmission coefficient, equal to the sum of the transmission coefficients over the occupied levels at the Fermi energy. Assuming that the modes in the constriction do not mix, and that the transmission coefficients are 1 (0) if E_F is above (below) the bottom of a given subband at the center of the constriction, one obtains Eq. (1). These assumptions are quite restrictive since they are equivalent to neglecting effects of nonideal electron injection, mode mixing, and partial reflection of the wave field in the vicinity of the constriction. Glazman *et al.*[9] have demonstrated their validity in the adiabatic limit, where the width of the constriction is assumed to vary very slowly, and obtained exponentially sharp CP's. The adiabatic and nearly adiabatic regimes have also been discussed by Yacoby and Imry.[10]

On the other hand, one can consider NBC's with abrupt geometries. In this case the CP's are modulated by resonant transmission due to longitudinal resonances ("organ-pipe" modes) along the constriction.[11-20] Some experimental evidence suggestive of these resonances has been obtained by Hirayama, Saku, and Horikoshi.[21] In the abrupt models there is a strong impedance mismatch between the NBC's and the 2DEG's at their ends, and the effects of current injection, mode mixing, and reflection are included in the calculations. Tapering the constrictions, or ramping the potential in them,[12,13,15,16,20] reduces the impedance mismatch and weakens the resonant modulation.

From the outset, it has been recognized that realistic NBC's are not fully adiabatic or completely sharp. The constriction is just a *finite* part of a large 2DEG; its width changes noticeably over a very small region of the system. With this in mind, Glazman and Jonson[22] have stressed the lack of *global* adiabaticity in ballistic devices in the absence of magnetic fields, and pointed out the importance of distinguishing between local and global adiabatic regimes. More recently, Laughton *et al.*[23] and Nixon, Davies, and Baranger[24] have shown that accurate conductance quantization may still be possible even when adiabaticity is significantly violated by scattering due to potential irregularities. Ulloa, Castaño, and Kirczenow,[25] Castaño, Kirczenow, and Ulloa,[26] and Lent and Leng[27] have considered nonadiabatic effects in periodically modulated one-dimensional ballistic conductors.

However, the elegance and simplicity of the adiabatic theory and its good agreement with experiments are very appealing, and the adiabatics is widely accepted as the fundamental explanation of quantized ballistic conductances. In this paper, which builds on the work of Yacoby and Imry,[10] we present results that strongly suggest that quantized conductances observed in real systems may *not* be adiabatic in origin. We consider model constrictions with a smooth geometry, but without taking the adiabatic limit. The Schrödinger equation is solved exactly, albeit numerically to find the wave function, reflection and transmission coefficients, and the two-point conductance of the system. The effects of mode mixing, reflection, and current injection are fully taken into account. Our main results are (a) G is a smooth function of E_F with quantized plateaus if the mixing between the different propagating modes is fully taken into account. (b) However, if mode mixing is neglected, the conductance G_u is strongly modulated by resonant transmission, a behavior that is anomalous since the constriction is smooth. This modulation appears because the effective potential for each transverse mode is *not* simply a smooth, featureless barrier as in the adiabatic limit, but exhibits a *pair* of peaks which induce strong multiple reflections unless significant nonadiabatic mode mixing intervenes. This shows that in such constrictions it is precisely the *nonadiabaticity* that is responsible for conductance quantization.

A schematic representation of the model (drawn to scale) is given in Fig. 1. The electrons are confined to the unshaded area by a lateral hard-wall potential. The constriction width $W(x)$ varies smoothly from W_e for $|x| > L/2$ to $W_0 = W(x=0)$ at the center of the constriction. We use an effective-mass Hamiltonian given by

$$H = -\hbar^2(\partial^2/\partial x^2 + \partial^2/\partial y^2)/2m^* + U(x,y) , \qquad (3)$$

where $U(x,y)$ is the confining potential. If $|y| \le W(x)/2$, $U(x,y)=0$; $U(x,y)=\infty$ otherwise.

Ignoring, just for the moment, the motion in the x direction, the normalized transverse wave functions in the y direction are given by

$$\phi_{nx}(y) = \left[\frac{2}{W(x)}\right]^{1/2} \sin\left[\frac{n\pi}{W(x)}[y - W(x)/2]\right] \qquad (4)$$

for $|y| \le W(x)/2$ $n = 1,2,\ldots$. Here x is treated as a parameter. In terms of this (locally) complete basis of transverse eigenfunctions the wave function can be expanded as follows,

$$\Psi(x,y) = \sum_{n=1}^{\infty} A_n(x)\phi_{nx}(y) . \qquad (5)$$

To find the expansion coefficients, $A_n(x)$, substitute (5) in the Schrödinger equation, multiply by $\phi_{mx}(y)$ and integrate over y. Since the ϕ's are orthonormal we obtain a set of coupled differential equations as in Ref. 10:

$$\sum_{n=1}^{\infty}\left[\delta_{mn}\frac{\partial^2}{\partial x^2} + 2\alpha_{mn}(x)\frac{\partial}{\partial x} + \beta_{mn}(x) + \delta_{mn}\left[\frac{2m^*E_F}{\hbar^2} - \frac{n^2\pi^2}{W(x)^2}\right]\right]A_n(x) = 0 , \qquad (6)$$

where

$$\alpha_{mn}(x) \equiv \int_{-W(x)/2}^{W(x)/2} \phi_{mx}(y)\frac{\partial}{\partial x}\phi_{nx}(h)dy , \qquad (7a)$$

$$\beta_{mn}(x) \equiv \int_{-W(x)/2}^{W(x)/2} \phi_{mx}(y)\frac{\partial^2}{\partial x^2}\phi_{nx}(y)dy . \qquad (7b)$$

From now on the unit of energy will be $E_0 = \hbar^2 n^2/2m^* W_0^2$ and the unit of length $W_0 = W(x=0)$. The specific functional form of $W(x)$ is quite arbitrary; we only require the continuity of $W'(x) = dW(x)/dx$ and $W''(x) = d^2W(x)/dx^2$. In this work, we have chosen $W(x)$ as follows:

$$W(x) = \frac{W_e W_0}{(W_e - W_0)\cos(x\pi/L)^4 + W_0} , \quad \text{if } |x| \le L/2$$

and

$$W(x) = W_e, \quad \text{if } |x| \ge L/2 .$$

This form is represented in Fig. 1 for $W_e = 6W_0$, and $L = 2W_0$. To simplify the discussion, we now rewrite (6) in a more transparent form. We define an effective potential

$$V_n(x) = \frac{n^2}{W(x)^2} + \left[\frac{W'(x)}{\pi W(x)}\right]^2 (1 + n^2\pi^2/3) , \qquad (8)$$

and since $\alpha_{nn}(x) = 0$ we obtain

$$\left[\frac{\partial^2}{\partial x^2} - \pi^2 V_m(x) + \pi^2\epsilon\right]A_m(x) = -\sum_{n\ne m}^{\infty} [2\alpha_{mn}(x)\partial/\partial x + B_{mn}(x)]A_n(x) , \qquad (9)$$

where $\epsilon = E_F/E_0$. In (9), the right-hand side represents mode mixing. If this term is neglected, the left-hand side becomes a set of decoupled one-dimensional Schrödinger equations; in this case, the only remaining effect of the constriction would be through the effective potential

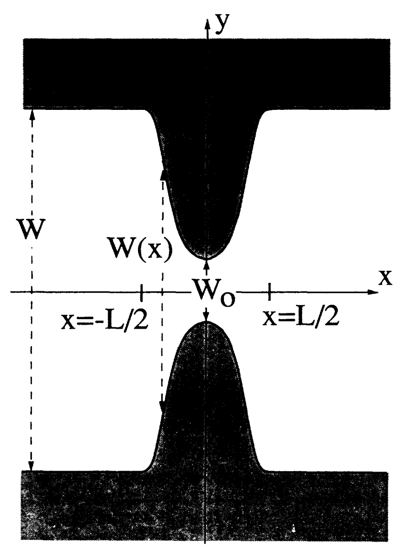

FIG. 1. Schematic representation of the model constriction used, drawn to scale. The shaded areas are inaccessible to the electrons. The width at the center of the constriction is W_0. For $|x| > L/2$ the width is W_e. The constriction width varies smoothly. $W_e = 6W_0$ and $L = 2W_0$.

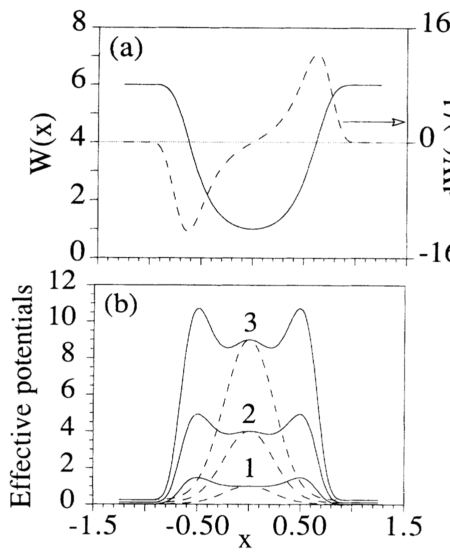

FIG. 2. (a) $W(x)$ of the NBC and $dW(x)/dx$ as functions of x. (b) Effective potentials $V_n(x)$ (solid lines), and the transverse mode energies $\epsilon_n(x)=n^2/W(x)^2$ (dashed lines) vs x for $W_e=6W_0$ and $L=2W_0$. Each pair of curves is labeled by the corresponding mode index.

