Theory of conduction through narrow constrictions in a three-dimensional electron gas

J. A. Torres, J. I. Pascual, and J.J. Sáenz
Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
(Received 27 December 1993)

An exact calculation of the quantum conduction through a curvilinear constriction in a three-dimensional electron gas is presented. We show that the conductance behavior presents significant differences with respect to the two-dimensional case. Importantly, we find that the conductance of a circular point contact deviates from the classical Sharvin result and the conductance per unit area is not constant except in the limit of macroscopic areas. We show that quantum finite-size effects can be taken into account by a simple semiclassical correction to the Sharvin formula. Recent experiments and calculations on quantum constrictions formed in atomic-scale point contacts are discussed.

The discovery[1] of the quantization of conductance of a narrow constriction in a two-dimensional electron gas (2DEG) has been a breakthrough in the field of ballistic transport in mesoscopic systems. This phenomenon is the consequence of the quantization of the transversal momentum of the electrons confined in a constriction with a width of the order of the Fermi wavelength. The effect of different confining potentials has been the object of detailed calculations[2–5] based on Landauer's[6] scattering approach to electric transport. For a long constriction, the conductance is directly proportional to the integer number of propagating modes or conductance channels and increases with the constriction width in steps of $2e^2/h$ each time a new channel opens up. Even in the case of extremely short constrictions, where the transverse quantization is not well defined, the conductance shows an oscillatory quantum behavior[3] superimposed on the classical two-dimensional Sharvin conductance.[7] This quantum behavior should not be restricted to a 2DEG and was also expected to describe the conduction in a small metallic point contact. Here, our main objective is to study the effects of the size and geometry on the quantum conductance of a small connecting constriction between two three-dimensional electron gas (3DEG) reservoirs. Although the general behavior of the conductance resembles that of a 2DEG point contact, we have found significant features in the 3DEG. In particular, we will see that the classical Sharvin formula for the conductance of a circular contact is not a good approximation for finite contact areas in contrast with the 2DEG case. We will also discuss the possibility of observing conductance quantization effects in actual experiments on atomic-scale point contacts.[8–11]

Our discussion can be considered as a generalization to a three-dimensional system of the theory of conduction in curvilinear constrictions in a 2DEG of Yosefin and Kaveh (YK).[5] Following YK, we start with the observation that the free Schrödinger equation can be separated in several coordinate systems.[12] If the boundary of the constriction coincides with surfaces ϑ =const, in one of these systems quasi-one-dimensional conduction channels can be defined. As in the 2DEG case, the conductance G is given by the Landauer formula

$$G = \frac{2e^2}{h} \sum_m \sum_l T_{ml}, \tag{1}$$

where T_{ml} is the transmission probability of the subband ml and the sum runs over the total number of occupied subbands. In the case of a quantum constriction in a 3DEG each subband is defined by two quantum numbers l and m, since the electrons are confined in two spatial directions. We will discuss three-dimensional constrictions with hyperbolic geometry (Fig. 1) since this approximates the shape of the quantum constrictions formed in actual scanning tunneling microscopy (STM) experiments.[9–11] Moreover, by choosing the parameters appropiately, this geometry allows us to analyze the problem of quantum point contacts for the short-contact-constriction case of a circular hole (i.e., a Sharvin point contact).

Spheroidal oblate coordinates $(\mu, \vartheta, \varphi)$ can be defined by[12]

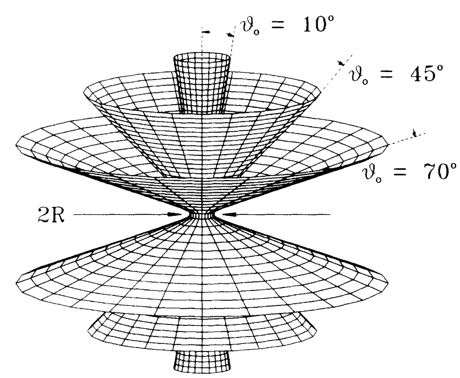

FIG. 1. Geometry of connective constrictions with variable cross section. Two parameters define the hyperbolic constriction geometry: the radius R of its narrowest section and its asymptotic opening angle ϑ_0, which can go from 0 (a cylindrical wire) to 90° (a circular hole).

