Magnetic switching and thermal enhancement of quantum transport through nanowires

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Magnetic-field switching and blockade of quantum transport through three-dimensional metallic and semimetallic nanowires with a small number of conducting channels are proposed. Temperature enhancement of magnetotransport in such wires is predicted. [S0163-1829(96)51620-6]

Early investigations of ballistic electronic transport through microconstrictions led to the discovery of conductance quantization. Initially this phenomenon was observed in two-dimensional semiconducting structures, manifesting itself in $2e^2/h$ steplike variations of the conductance as a function of the transverse size of the narrowing (see review in Ref. 1). Underlying the phenomenon is the discrete character of the electronic modes (conducting channels) propagating through the constriction. Theoretical analysis of the generation and properties of small three-dimensional (3D) constrictions and nanowires, including mechanical[2,3] and electrical (conductance quantization) (Ref. 4) characteristics, the applications of modern experimental techniques to investigations of such systems, and their fundamental as well as potential technological significance, motivated intensifying research efforts of such systems.[5–13]

In the absence of an applied magnetic field the number of propagating modes, and thus the conductance in such structures, is determined by the minimum cross section of the constriction. However, shifting of the electronic energy levels under the influence of an applied magnetic field may lead to significant changes in the conductance. Indeed, analysis of the effect of a longitudinal magnetic field on quantum transport in relatively wide wires, characterized by a large number of conducting channels,[14] described the appearance of steplike fluctuations of the magnetoconductance of 3D microwires, on a scale corresponding to a small fraction of the magnetic flux quantum $\phi_0 = hc/e$. It is likely that such fine fluctuating features have been observed in recent experiments.[15,16]

Most observations of well-defined quantized conductance features have been reported for metallic nanowires with a small number of conducting channels.[5–11] In this paper we investigate quantum magnetotransport in such systems, and propose a magnetic switch effect and the occurrence of magnetic blockade of quantum transport in metallic and semimetallic nanowires. Additionally, we demonstrate that under appropriate conditions (depending on parameters of the wire and on the applied magnetic field), an enhancement of the magnetoconductance with increasing temperature may occur in such systems. This effect originates from temperature broadening of the Fermi distribution, which can result in an increase of the number of conducting channels in a magnetic field.

We consider ballistic electronic transport through 3D nanowires (nanoconstrictions, see inset to Fig. 1) between two bulk reservoirs. The cross sections of the nanowire perpendicular to the axis of the wire are taken for convenience to be circles of radii $a(z)$, with that in the narrowest part of the constriction denoted by $a_0 = a(0)$. We assume also that the function $a(z)$ describing the shape of the wire is smooth on the scale of k_F^{-1} (where k_F is the Fermi wave vector; such smoothness of $a(z)$ may be realized for constrictions with large radii of curvature, R). The applied magnetic field H is oriented parallel to the axis of the wire (z direction).

The conductance of the wire, G, is determined by a Landauer-type formula[17,18]

$$G = \frac{2e^2}{h} \sum T_{mn;m'n'}, \tag{1}$$

where $T_{mn;m'n'}$ is the transmission probability for the incident mn channel and the sum extends over all incident and transmitted channels. To calculate the transmission probability we need to solve the single-particle Schrödinger equation with a hard-wall boundary condition at the surface of the wire, $r = a(z)$. The slow variation of the function $a(z)$ describing the shape of the constriction [we assume that $a'(z)$, $a(z)a''(z) \ll 1$] allows us to use the adiabatic method of separation of transverse and longitudinal variables,[19] and the wave function can be written in the form