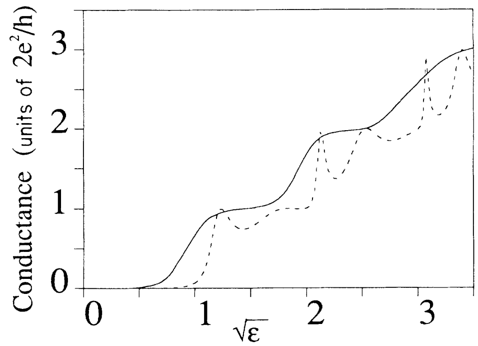

FIG. 3. The exact conductance G (solid line) is a smooth function of $\sqrt{\epsilon}=(E_F/E_0)^{1/2}$, for $W_e=6W_0$ and $L=2W_0$. In the adiabatic approximation the conductance G_u (dashed line) has strong resonances due to reflections between the peaks in the effective potentials shown in Fig. 2(b).

$V_m(x)$ for each mode. This is an adiabatic approximation in the sense that the modes propagate through the constriction without mixing.

We solve the system of Eqs. (9) numerically in order to calculate the *exact* conductance G. The numerical technique required the use of backward differentiation formula methods since (9) is a system of stiff differential equations, a detailed account will be published elsewhere. We also solve the decoupled system obtained by neglecting the right-hand side of (9) to obtain the adiabatic approximation G_u to the conductance.

In Fig. 2(a) we plot $W(x)$ and $W'(x)$ vs x for $L=2W_0$ and $W_e=6W_0$. In Fig. 2(b) we plot the effective potential $V_n(x)$ (solid line) and $\epsilon_n(x)=n^2/W(x)^2$ (dashed line) versus x for several different mode indices, n, as indicated by the numbers next to each pair of curves. Notice that where $|W'(x)|$ is maximal $V_n(x)$ has peaks that are higher than $V_n(x=0)$. These peaks become more pronounced for higher mode numbers. Thus we see that the effective potentials for the transverse modes are qualitatively different from a simple potential barrier, and have "mirrors" at the ends of the constriction. If W_e is increased the peaks become progressively more dominant. On the other hand, $\varepsilon_n(x)$ is a smooth featureless barrier, similar to the effective potential found in the adiabatic limit. By itself it would give rise to a transmission coefficient for any decoupled mode, which would rise smoothly from zero to 1 as E_F is increased.

In Fig. 3 the solid line is G, the exact conductance of the system, and the dashed line is G_u, the conductance when mode mixing is neglected. Notice that G and G_u are very different. G_u is strongly modulated by transmission resonances caused by multiple reflections between the peaks in the effective potential; this resonant modulation is stronger for the higher modes since for them the peaks are larger. However, G in which *no* approximations are made and mode mixing is fully taken into account is a *smooth* function of E_F and has conductance plateaus at the quantized values. These contrasting results for G and G_u illustrate that *a priori* neglect of nonadiabatic mode mixing is not warranted even though we have a constriction of smooth appearance and the conductance exhibits quantized plateaus.

It is important to emphasize that our results apply to other constriction shapes as well; the important ingredient is the qualitative behavior of $W(x)$ that includes a smooth change of width over a *finite* region. For larger external widths than the ones presented in this work, we expect that this breakdown of adiabaticity would be even more pronounced since the nonmonotonic features of the effective potentials will become more dominant. If the constriction is asymmetric, the peaks at its two ends would be different and the effects of resonant transmission for the decoupled modes would be less pronounced. This would tend to lessen the differences between G and G_u.[28]

In conclusion, we have presented evidence that nonadiabatic mode mixing may play an unexpectedly important role in the development of quantized conductance plateaus in smooth but finite ballistic constrictions, showing that it is not necessary to use adiabatic approximations to explain quantum electronic transport in realistic ballistic nanostructures. We hope that these results will stimulate further research and discussion leading to a more comprehensive understanding of ballistic quantum transport phenomena.

Note added. After submission of this paper we received a copy of work prior to publication by Bryant[29] in which the importance of nonadiabatic mode mixing in current-injection phenomena in vertical quantum-dot systems is demonstrated.

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*Permanent address.

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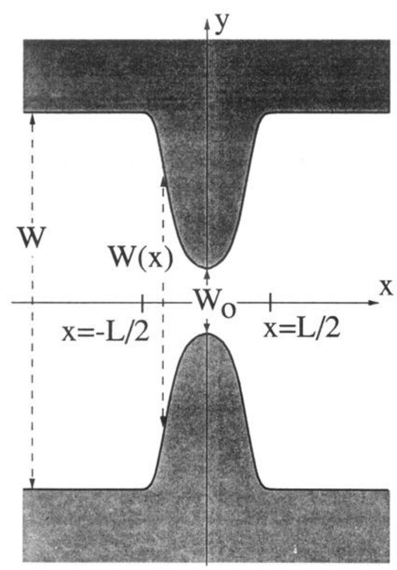

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