Nonlinear magnetoconductance of nanowires

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Quantum magnetoconductance properties of three-dimensional nanowires are studied in the nonlinear (finite-voltage) regime. In the absence of a magnetic field a finite applied voltage leads to the appearance of new plateaus in the differential conductance of the wires, as well as shifts in the locations of the conductance steps. For wires that are symmetric with respect to the plane of the narrowest cross section the new plateaus are characterized by heights that are integer multiples of e^2/h. When placed in a longitudinal magnetic field the conductance as a function of the field strength, and, in particular, magnetic-field-induced switching between quantized conductance levels, can be similarly affected by an applied-finite voltage. This indicates possible experimental control of quantum transport in three-dimensional wires by external fields. [S0163-1829(97)05648-8]

The conductance of ballistic microconstrictions (or wires) connecting macroscopic reservoirs can be described by a Landauer type expression[1,2]

$$G=(2e^2/h)\sum_{\alpha,\alpha'} T_{\alpha\alpha'}, \tag{1}$$

where $T_{\alpha\alpha'}$ is the transition probability from the incident channel α into the transmitted one α'; in the classical limit (i.e., when the electron Fermi wavelength λ_F is much smaller than the contact size), the above expression reduces to the well-known Sharvin conductance[3] $G_{\mathrm{Sh}}=(2e^2/h)k_F^2S/4\pi$, where k_F is the Fermi wave vector and S is the cross-sectional area.

In quantum wires, where the cross-sectional dimension is comparable with λ_F, Eq. (1) describes a stepwise (rather than continuous) variation of G in units of $2e^2/h$, as the transverse size of the constriction is varied. Such behavior occurs in two-dimensional (2D) wires,[4] as well as in three-dimensional (3D) ones;[5–7] in the latter the magnitudes of the conductance steps reflect the degeneracies of the conducting channels[5] (i.e., transverse electronic states), an effect that is absent in 2D wires. However, while the general manifestation of conductance quantization is similar in 2D and 3D wires, these systems differ rather significantly. Particularly, 2D constrictions in semiconductor heterostructures (confined 2D electron gas) can be reproducibly created and controlled through gate-voltage techniques,[4] while experimental methods[7] used in studies of 3D wires (e.g., tip-based methods, mechanical break junctions, and pin-plate setups) do not allow such control and reproducibility. Thus, the evolution of the physical characteristics of a 3D wire during elongation (e.g., atomic structure, morphology, cross-sectional size and shape, and effective length related to the axial radius of curvature of the wire) may be viewed as resulting in the development, in the course of the experiment, of a sequence of wires corresponding to a succession of elongation stages.

Due to the above considerations, pertaining mainly to the methods of preparing 3D nanowires, as well as for potential technological reasons, it is desirable to explore transport measurements where added measures of control may be gained through the application of variable external fields. To this end we have investigated recently[8–10] the influence of magnetic fields on the conductance and thermopower of quantum wires. In these studies it was shown that shifting of electronic energy levels in a magnetic field can change the number of conducting channels in 3D wires in a controlled manner (without affecting their atomic structure), resulting in the appearance of new features such as magnetic-field splitting of conductance steps and magnetic switching and/or blockade of electronic transport. In this paper we investigate quantum magnetotransport in wires in the nonlinear (finite-voltage) regime. Specifically, we demonstrate the appearance of new conductance plateaus and shifts of the conductance steps due to an applied finite voltage. The latter may facilitate observation of the magnetic-field effects in quantized conductance measurements suggested by us earlier.[10]

Consider ballistic electronic transport through a 3D nanowire connecting two reservoirs with a bias voltage applied between them (i.e., $-V/2$ in the left (or lower) one and $V/2$ in the right (or upper) one; see inset in Fig. 1). Assuming that the wire is symmetric,[11] the current through the nanowire has the form

$$I=\frac{2e}{h}\int dE\left[f\left(\frac{E-eV/2-\mu}{k_BT}\right)-f\left(\frac{E+eV/2-\mu}{k_BT}\right)\right]\sum_{\alpha,\alpha'} T_{\alpha\alpha'}(E), \tag{2}$$

where μ is the chemical potential, T is the temperature, k_B is the Boltzmann constant, and f is the Fermi function. To calculate the transmission coefficients $T_{\alpha\alpha'}$ we model the nanowire for convenience as a constriction whose transverse cross sections perpendicular to its z axis are circles of radii $a(z)$; $a_0\equiv a(0)$ is the radius at the narrowmost part of the constriction. Additionally, limiting ourself to wires of adiabatic shape, where the transmission probability has a diagonal form in the channel index (i.e., no mode mixing),[10,12] allows one to write