$$x = a \cosh\mu \sin\vartheta \cos\varphi,$$
$$y = a \cosh\mu \sin\vartheta \sin\varphi, \quad (2)$$
$$z = a \sinh\mu \cos\vartheta,$$
$$(-\infty < \mu < \infty), \quad (0 \le \vartheta \le \pi/2),\ (0 \le \varphi \le 2\pi),$$

where $2a$ is the distance between the foci. The constriction is defined by the surface $\vartheta = \vartheta_0 =$ constant and the radius of the narrowest section of the constriction is given by $R = a \sin\vartheta_0$ (see Fig. 1). Assuming electron wave functions of the form

$$\Psi(\mu,\vartheta,\varphi) = \{\cosh\mu \sin\vartheta\}^{-1/2} \mathcal{J}(\mu)\mathcal{S}(\vartheta)\Phi(\varphi), \quad (3)$$

the Schrödinger equation inside the constriction separates into

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0, \quad (4a)$$

$$\frac{d^2\mathcal{S}}{d\vartheta^2} + \left\{\epsilon_{ml} - f^2 \sin^2\vartheta - \frac{m^2 - 1/4}{\sin^2\vartheta}\right\}\mathcal{S} = 0, \quad (4b)$$

$$\frac{d^2\mathcal{J}}{d\mu^2} + \left\{-\epsilon_{ml} + f^2 \cosh^2\mu + \frac{m^2 - 1/4}{\cosh^2\mu}\right\}\mathcal{J} = 0, \quad (4c)$$

where m and ϵ_{ml} are the two separation constants and, for the electrons at the Fermi level, $f = 2\pi a/\lambda_F$. From the azimuthal boundary conditions we have $m =$ integer. Now, for a fixed azimuthal number m, using Eq. (4b) and the Sturm-Liouville[12] boundary conditions $\mathcal{S}(\vartheta_0) = 0$ and $\mathcal{S}(0) =$ finite, one can determine the set of transverse functions $\mathcal{S}_{ml}(\vartheta)$ together with the corresponding values of the separation constant $\{\epsilon_{ml}\}_{l=0,1,2,\ldots}$. This problem can be easily solved for $\vartheta_0 \to 0$, i.e., for an almost perfectly cylindrical wire of constant section. In this simple case, we have cylindrical symmetry and $\{\vartheta_0\sqrt{\epsilon_{ml}}\}$ becomes the set of zeros of Bessel functions. However, in general, this problem has to be solved by numerical methods.

Since the Schrödinger equation is separable there is no channel or mode mixing and the calculation of the transmission probability T_{ml} of a wave incident from the $\{ml\}$th left-hand-side channel ($\mu < 0$) is reduced to that of a one-dimensional problem. Moreover, T_{ml} can be calculated *exactly* from Kemble's method[13,5] and is given by

$$T_{ml} = \left\{1 + \exp\left(\frac{\pi}{f}[\epsilon_{ml} - (m^2 - 1/4) - f^2]\right)\right\}^{-1}, \quad (5)$$

which, except for the $(m^2 - 1/4)$ factor, is the same as that obtained by YK.

In Fig. 2 we plot the calculated conductance G of a quantum constriction versus the area of the narrowest section and as a function of the opening angle of the constriction ϑ_0. When the opening angle ϑ_0 is small the constriction has an elongated shape and G presents quantum jumps at integer multiples of $2e^2/h$. As in two-dimensional long constrictions, these jumps appear every time a new quantum channel in the constriction goes below the Fermi energy. In the three-dimensional case,

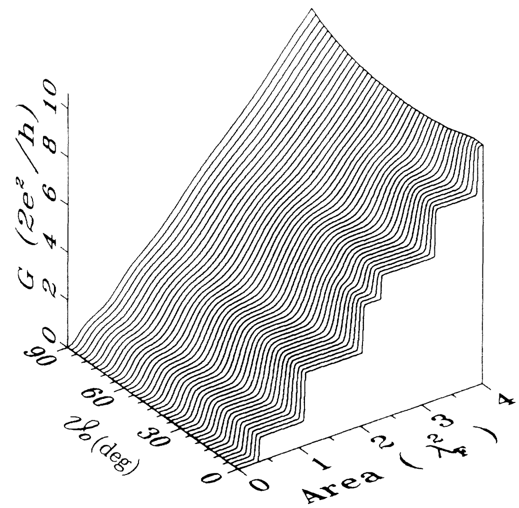

FIG. 2. Conductance G of a quantum constriction as a function of the area of the narrowest section and the opening angle of the constriction ϑ_0.

because of the azimuthal degeneration of the transverse modes (electrons with quantum numbers m and $-m$ have the same transverse momenta) steps of one ($m = 0$) or two quantum conductance units can be observed. As the opening angle increases, the stepped structure smooths out and when ϑ_0 goes to 90° it evolves into smooth quantum oscillations that reflect an underlying periodicity in the original stepped structure. It is interesting to note that, as in the 2DEG case, these oscillations occur approximately each time the diameter of the contact (i.e., $2R$) increases by $\lambda_F/2$.

