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Magnetomechanics of mesoscopic wires

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We have studied the force in mesoscopic wires in the presence of an external magnetic field along the wire using a free electron model. We show that the applied magnetic field can be used to affect the force in the wire. The magnetic field breaks the degeneracy of the eigenenergies of the conduction modes, resulting in more structure in the force as a function of wire length. The use of an external magnetic field is an equilibrium method of controlling the number of transporting channels. Under the least favorable circumstances (on the middle of a low conduction step) one needs about 1.3 T to see an abrupt change in the force at fixed wire length for a mesoscopic bismuth wire.

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I. Introduction

Thc electrical conductance in a ballistic wire with dimensions comparable to the Fermi wavelength increases in steps of $G_0 = 2e^2/h$ as the cross section increases. This conductance quantization is observable at room temperature in metallic nanowires formed by pressing two pieces of metal together into a metallic contact. When the two pieces are separated, the contact is stretched into a nanowire, a wire of nanometer dimensions. Several experiments varying this principle have been performed, e.g., using scanning tunneling microscopy [1], mechanically controlled break junctions [2], or just plain macroscopic wires [3]. Although most nanowire experiments have been performed on metals, conductance quantization has been seen in bismuth at 4 K [4]. Since bismuth has a Fermi wavelength $\lambda_F = 26$ nm [4], these semimetal «nanowires» are larger than the metallic nanowires.

The stepwise variation of the conductance in such a mesoscopic wire is accompanied by an abrupt change of the force in the wire [5]. Using a free-electron model, neglecting all atomic structure of the wire, it has been shown [6–9] that the size of the electronic contribution to the force fluctuations are comparable to the experimentally found values and that the qualitative behavior, i.e., the abrupt change that accompanies the conductance steps, is the same.

In the wire the transverse motion of the electrons give rise to quantized modes α of energy E_α . In the simplest version of the Landauer formalism, a mode is considered fully transmitting (open) if $E_F > E_\alpha$ and closed otherwise [10]. Each open mode contributes an amount e^2/h to the conductance, if modes with different spin are considered separately. When the wire is elongated, the cross section decreases, more and more modes are pushed above the Fermi level and closed, thus decreasing the conductance stepwise. This has been shown in two dimensions [11] and in three dimensions [12].

It has been suggested [13] that the conductance and the mechanical force in a nanowire can be controlled by an applied driving voltage. This effect originates from the injection of additional electrons with voltage dependent energy, because of the different chemical potentials of the two reservoirs. Since relatively large applied voltage is needed, one will have to worry about heating in this case.

The eigenenergies of the transverse motion can be affected by an external magnetic field B perpendicular to the cross section of the wire. This will show up in the conductance and in the force as a function of B. The effect of magnetic field on the conductance has been considered in Ref. 14. To use an external magnetic field is an equilibrium method of controlling the number of transporting channels, without significant risk of relaxation.

Because of band bending, due to the small size of the wire, the eigenenergies will have to be corrected. This can, however, be taken care of by introducing an effective Fermi energy $\tilde{E}_F$ in the wire. Assuming that the number of electrons (per unit volume) is constant, $\tilde{E}_F$ can be determined self-consistently and will vary with wire length and magnetic field.

In this paper we present force calculations for different applied magnetic fields and wire lengths, using a free-electron model. We take into account the effect of band bending, adjusting the Fermi energy in the wire. In order to resolve any effect for moderate magnetic fields, a low cyclotron effective mass (which enters in the cyclotron frequency) is needed, which can be found in semimetals. Metals are less favorable since, because of a larger cyclotron effective mass (larger Fermi energy), we would need a larger magnetic field in order to resolve any effect. For numerical estimates we have used values for bismuth, a typical semimetal. For bismuth the spin splitting is also important, since it has a large spectroscopic spin splitting factor g.

II. Model

We consider a cylindrical ballistic wire of length L with circular cross section and a parabolic confining potential

$$\omega(r) = \frac{\omega_0^2 m^* r^2}{2} \equiv E_F \frac{r^2}{R^2} , \quad (1)$$

using cylindrical coordinates (r, φ, z); here m^* is the effective electron mass. The wire is along the z direction. The last equality in Eq. (1) defines ω_0. In this equation E_F is the zero-B-field bulk value, yielding a magnetic-field-independent confining potential. We assume that the volume $V = \pi R^2 L$ of the wire is kept constant during elongation, which makes R and L mutually dependent.

With the above confining potential and an applied magnetic field along the wire, the Schrödinger equation has been solved [15]. If also spin is included, the eigenenergies are

$$E_\alpha = \hbar \left(\frac{\omega_c^2}{4} + \omega_0^2 \right)^{1/2} n + \frac{1}{2} l\hbar\omega_c + sg\mu_B B, \quad (2)$$

$$n = 2m + |l| + 1, \quad m = 0, 1, 2, \ldots,$$

$$l = 0, \pm 1, \pm 2, \ldots, \quad s = \pm 1/2, \quad \alpha = \{m, l, s\} ,$$

where $\omega_c = eB/m^*$ is the cyclotron frequency; μ_B is the Bohr magneton; $sg\mu_B$ is the magnetic moment associated with the electronic spin.