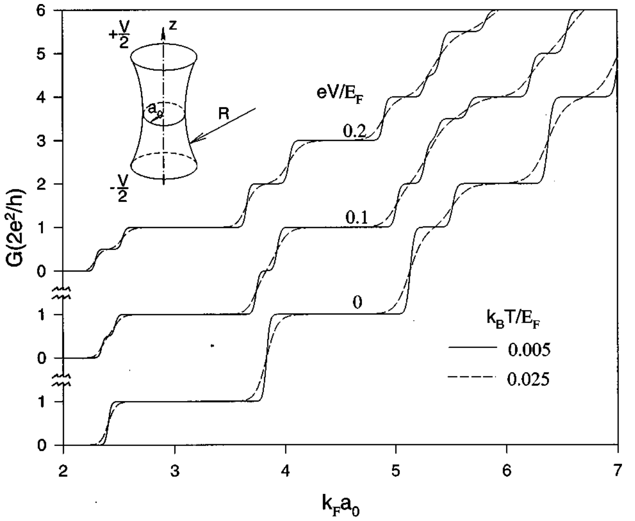

FIG. 1. Conductance (G, in units of $2e^2/h$) of a 3D wire plotted vs the dimensionless parameter $k_F a_0$, with $H=0$ and $R/a_0=200$. The different curves correspond to the three marked values of the applied voltage (V in units of E_F/e, where E_F is the Fermi energy). Results for two different temperatures (T, in units of E_F/k_B) are given for each case. In the inset we show schematically the geometry of the nanowire. $a_0 \equiv a(0)$ is the radius of the narrowmost cross section and R is the axial radius of curvature.

$$T_{\alpha\alpha}^{-1}(E)=1 + \exp\{-2\pi[E-E_\alpha(0)]/[-(\hbar^2/m^*)E''_\alpha(0)]^{1/2}\}, \quad (3)$$

where $E_\alpha(0)$ are the transverse electronic energy levels in the narrowmost part of the wire ($z=0$), which we calculate in the hard-wall potential approximation; $E''_\alpha(0) \equiv \partial^2 E_\alpha(0)/\partial z^2$, α denotes the quantum numbers m and n ($m=0,\pm 1,...$; $n=1,2,...$), and m^* is the electron's effective mass. The (differential) conductance of the wire is given by $\partial I/\partial V$.

We examine first the conductance of the nanowire in the absence of a magnetic field. In this case the positions of the conductance steps are determined by the sequence of zeros of the Bessel function and the magnitude of the applied voltage. Variation of the conductance as a function of the dimensionless parameter $k_F a_0$ is shown in Fig. 1 for several values of the applied voltage V. The bottom curve corresponds to $V \rightarrow 0$, and the conductance exhibits a standard $1g_0, 3g_0, 5g_0, 6g_0, \ldots$ sequence of plateaus ($g_0 = 2e^2/h$), reflecting the degeneracies of the zeros of the Bessel function, as predicted in Ref. 5 and observed in mechanical break-junction measurements of sodium.[13] Increase of the applied voltage leads to the appearance of a new sequence of conductance plateaus;[14] $0.5g_0, 1g_0, 2g_0, 3g_0, 4g_0, 5g_0, 5.5g_0, 6g_0, \ldots$ for $eV/E_F=0.1$ (see middle curve in Fig. 1). The occurrence of steps with heights of multiples of half-integer quanta (i.e., $g_0/2$) in the differential conductance for finite voltage has been discussed previously for 2D microconstrictions.[11] The origin of the occurrence of such steps is that at finite voltage V across the wire the effective chemical potentials for the left- and right-moving electrons are shifted by $eV/2$ and $-eV/2$, respectively [see Eq. (1)]; equivalently one may say that the energy levels of left- and right-moving electrons are shifted as $E_{mn}(0)+eV/2$ and $E_{mn}(0)-eV/2$. The above mentioned degeneracies of some of the electronic levels occurring in our 3D nanowires (which are absent in the 2D case) are the source of the differences between the sequence given above and that described in the 2D case[11] (the half-integers originate from singly degenerate levels).