$$\psi = R_z(r) e^{imz} Z(z), \tag{2}$$

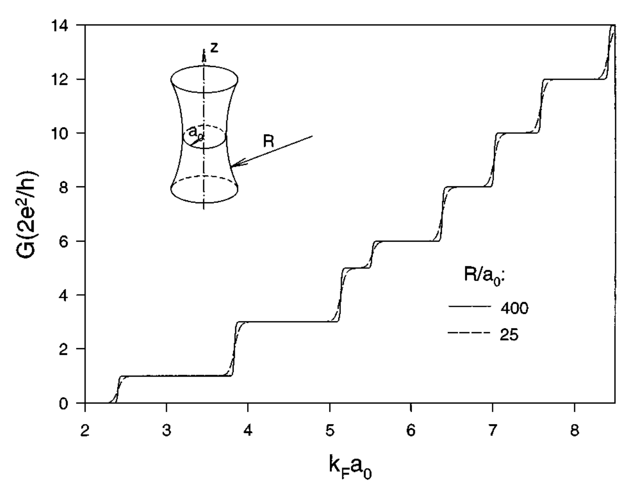

FIG. 1. Conductance (G, in units of $2e^2/h$) of a 3D wire vs k_Fa_0 with $H=0$, plotted for two values of R/a_0. Inset: geometry of a nanowire. a_0 is the radius of the narrowmost cross section and R is the radius of curvature.

where m is the magnetic quantum number ($m=0$, ± 1, $\pm 2, \ldots$), and the radial part of the wave function, $R_z(r)$, obeys the equation

$$-\frac{\hbar^2}{2m^*}\left\{\frac{d}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{m^2}{r^2}-\frac{eHm}{\hbar c}-\frac{e^2H^2}{4\hbar^2c^2}r^2\right\}R_z(r)$$
$$=E_{mn}[a(z)]R_z(r), \tag{3}$$

with the boundary condition $R_z[r=a(z)]=0$. Here m^* is the electron effective mass and for the vector potential we use the cylindrical coordinate gauge $A=(A_r,A_\phi,A_z)$ with $A_\phi=Hr/2$ and $A_r=A_z=0$. The solutions to this equation may be expressed in terms of the confluent hypergeometric function,[20]

$$R_z(r)=e^{\xi/2}\xi^{|m|/2}F\left[-\left(\frac{E_{mn}[a(z)]}{\hbar\omega_c}-\frac{|m|+m+1}{2}\right),|m|+1,\xi(r)\right]. \tag{4}$$

Here $\xi(r)=m^*\omega_c r^2/2\hbar=H\pi r^2/\phi_0$, and $\omega_c=eH/m^*c$ is the cyclotron frequency. The transverse adiabatic energy levels $E_{mn}(z)$ are expressed according to the boundary condition in terms of the zeros of the confluent hypergeometric function F(the zeros of this function are indexed by n) (Ref. 21).

The motion of the electron through the wire (z direction) is described by the longitudinal part of the wave function, which is the solution of

$$-\frac{\hbar^2}{2m^*}\frac{d^2Z}{dz^2}+E_{mn}[a(z)]Z(z)=EZ(z). \tag{5}$$

Near the narrowmost part of the constriction, $z=0$, the effective potential $E_{mn}[a(z)]$ in Eq. (5) may be expanded [as in Ref. 19] to second order with respect to the variable z, i.e.,

$$E_{mn}[a(z)]=E_{mn}[a_0]+\frac{1}{2}\frac{\partial^2E_{mn}[a_0]}{\partial z^2}z^2, \tag{6}$$

where $\partial^2E_{mn}[a_0]/\partial z^2=(\partial E_{mn}[a_0]/\partial a)(\partial^2a_0/\partial z^2)<0$ (the inequality follows from numerical analysis of the spectrum). In this case the transmission probability has a diagonal form (no modes mixing) (Ref. 20)

$$T^{-1}_{mn;mn}=1+\exp\{-2\pi[E-E_{mn}(a_0)]/[(-\hbar^2/m^*)$$
$$\times\partial^2E_{mn}(a_0)/\partial z^2]^{1/2}\}. \tag{7}$$

In the absence of tunneling the transmission coefficient transforms to a step function, $\theta[E-E_{mn}(a_0)]$, accordingly, the threshold energy for each channel in the plane $z=0$ is equal to $E_{mn}(a_0)$. Channels with energies $E>E_{mn}(a_0)$ pass through the wire with unit probability while others are reflected. Consequently, in this case the transmission probability [and thus the conductance, see Eq. (1)] is a sharp stepwise function of the transverse size of the constriction and the magnetic-field strength.