Since our system is open, the electronic contribution to the force in the wire is given by the derivative of the grand potential $\Omega = E - \mu N$ with respect to elongation. Here E is the total energy of the electrons in the wire, μ is the chemical potential, and N is the number of electrons in the wire. If the Fermi energy E_F is much higher than the thermal energy (as in metals or at low temperature), we have $\mu \approx E_F$. The grand potential is then [9]

$$\Omega(E_F) = -\sum_\alpha \frac{4}{3} L \left(\frac{2m^*}{\pi^2 \hbar^2} \right)^{1/2} (E_F - E_\alpha)^{3/2} , \quad (3)$$

where the sum is over all open modes. The force in the wire is given by

$$F = -\frac{\delta\Omega}{\delta L} , \quad (4)$$

which in general has to be calculated numerically.

The magnetic field affects the system primarily by splitting the otherwise degenerate eigenenergies of the conduction modes [Eq. (2)]. Since then the conduction modes will open one-by-one, this will cause more structure in the force and conductance when displayed as functions of wire length. Subsequently, when applying an external magnetic field we will see the (clearest) effect when the highest open level or the lowest closed level goes through the Fermi level (whichever happens first). If one does not adjust the Fermi energy for band bending but uses the bulk Fermi energy for zero magnetic field, one can analytically calculate the B field needed when the wire is kept at a specified length. The least favorable situation would be on the middle of a conduction step.

III. Results and discussion

We have used numerical values for bismuth, a typical semimetal with $E_F = 25$ meV [4]. Bismuth has an anisotropic Fermi surface resulting in different effective masses in different directions, between $0.009m_e$–$1.8m_e$ [16]. The cyclotron effective mass is in the range $0.009m_e$–$0.13m_e$ [16]. Assuming an isotropic Fermi surface and an quadratic dispersion relation, both effective masses are the same: $m^* = 0.07m_e$ for $E_F = 25$ meV. The spectroscopic splitting factor g can be as high as 260 or an order of magnitude smaller, depending on the direction of the magnetic field [17]. With $g = 20$ the spin splitting is roughly of the same order as the Landau level distance, and becomes dominant for g as large as 200. We have used $g = 20$. The wire volume was kept constant at 30 000 nm^3 [3].

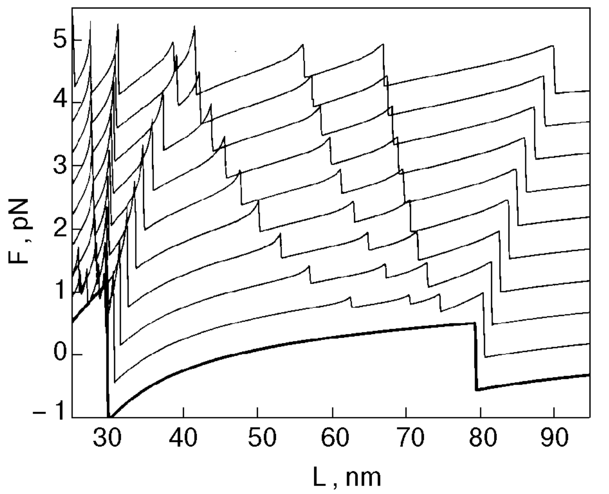

Fig. 1. The force in a mesoscopic wire as a function of wire length for different magnetic fields. The lowest, thick, curve is for $B = 0$. The next lines, each displaced by 0.5 pN, are for $B = 0.5$; 1T etc., the uppermost line being for $B = 4.5$ T. The splitting of the eigenenergies of the conduction modes is clearly visible: for larger B fields the curves have more structure, since now every mode closes one-by-one when the wire is elongated. We have used the spectroscopic splitting factor $g = 20$ and an effective Fermi energy $\tilde{E}_F$.

To find the effective Fermi energy of the wire we have adjusted the value in order to keep the number of electrons constant, with a tolerance of 10^{-4}%.

Figure 1 shows the force in the wire as a function of wire length for different magnetic fields. For nonzero fields the force curves show more structure, since now the eigenenergies of the conduction channels are nondegenerate and close one-by-one, each time resulting in a sharp change of the force.

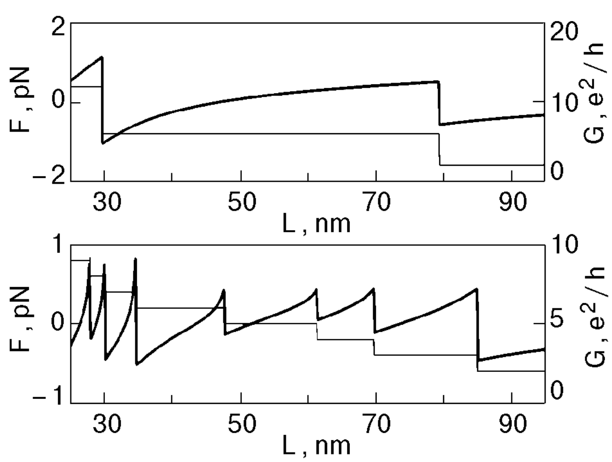

Fig. 2. The force (thick line) and the conductance in a mesoscopic wire for two different magnetic fields, in the upper figure $B = 0$, and in the lower figure $B = 2.5$ T. We clearly see that the abrupt change in the force happens when a channel closes, i.e., when there is a step in the conductance. We have used an effective Fermi energy $\tilde{E}_F$.

