Shape effects on conductance quantization in three-dimensional nanowires: Hard versus soft potentials

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Effects of the shapes of the cross sections of three-dimensional nanowires on electronic conductance quantization are studied for both hard- and soft-wall potentials. In both models the quantum conductance is determined by both the area and shape of the narrowmost part of the nanowire. For the hard-wall potential the semiclassical (Weyl) correction to the Sharvin formula provides an adequate approximation to the average quantized conductance. For nanowires modeled by soft-wall potentials, the average quantum conductance may be well estimated using a classical approximation. [S0163-1829(97)09128-5]

The character of ballistic electronic transport in wires (constrictions) is determined by the ratio between their transverse size and the wavelength of the electrons. In wide constrictions, when the electronic wavelength is small compared to the transverse size, electronic transport is classical in nature, and the conductance through the constriction is determined by the Sharvin expression[1]

$$G_{\rm sh}=\frac{2e^2}{h}\,\frac{k_F^2 S}{4\pi}, \tag{1}$$

where k_F is the Fermi wave vector of the electrons, and S is the cross-sectional area. With a decrease of the transverse size, quantum effects become important, resulting in conductance quantization, exhibited by a steplike variation of the conductance in units of $2e^2/h$. Initially studied in two-dimensional (2D) semiconductor structures (see a review in Ref. 2), this phenomenon can also occur, under appropriate conditions, in three-dimensional (3D) metallic nanowires.[3–19] The geometry of 2D constrictions may be described by the transverse size of the narrowmost part (so called bottleneck) of the constriction and by its length (along the axis), and knowing these parameters is sufficient for a description of transport through such constrictions in both the classical and quantum regimes. The situation is different for 3D wires. Classical transport through such constrictions is determined according to Sharvin's formula by the cross-sectional area, while for a description of the transport in the quantum regime additional information about the cross-sectional shape is necessary. As we will show below, the shape influences the quantum transport characteristics in a significant manner.

We investigate shape effects of the cross sections of 3D nanoconstrictions (nanowires) on quantum transport through such nanowires connecting bulk reservoirs. We model the constrictions using either hard- or soft-wall potentials, and compare the results for the quantum conductance in these cases.

Consider ballistic electronic transport through 3D constrictions with an arbitrary shape of the cross sections. We assume that all the cross sections along the nanoconstriction are geometrically similar, and that their size changes slowly on the scale of k_F^{-1}. Such geometries pertain to constrictions with sufficiently large radii of curvature along the constriction (i.e., axial radii of curvature).

The conductance of the constriction, G, is determined by a Landauer-type expression[20,21]

$$G=\frac{2e^2}{h}\sum T_{mn;m'n'}, \tag{2}$$

where $T_{mn;m'n'}$ is the transmission probability for the incident mn channel, and the sum runs over all incident and transmitted channels. The transmission probability $T_{mn;m'n'}$ may be calculated from the solution of the single-particle Schrödinger equation.

In the hard-wall potential model the electronic wave function $\psi(\mathbf{r})$ satisfies the potential-free Schrödinger equation with the Dirichlet boundary condition $\psi|_{\sigma(z)}=0$, where $\sigma(z)$ is the surface of the constriction and z is the coordinate in the direction of the constriction axis. The smoothness of the function $\sigma(z)$ allows us to use the method of adiabatic separation of variables,[22] with the equations for the transverse [Eq. (4)], and longitudinal [through the constriction, Eq. (5)] directions given by

$$-\frac{\hbar^2}{2m^*}\,\Delta_{xy}R_z(x,y)=E_{mn}(z)R_z(x,y), \tag{3}$$

$$-\frac{\hbar^2}{2m^*}\,\frac{d^2Z(z)}{dz^2}+E_{mn}(z)Z(z)=EZ(z), \tag{4}$$

where m^* is the effective mass of the electron.