In zero magnetic field Eq. 3 reduces to the Bessel equation and the transverse energy levels $E^{(0)}_{mn}$ are given by the expression

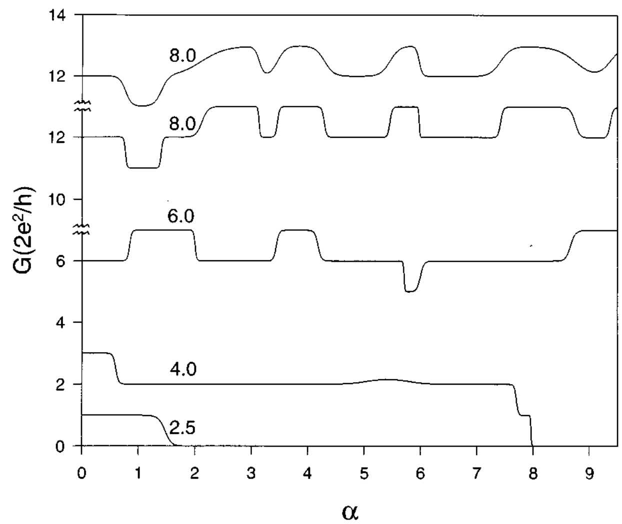

FIG. 2. Conductance (G, in units of $2e^2/h$) of 3D wires vs the dimensionless magnetic flux $\alpha=\phi/\phi_0$. The different curves correspond to the marked values of k_Fa_0. The four lower curves describe conductance behavior for long wires ($R/a_0=400$), and the upper one corresponds to a shorter wire ($R/a_0=25$) where smearing of the steps due to tunneling becomes significant.

$$E^{(0)}_{mn}=\frac{\hbar^2\gamma^2_{mn}}{2m^*a^2(z)}. \tag{8}$$

In this case the positions of the conductance steps are determined by the sequence of zeros of the Bessel function, γ_{mn}, and the step heights (single or double) depend on the m degeneracy of the energy levels;[4] see Fig. 1, where the conductance in units of $2e^2/h$ is plotted versus k_Fa_0 for two values of the parameter $(a_0a_0'')^{-1}=R/a_0$. Note the increased smearing of the steps due to tunneling effects in the shorter wire[4] (dashed line).

To obtain the magnetic-field dependence of the conductance we compute the zeros of the confluent hypergeometric function $F\{-[k^2_{mn}a^2_0/4\alpha-(|m|+m+1)/2],|m|+1,\alpha\}$, where $k^2_{mn}=2m^*E_{mn}(a_0)/\hbar^2$, and $\alpha=\pi a^2_0H/\phi_0$ is the magnetic flux through the narrowmost part of the constriction in units of ϕ_0. The dependence of the conductance on the dimensionless flux α for different values of the parameter k_Fa_0 (i.e., for several values of the number of conducting channels, see Fig. 1) is displayed in Fig. 2. The behavior of the conductance demonstrates a ''magnetic switch'' (on and off) effect and ''magnetic blockade'' of the quantum electronic transport in wires with small values of k_Fa_0 (i.e., small number of transport channels, see, for example, the curves for $k_Fa_0=2.5$ and 4 in Fig. 2). Note that for a nanowire with the same geometry (i.e., same R/a_0) smearing of the magnetic steps is larger (compare upper curve in Fig. 2 with the dashed line in Fig. 1). This is due to the slow dependence of the energy levels on the magnetic field resulting in the increased role of tunneling effects. [The cause of the local maximum near $\alpha\sim 5.5$ in the curve for $k_Fa_0=4$ is discussed below in the context of Fig. 4(a).]