For a larger voltage, $eV/E_F=0.2$, a new sequence $0.5g_0, 1g_0, 2g_0, 3g_0, 4g_0, 4.5g_0, 5.5g_0, 6g_0, \ldots$ occurs (see upper curve in Fig. 1). Such sequences may occur when $eV > \Delta E_{mn}$, where ΔE_{mn} is the spacing between neighboring energy levels with different m degeneracies, i.e., $E_{0,n}(0)$ and $E_{m,n'}(0)$, $m \neq 0$ (in the above sequence $n=2$ and $n'=1, m=\pm 2$) leading to reordering of the energy levels; note that since the higher-energy levels are more densely spaced such reordering occurs for them first, being reflected in the occurrence of the new features further on in the conductance sequence (compare the middle and upper curves in Fig. 1). Additionally, deviation of the transverse cross section of the nanowire from a circular shape leads to removal of the degeneracies of the energy levels.[15] Under finite voltage this will result in the appearance of conductance plateaus only at half-integer values of g_0. We remark also that for a finite voltage applied to wires that are nonsymmetric in the axial (z) direction, because of the asymmetry of the potential drop, the conductance values at the plateaus may differ from those in symmetric constrictions (as is the case here) where they occur at integer multiples of $g_0/2$. Increasing the temperature leads to progressively larger smearing of the conductance steps as illustrated also in Fig. 1 (compare solid and dashed lines).

In a longitudinal magnetic field the energy levels in Eq. (3) are determined by the zeros of the confluent hypergeometric function.[10] In Figs. 2(a) and 3(a) we display the dependence of the conductance, for several values of V, on the dimensionless flux φ/φ_0 ($\varphi = \pi a_0{}^2 H$ is the magnetic flux through the narrowmost part of the wire and $\varphi_0 = hc/e$ is the quantum of flux) for wires with $k_F a_0 = 5.4$ and 2.55 (corresponding, respectively, to five and one conducting channels at $H=0$ and $V \rightarrow 0$). Already for $V \rightarrow 0$ [see bottom curves in Figs. 2(a) and 3(a)] the magnetic field can cause switching between conductance plateaus, due to shifts of the energy levels.[10] The behavior of the conductance shown in Figs. 2 and 3 (for $V \neq 0$) illustrates that the magnetic switch effect (i.e., transitions between conductance values as a function of the magnitude of the applied magnetic field) can be influenced significantly by an applied voltage, with the origins of the effects being similar to those discussed above for the magnetic-field-free case. Since the conductance can be influenced either by an applied magnetic field, an applied voltage, or combinations of the two, we show in Figs. 2(b) and 3(b) the conductances of the two wires as functions of both V and φ/φ_0.

The above analysis demonstrates that quantum transport in 3D nanowires can be controlled by external fields, i.e., magnetic field and/or a finite voltage, while maintaining the atomic structure and geometric characteristics of the wire unchanged. A magnetic field as well as a finite voltage shift the electronic energy levels and may lead to changes in the number of conducting channels. Additionally, a finite voltage