Near the narrowmost part of the constriction at $z=0$, the effective potential for the longitudinal motion, $E_{mn}(z)$, may be expanded to second order with respect to the variable z. In this approximation the transmission probability has a diagonal form (no mode mixing) (Ref. 23)

$$T_{mn;mn}^{-1}=1+\exp\{-2\pi[E-E_{mn}(0)]/[(-\hbar^2/m^*)\times E''_{mn}(0)]^{1/2}\}, \tag{5}$$

where $E''_{mn}(0)\equiv\partial^2 E_{mn}(0)/\partial z^2$. Taking into account the similarity relation $E_{mn}(z)/E_{mn}(0)=S(0)/S(z)$, where $S(z)$ is the area of the cross section at z, we can express the second derivative of the energy in the form

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$$E''_{mn}(0) = -E_{mn}(0)\,\frac{S''(0)}{S(0)}. \tag{6}$$

In this case the conductance of the constriction can be defined in terms of the electronic energy levels at the narrowmost part $E_{mn}(0)$ and the geometrical factor $S''(0)/S(0)$ [see Eqs. (2), (5), and (6)].

To calculate the conductance of the constriction, we need to define its geometry. When all the cross sections of a nanowire are circles a sequence of conductance steps of heights $1g_0, 2g_0, 2g_0, 1g_0, \ldots$, where $g_0 = 2e^2/h$, reflecting the cylindrical degeneracy of the electronic levels, will occur. Such a predicted sequence of quantized conductance steps[3] has been recently observed in conductance measurements of sodium nanojunctions.[11c] Deviation from circular symmetry leads to restoration of single-step (g_0) behavior of the conductance, depending on the constriction shape. To demonstrate such effects, we consider constrictions with elliptic cross sections. In elliptic coordinates $x = C\cosh\mu\cos\theta$ and $y = C\sinh\mu\sin\theta$ [here $C = C(z)$], Eq. (3) transforms to the Mathieu equation with the boundary condition that the wave function should vanish on the surface of the constriction $\mu = \mu_0$. Under such conditions, the transverse electronic energy levels may be expressed in terms of the zeros of the Mathieu function, q_{mn},

$$E_{mn}(z) = \frac{\hbar^2 q_{mn}^2 \pi \sinh\mu_0 \cosh\mu_0}{2m^* S(z)}. \tag{7}$$

Substituting Eqs. (6) and (7) into Eq. (5), for the conductance of the constriction we obtain the following expression:

$$G = \frac{2e^2}{h}\sum_{mn}\left(1 + \exp\left\{-2\pi\left(\frac{2\pi}{S''(0)}\right)^{1/2}\left[\left(\frac{k^2 S(0)}{\pi}\right)^{1/2} - q_{mn}\sinh\mu_0\cosh\mu_0\right]\right\}\right)^{-1}, \tag{8}$$

where $k^2 = 2m^*E/\hbar^2$.

To evaluate the energy dependence of the conductance, we compute the zeros of the Mathieu function. The dependence of the conductance on the dimensionless parameter $\chi = [k^2 S(0)/4\pi]^{1/2}$ for constrictions with various values of the ratio of elliptic axes (solid lines marked 2 and 3 correspond to $\coth\mu_0 = 1.13$ and 5.06, respectively), and a constant value of the cross-sectional area, are displayed in Fig. 1; the dotted line corresponds to the classical (Sharvin) conductance, $G_{sh} = (2e^2/h)[k^2 S(0)/4\pi]$, and the dashed lines represent semiclassical results. The latter are described by Weyl's corrections to the number of transverse states (channels), which for the Dirichlet boundary condition have a form (see, for example, Ref. 24)

$$G_W = \frac{2e^2}{h}\left[\frac{S(0)k^2}{4\pi} - \frac{L(0)k}{4\pi}\right], \tag{9}$$

where $L(0)$ is the perimeter of the cross section.[25] Note that increasing the eccentricity of the constriction's cross sections while maintaining a constant value of the cross-sectional area (with this condition the classical conductance value remains constant) results in a decrease of the values of the quantum conductance. Additionally, note that in Fig. 1 we plotted the conductance for a relatively short constriction with $[2\pi/S''(0)]^{1/2} = 3$ [$S''(0) = \pi\sinh(2\mu_0)CC'' = \pi\sinh(2\mu_0)C/R$, where C gives the locations of the focii of the elliptical cross section $(\pm C,0)$, and R is the axial radius of curvature of the nanowire], which yields smearing of some steps due to tunneling effects.