The magnetic-field behavior of the conductance (e.g., the magnitude of the applied field for which a switch to a different conductance level occurs) is very sensitive to the transverse size of the constriction in the wire. Figure 3 portrays

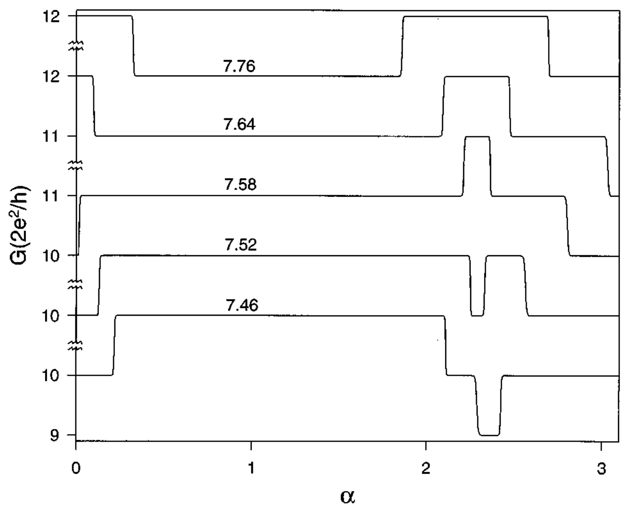

FIG. 3. Conductance (G, in units of $2e^2/h$) of very long 3D nanowires vs $\alpha = \phi/\phi_0$. The different curves correspond to the marked close values of $k_F a_0$.

such a behavior for different but relatively close values of the parameter $k_F a_0$, illustrating that for wires characterized by the same zero-field conductance switching may occur for a broad range of magnetic-field strengths, depending on small variations in the transverse dimensions of the wire.

In the above we discussed the conductance behavior of long nanowires, where tunneling effects are small, and at zero temperature. In shorter wires tunneling becomes more important leading not only to ordinary ''smearing'' of the conductance steps (see Fig. 2) but under some circumstances to increase of the conductance. In Fig. 4(a) we plotted the conductance versus the magnetic flux for wires with different lengths. The increase of the conductance (maximum in the vicinity of $\alpha \approx 3$) is related to the flux dependence of the transverse energy levels [see Fig. 4(c)]. This behavior of the conductance originates from a finite probability of tunneling in a short wire of the second channel near $\alpha \approx 3$. Even more remarkable is the influence of the temperature on the conductance demonstrated in Fig. 4(b), where the conductance of a long wire (where tunneling is insignificant) is plotted versus flux for different temperatures. The predicted temperature enhancement of the quantum transport is due in this case to an increase of the transmission probability of a quantum channel located in the vicinity of the top of the temperature broadened Fermi distribution. Consequently, through variation of the applied magnetic field one may achieve conditions that would result in enhancement of the conductance, of tunneling or thermal origins.

We turn now to issues pertaining to experimental observations of the predicted magnetic switch and blockade effects in nanowires. As aforementioned, the sharp steps in the conductance as a function of H (Fig. 2) are caused by shifts of the electronic energy levels in the presence of a magnetic field. The change in the magnetic flux required to shift energy levels by an amount of the order of the average spacing between transverse energy levels in 3D wires of common metals, i.e., $\sim \epsilon_F/(k_F a_0)^2$, may be large (e.g., about one flux quantum ϕ_0), and consequently for wires with a small number of conducting channels may require excessively large magnetic fields. This suggests semimetallic or semiconducting nanowires as the most suitable systems for observation of the magnetic switch and blockade effects described above. For example, in bismuth the Fermi wave vector is $\sim 2\times10^6$ cm^{-1}. For $k_F a_0 = 2.5$ (i.e., $a_0 \sim 10^{-6}$ cm), corresponding to a single conducting channel (see Fig. 1), the magnetic field needed to create a magnetic flux quantum in the wire is about $H = \phi_0/\pi a_0^2 \sim 10$–15 T, which is readily accessible experimentally. For thicker wires with a larger number of channels, observation of the switch effect would require even lower fields. Note also that at low temperatures the conditions for ballistic transport are readily satisfied in bismuth wires and whiskers, even on the micron scale. Finally, for Bi the temperatures used in Fig. 4(b) describing the temperature enhancement of the conductance range between 1 and 20 K.