An important result is that the conductance deviates from the classical prediction given by the Sharvin formula[7] at small contact areas. Using a semiclassical treatment Sharvin showed that the conductance of a circular contact of radius R, in the ballistic regime, i.e. when R is smaller than the electron mean free path, is given by

$$G_S = \frac{2e^2}{h}\pi A, \quad (6)$$

where A is the contact area in units of the square Fermi wavelength λ_F, $A = \pi(R/\lambda_F)^2$. In Fig. 3 we have plotted the Sharvin conductance G_S, together with the exact results for three different angles. As can be seen, even for the case of a circular hole, the exact result does not follow Eq. (6).

This result is quite different from that obtained for a 2DEG in which the small quantum oscillations in the conductance are superimposed on the classical Sharvin conductance.[3] The deviation in the 3DEG case arises as a consequence of quantum finite-size effects. In the classical limit $\lambda_F/R \to 0$ (i.e., $A \to \infty$) the asymptotic value of the conductance G_∞ is proportional to the number of propagating modes. From Eqs. (1) and (5), G_∞ can be written as $(2e^2/h)N$, N being the average number of modes ml such that $\epsilon_{ml} \le (m^2 - 1/4) + f^2$. An analysis

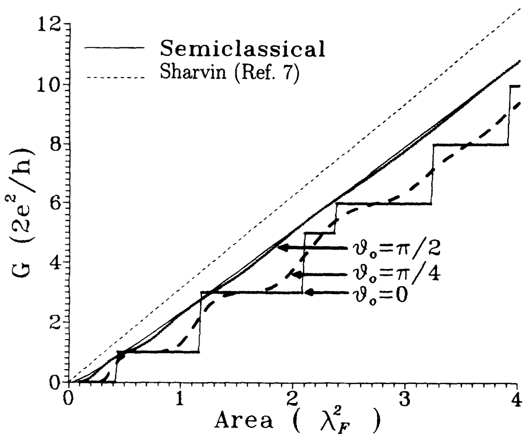

FIG. 3. Exact quantum mechanical calculation for three different opening angles ϑ_0 (taken from Fig. 2) together with the classical result of Sharvin, $G_S = (2e^2/h)\pi A/\lambda_F^2$ (dashed line). A clear deviation of the Sharvin conductance from the exact result is evident. The semiclassical approximation given by Eq. (8) (continuous line) reproduces quantitatively the exact quantum results for a circular hole.

of the eigenvalues ϵ_{ml} in Eq. (4b) within the semiclassical approximation[12,13] shows that $N \approx \pi A$ and $G_\infty \approx G_S$ (notice that in the semiclassical limit N does not depend on the details of the constriction geometry). In other words, the Sharvin result is the leading term in the asymptotic expansion of the conductance in the limit $A \to \infty$.

We can go further than this, however, for we note that, for a *constant* cross section wire, N is given by the average number of modes with transverse momentum less than $k_F = 2\pi/\lambda_F$. In this case, it is well known (see, for example, Eq. 6.3.54 in Ref. 12) that N is given by $\approx (\pi A - L/2)$ where L is the perimeter of the cross section in units of λ_F. This result holds for rectangular, triangular, and circular cross sections and presumably holds for cross sections of any shape.[12] Detailed counting shows that, for a curvilinear constriction, the perimeter correction changes as a function of the opening angle. In particular, for a circular hole, we find

$$G_\infty \approx 2e^2/h(\pi A - L/4), \tag{7}$$

i.e., the perimeter correction is half of that corresponding to the cylindrical constriction. The same result is obtained from a simple qualitative argument. As a consequence of the quantum uncertainty of the electron wave in the contact, since the transverse momentum cannot exceed k_F, we have $2Rk_F \gtrsim 1$. Then, we would expect that the transmission through the contact would be suppressed for $R/\lambda_F \approx 1/(4\pi)$ (except a small contribution coming from the evanescent modes). Then, if we assume that the conductance is approximately given by Eq. (6) but with an effective contact radius $R_E = R - \lambda_F/(4\pi)$, we have