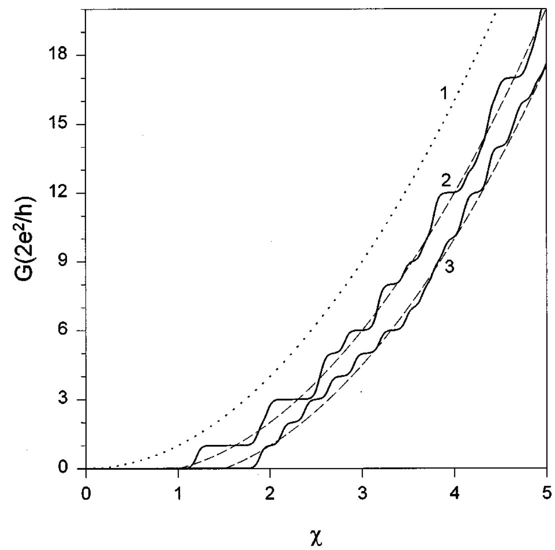

FIG. 1. Conductance (G, in units $2e^2/h$) of 3D asymmetric constrictions modeled by a hard-well potential, plotted vs the dimensionless parameter $\chi = [k^2 S(0)/4\pi]^{1/2}$, where k is the wave vector of the electrons, and $S(0)$ is the cross-sectional area of the narrowmost part of the constriction. Solid lines 2 and 3 correspond to different shapes of the elliptic cross sections of the constrictions (the ratios of elliptic axes are 1.13 and 5.06, respectively), while maintaining a constant value of the cross-sectional area of the constrictions. Dashed lines correspond to calculated conductance in the semiclassical limit (Weyl's corrections), and the dotted line (marked 1) corresponds to Sharvin's conductance. Here we used $[2\pi/S''(0)]^{1/2} = 3$.

In the soft-wall potential model the constriction is modeled by a confining potential which characterizes the shape and extent of the constriction. Expressing the confining potential in the form $V(x,y,z) = U(x,y) - F(z)$, with $F(z) \geqslant 0$ and $F(0) = 0$, and again separating the transverse and longitudinal variables, the equation describing the motion of the electron through the constriction has the same form as Eq. (4) with the effective potential $E_{mn} - F(z)$, where E_{mn} are the transverse energy levels of the electron in the potential $U(x,y)$. Assuming smoothness of the confining potential and expanding it to second order near the bottleneck (i.e., near $z = 0$), for the transmission coefficient we obtain

$$T^{-1}_{mn;mn} = 1 + \exp\left\{-2\pi(E - E_{mn}) \Big/ \left[\frac{\hbar^2}{m^*}F''(0)\right]^{1/2}\right\}. \tag{10}$$

For calculations of the conductance we use a 3D generalization[14] of the Büttiker model.[26] The confining potential in such a model has a form[14]

$$V(x,y,z) = V_0 - \tfrac{1}{2}m^*\omega_z^2 z^2 + \tfrac{1}{2}m^*(\omega_x^2 x^2 + \omega_y^2 y^2). \tag{11}$$