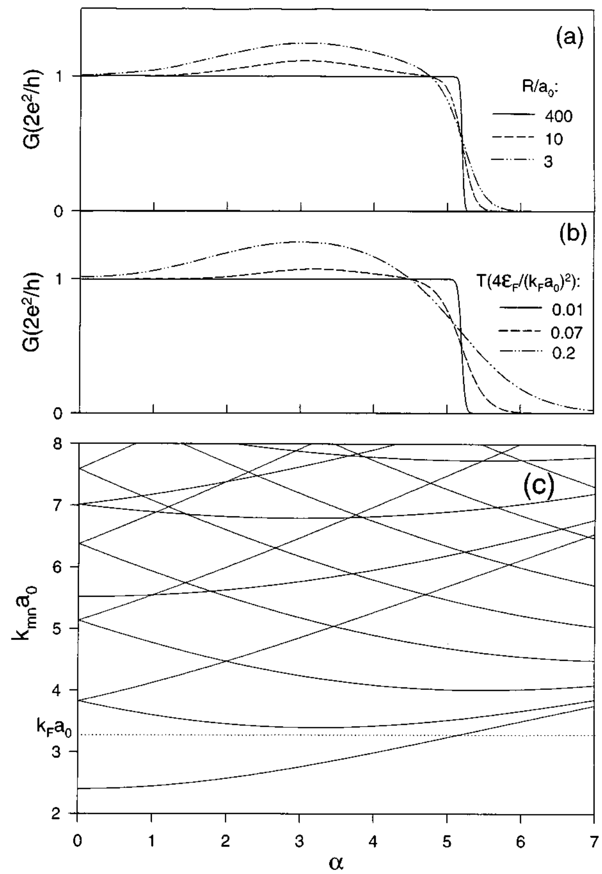

FIG. 4. (a) and (b) Conductance (G, in units of $2e^2/h$) of 3D nanowires vs α for $k_F a_0 = 3.3$ corresponding to one channel at zero magnetic field (see Fig. 1). In (a) the different curves correspond to various lengths of the nanowire (i.e., different values of R/a_0), as denoted. In (b) the different curves correspond to various temperatures, measured in units of $4\epsilon_F/(k_F a_0)^2$, where ϵ_F is the Fermi energy. (c) Dependence of $k_{mn}a_0$ $[k_{mn}^2 = 2m^* E_{mn}(a_0)/\hbar^2]$ as a function of α for different values of the quantum numbers m and n. The dotted line corresponds to the value $k_F a_0$ used in (a) and (b).

The experimental situation becomes more complicated in normal metallic nanowires. For typical metals, for example, gold or sodium with well-defined conductance step structures,[6–9] the Fermi wave vector is $\sim 10^8$ cm^{-1}. For $k_F a_0 = 8$, corresponding to twelve conducting channels (Fig. 1), the magnetic-field strength ($\sim 10^3$ T) required in order to create a flux quantum is beyond current normal capabilities.

Consequently we suggest that to observe magnetic-switch steps in such systems it would be necessary to select wires with the largest transverse energy level located near the Fermi energy, corresponding to positions in Fig. 1 in the vicinity of the thresholds for opening or closing of a quantum conductance channel. This could be achieved by varying slightly the wire's cross-sectional radius (e.g., through mechanical manipulation of the wire, such as slight elongation or compression). In this case, as seen from Fig. 3, one may find configurations for which magnetic switching and thermal enhancement of the quantum transport can be reached for accessible values of the applied magnetic field.

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