$$G_\infty \approx \frac{2e^2}{h}\pi A \left\{ \left(1 - \frac{\lambda_F}{4\pi R}\right)^2 \right\}, \tag{8}$$

which except for a negligible constant term is the same as that given in Eq. (7). In Fig. 3 we have also plotted Eq. (8) together with the Sharvin and the exact results. As can be seen, except for the weak quantum oscillations, our semiclassical approximation reproduces nicely the exact results. It is worth noticing that finite-size effects are also present in the two-dimensional case.[3,4] However, in a 2DEG, where the conductance is linear with the constriction radius, this quantum finite-size effect manifests itself as a slight displacement of the entire curve from the origin[4] and does not modify the general behavior of the conductance.

We would like to discuss now some results relevant in the understanding of recent experiments on atomic-scale metallic point contacts. By changing the area of the contact, reproducible jumps in the conductance have been observed in atomic-scale metallic junctions[8] and STM point contacts[9] at low temperatures. Very recently, a steplike behavior of the conductance has also been found in the formation of gold nanostructures by a STM operating in air at "room temperature."[10] Molecular dynamics simulations[14] showed that when the STM tip is receded, after contact, the tip motion leads to the formation of a connective constriction which elongates in steps, this elongation being produced by atomic rearrangements as the tip retracts. These mechanical instabilities produce discrete variations of the contact cross section resulting in discrete jumps in the ballistic conductance.[4,8,15] Our results show that in spite of this fact conductance quantization effects can be observed experimentally.

For a metallic contact, where λ_F is of the order of the atomic radius r_0 ($\lambda_F \approx \pi r_0$), the Sharvin formula would be equivalent to a quantum conductance channel per atom in the constriction. Since the actual contact area in the experiments changes in atomic increments, this would imply jumps in the conductance in the form of integer multiples of $2e^2/h$ even in the cases where the conductance is not quantized. However, the conductance per unit area is far from being constant and, therefore, the conductance *per atom* is not constant.[15] To stress this fact, in Fig. 4 we show the conductance per unit area as a function of the contact area for the two limiting cases of a cylindrical constriction ($\vartheta_0 = 0$) and a circular hole ($\vartheta_0 = \pi/2$). The results for the Sharvin formula and our semiclassical approximation are also shown. For large opening angles, an atomic increment in the constriction cross section would result in a jump in the conductance which, in general, will not be an integer multiple of the quantum of conductance. On the other hand, for small angles, where the conductance is quantized, the jumps must be in the form of integer multiples of $2e^2/h$ independently of the number of atoms forming the narrow constriction structure. Notice that in this case the number of quantum channels is directly related not to the number of atoms but to the number of propagating modes: An atomic change of the constriction cross section does not necessarily imply a change in the conductance. In a typical STM experiment the contact geometry changes with the tip motion. After tip indentation, the contact is not long enough to allow conductance quantization. During the formation of the connective constriction as

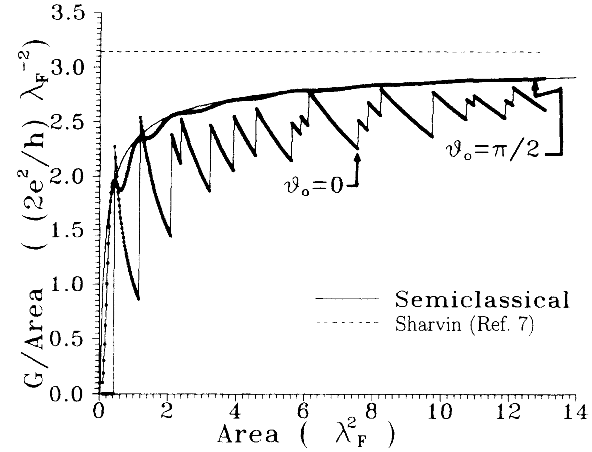

FIG. 4. Conductance per unit area as a function of the contact area for the two limiting cases of a cylindrical wire ($\vartheta_0 = 0$) and a circular hole ($\vartheta_0 = \pi/2$). The results for the Sharvin formula (dashed line) and for our semiclassical approximation (continuous line) are also shown.

the tip retracts, the experiments[9,10] show different structures and jump magnitudes depending on the particular experiment. As the constriction becomes longer and narrower the conductance should show quantization effects. As a matter of fact, Pascual *et al.*[10] have found reproducible jumps at integer multiples of $2e^2/h$ just before the breaking of the contact. From our discussion above, this represents the experimental observation of quantized conductance in metallic point contacts.