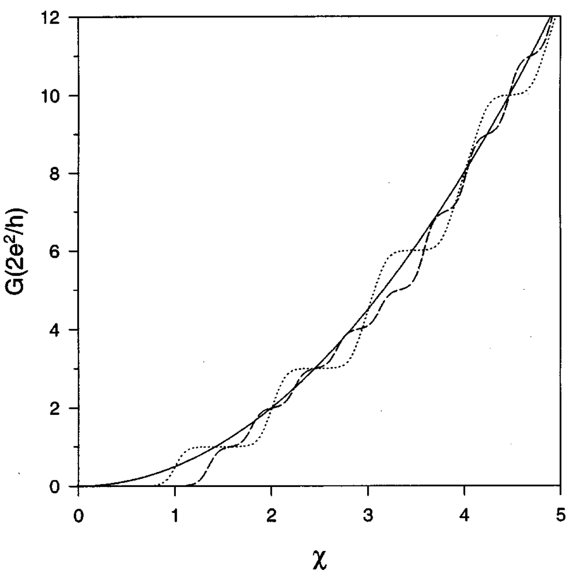

FIG. 2. Conductance (G, in units $2e^2/h$) of 3D asymmetric constrictions modeled by a soft (harmonic) potential, plotted vs the dimensionless parameter $\chi=[k^2S_k(0)/4\pi]^{1/2}$, where $S_k(0) = \pi\hbar^2k^2/m^{*2}\omega_x\omega_y$ is the effective area of the narrowmost cross section, and ω_x and ω_y are the effective frequencies of the confining potential (see text). Dotted and dashed lines correspond to different shapes of the elliptic cross sections of the constrictions (the ratios of the effective elliptic axes, are given by $\omega_y/\omega_x=1.13$ and 5.06, respectively). The solid line corresponds to the classical value of the conductance, which is equal in this model to one-half of the Sharvin conductance. The parameter $[(2\pi/S_k''(0)]^{1/2} =(\omega_x\omega_y)^{1/2}/\omega_z=3$, as in Fig. 1.

The parameter ω_x/ω_y describes the degree of anisotropy of the cross section of the constriction [being spherical when $\omega_x/\omega_y=1$)].

For the confining potential given by Eq. (11) the conductance of the constriction, in the notation of Eq. (8), has the form

$$G=\frac{2e^2}{h}\sum_{mn}\left(1+\exp\left\{-2\pi\left(\frac{2\pi}{S_k''(0)}\right)^{1/2}\left[\left(\frac{k^2S_k(0)}{\pi}\right)^{1/2} -\left(\frac{\omega_x}{\omega_y}\right)^{1/2}(n+\tfrac{1}{2})-\left(\frac{\omega_y}{\omega_x}\right)^{1/2}(m+\tfrac{1}{2})\right]\right\}\right)^{-1}. \tag{12}$$

Here $S_k(0)=2\pi(E-V_0)/m^*\omega_x\omega_y=\pi\hbar^2k^2/m^{*2}\omega_x\omega_y$ is the effective area of the narrowmost part of the nanowire, and the parameter $[2\pi/S_k''(0)]^{1/2}=(\omega_x\omega_y)^{1/2}/\omega_z$ determines its effective axial length. In Fig. 2 we display the conductance of the constriction modeled by the soft potential given in Eq. (11) for the same values of the geometrical parameters as in Fig. 1. Curves corresponding to two values of the ratio of effective elliptic axes ω_y/ω_x are shown. It is of interest to compare the quantized values of the conductance with their classical analogs $G_{\rm soft}^{\rm cl}$. Substituting the classical expression for the transmission probability $T^{\rm cl}=S_k(0)/S$, where S is the total area, into the Landauer expression [Eq. (2)] and integrating over all values of the wave vectors, we obtain

$$G_{\rm soft}^{\rm cl}=\left(\frac{2e^2}{h}\right)\frac{1}{2}\frac{k_F^2S}{4\pi}\equiv\frac{1}{2}G_{\rm sh}. \tag{13}$$

Note that the classical value of the conductance in the approximation of a harmonic confining potential is one half of the Sharvin value. From a plot of $G_{\rm soft}^{\rm cl}$ (the solid line in Fig. 2) we observe that for constrictions modeled by soft confining potentials the classical value of the conductance is close (unlike the case of constrictions with hard-wall potentials) to the average quantized conductance.

The analysis which we performed demonstrates the importance of shape corrections to quantum transport through 3D nanoconstrictions. Quantum transport through such constrictions is determined not only by the cross-sectional area but also by the shape of the cross section. Effects of this type have no analogs in two-dimensional quantum constrictions. Varying the shape of the cross section not only shifts the positions of the conductance steps but also changes the values of the conductance. For conductance calculations we used hard- and soft-wall model potentials. While both models lead to conductance quantization some significant distinctions occur. For nanowires made of typical metals (such as Au, Na, or Cu) with relatively small values of the screening lengths, the hard-wall model potential may be more appropriate.[18c,d] As seen from Fig. 1, shape effects are of importance in this case, and the Weyl correction [Eq. (9)] to the Sharvin formula yields an adequate description of the average behavior of the quantum conductance. For nanowires formed from semimetals, like Bi or Sb, where a soft-wall potential model may be used, the cross-sectional shape influences the quantized conductance, and its average behavior is well estimated (see Fig. 2) using a classical approximation [Eq. (13)]. Finally, these results indicate that in circumstances where shape effects are of importance, caution should be exercised in estimating cross-sectional areas from conductance measurements.

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