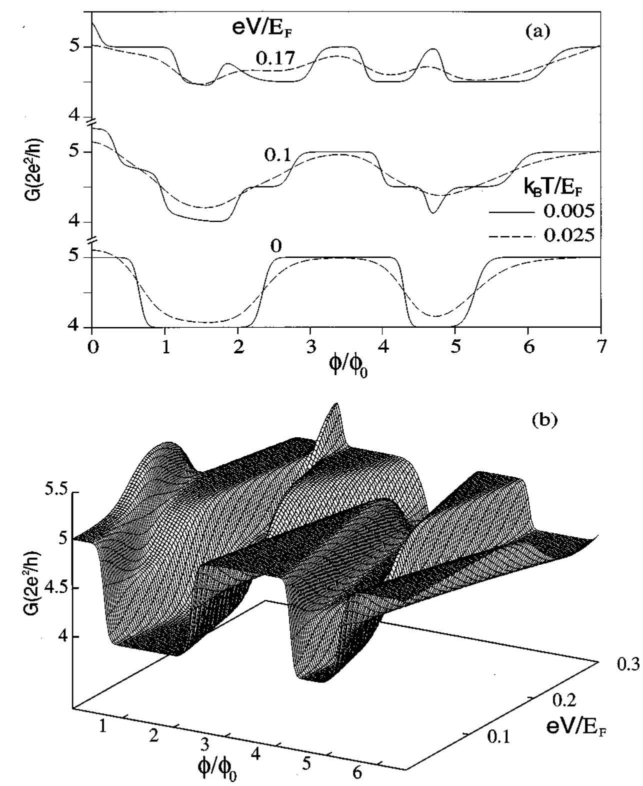

FIG. 2. (a) Conductance (G, in units of $2e^2/h$) of a 3D wire, plotted vs the dimensionless magnetic flux $\varphi/\varphi_0 = H\pi a_0{}^2 e/hc$, with $R/a_0 = 200$ and $k_F a_0 = 5.4$ (corresponding to five conducting channels for $H=0$ and $V \to 0$). Different curves correspond to the marked values of the applied voltage (V, in units of E_F/e), and in each case for two different temperatures (T, in units of E_F/k_B). (b) The conductance of the wire plotted vs φ/φ_0 and eV/E_F, for $k_B T/E_F = 5\times10^{-3}$.

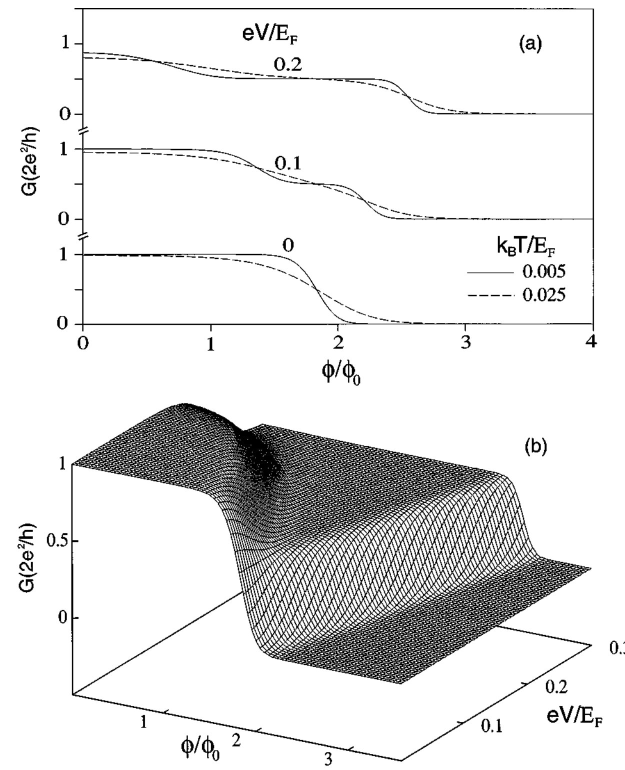

FIG. 3. Same as Fig. 2, but for a 3D wire with $k_F a_0 = 2.55$ (corresponding to one conducting channel for $H=0$ and $V \to 0$).

differentiates right- and left-moving electrons. This may be described in terms of different effective electrochemical potentials for opposite-moving electrons,[16,17] resulting in the appearance of fractional (in units of $2e^2/h$) plateaus in the quantum conductance.

To experimentally observe the effects discussed above applied magnetic fields with fluxes of the order of the flux quantum φ_0 (see discussion in Ref. 10), and voltages with eV of the order of the spacing between electronic energy levels in the nanowire, are required. While such conditions may be realized most easily in semimetallic wires (bismuth and antimony), the high sensitivity of the quantum transport to an applied voltage may allow also observation of magnetotransport effects in the nonlinear regime even in nanowires made from typical metals. Indeed, as illustrated in Figs. 2 and 3 the magnitude of the applied magnetic field required in order to switch between conductance values may be significantly lowered for certain values of the applied voltage. Furthermore, measurement of the conductance of a given wire (with fixed geometry) as a function of the applied voltage serves as an added measure of control in 3D wire experiments, and may allow identification of thresholds for opening (or closing) of conductance channels, which are the optimal conditions (i.e., requiring smaller magnetic fields) for observation of magnetotransport effects in 3D nanowires.

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