In summary, we have discussed some general properties of the ballistic transport through quantum constrictions in a three-dimensional electron gas. We have shown that the classical Sharvin formula deviates from the exact conductance at finite contact areas. The nonlinear behavior of the conductance arises as a consequence of the quantum uncertainty of the electron wave in the constriction. We have presented a simple semiclassical formula that accounts for this quantum finite-size effect. On the other hand, we have shown that an abrupt change in the contact area does not necessarily imply a change in the conductance. Moreover, we claim that the experimental observation of reproducible jumps of the conductance at *integer* multiples of $2e^2/h$ reflects the actual quantization of the conductance.

We gratefully acknowledge stimulating discussions with N. Agrait, A. Baró, N. García, J. Gómez-Herrero, J.M. Gómez, J. Méndez, J.G. Rodrigo, and J.M. Soler. We also gratefully acknowledge support from the Universidad Autónoma de Madrid (G. Precom.) and the DGICYT under Contract No. PB92-0081.

[1] B.J. van Wees, H. van Houten, C.W.J. Beenakker, J.G. Williamson, L.P. Kouwenhoven, D. van der Marel, and C.T. Foxon, Phys. Rev. Lett. **60**, 848 (1988); D.A. Wharam, T.J. Thorton, R. Newbury, M. Pepper, H. Ahmed, J.E.F. Frost, D.G. Hasko, D.C. Peacock, D.A. Ritchie, and G.A.C. Jones, J. Phys. C **21**, L209 (1988).

[2] G. Kirczenow, Solid State Commun. **68**, 715 (1988); L.I. Glazman, G.B. Lesovik, D.E. Khmelnitskii, and R.I. Shekhter, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 218 (1988) [JETP Lett. **48**, 239 (1988)]; A. Szafer and A.D. Stone, Phys. Rev. Lett. **62**, 300 (1989); N. García and L. Escapa, Appl. Phys. Lett. **54**, 1418 (1989).

[3] E.G. Haanappel and D. van der Marel, Phys. Rev. B **39**, 5484 (1989); L. Escapa and N. García, J. Phys. Condens. Matter **1**, 2125 (1989); A. Matulis and D. Šegžda, *ibid.* **1**, 2289 (1989).

[4] E. Tekman and S. Ciraci, Phys. Rev. B **43**, 7145 (1991).

[5] M. Yosefin and M. Kaveh, Phys. Rev. Lett. **64**, 2819 (1990).

[6] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).

[7] Y.V. Sharvin, Zh. Eksp. Teor. Fiz. **48**, 984 (1965) [Sov. Phys. JETP **21**, 655 (1965)].

[8] C.J. Muller, J.M. van Ruitenbeek, and L.J. de Jongh, Phys. Rev. Lett. **69**, 140 (1992).

[9] N. Agrait, J.G. Rodrigo, and S. Vieira, Phys. Rev. B **47**, 12 345 (1993).

[10] J.I. Pascual, J. Méndez, J. Gómez-Herrero, A.M. Baró, N. García, and Vu Thien Binh, Phys. Rev. Lett. **71**, 1852 (1993).

[11] L. Kuipers and J.W.M. Frenken, Phys. Rev. Lett. **70**, 3907 (1993).

[12] P.M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).

[13] L. Landau and E. Lifshitz, *Mécanique Quantique* (Mir, Moscow, 1967), p. 211.

[14] U. Landman, W.D. Luedtke, N.A. Burnham, and R.J. Colton, Science **248**, 454 (1990); U. Landman, W.D. Luedtke, and E.M. Ringer, in *Fundamentals of Friction: Macroscopic and Microscopic Processes*, Vol. 220 of *NATO Advanced Study Institute, Series E: Applied Sciences*, edited by I.L. Singer and H.M. Pollock (Kluwer, Dordrecht, 1992), p. 463.

[15] T.N. Todorov and A.P. Sutton, Phys. Rev. Lett. **70**, 2138 (1993). They found that the conductance does not vary linearly with the number of atoms in the contact. Since their calculation takes into account the atomic structure of the contact (by means of a tight-binding approach), it is not clear whether this result reflects a general property of a quantum point contact or depends on the particular crystal structure and material. Our calculation provides a simple explanation of this nonlinear behavior in terms of quantum finite-size effects.