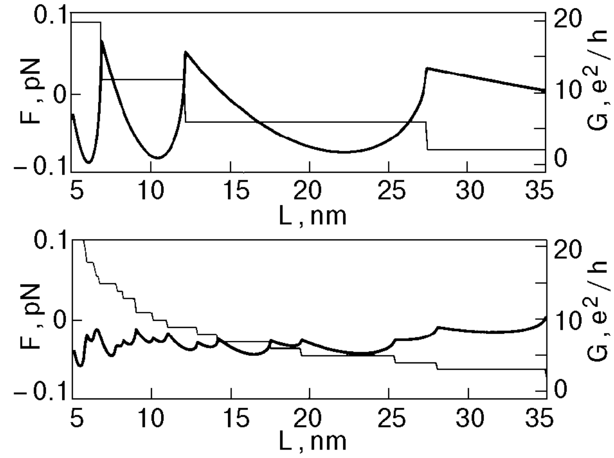

Fig. 3. The force (thick line) and the conductance in a mesoscopic wire for the less realistic case of a constant Fermi energy in the wire equal to the zero-B-field bulk value (25 meV). Results for two different magnetic fields are shown; in the upper figure $B = 0$, and in the lower figure $B = 2.5$ T.

The force and conductance for two particular magnetic fields, $B = 0$ and 2.5 T, are shown in Fig. 2. Each step in the conductance is accompanied by an abrupt change in the force. We also show the corresponding picture for the simplest possible case [9] when we use the bulk value of the Fermi energy, E_F , in Fig. 3. In this case the force is one order of magnitude smaller then in the more realistic case with $\tilde{E}_F$. This is because the effective fermi energy has to be larger then the bulk value in order to keep the number of electrons per unit volume in the wire constant in spite of the quantization of levels. Also, the conduction modes close much later in the $\tilde{E}_F$ case than in the simpler case when the wire is elongated. The reason for this is that the effective Fermi energy, as a function of wire length, follows each eigenenergy before intercepting it and closing the channel.

On the middle of the second conduction step ($G = 3G_0$, $n = 2$) the circumstances are least favorable to see the effect of the magnetic field. For the case with the zero-B-field bulk value of the Fermi energy ($L = 19.8$ nm), we have analytically calculated that one needs $B = 2.4$ T in order to see the highest open level go through the Fermi energy, thus giving a sharp change in the force as well as in the conductance. For higher conduction modes one will see the effect for smaller fields, since the splitting is proportional to l, whose absolute maximum is equal to n.

In Fig. 4 we see the force and the conductance as a function of magnetic field for a fixed wire length, $L = 54.6$ nm. This is for the case with an effective wire Fermi energy and a length corresponding to the middle of the second conduction step

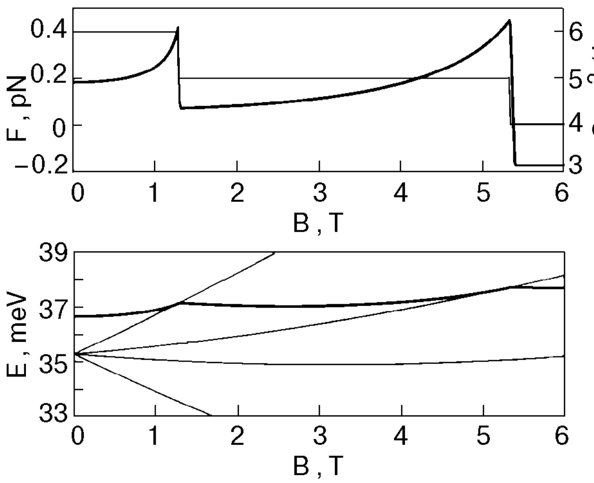

Fig. 4. In the upper figure we show the force (thick line) and conductance for $L = 54.6$ nm. This length corresponds to the middle of the second conduction step. In the lower figure we show the eigenenergies of the second conduction step and the effective Fermi energy of the wire (thick line). We see that when the highest level goes through the Fermi level (for approximately $B = 1.3$ T) there is a step in the conductance and an abrupt change in the force.

($G = 3G_0$, $n = 2$). We see that we need about 1.3 T before the highest open level goes through the Fermi surface, showing us the pronounced effect of the magnetic field. In the lower part of the same figure we also see the effective Fermi energy (thick line) and the eigenenergies of the second conduction steps. Notice how the Fermi level increases with the eigenenergy before it intercepts. However, these variations are small compared to the overall magnitude of the Fermi energy.

So far we have used the spectroscopic splitting factor $g = 20$. In Fig. 5 we show the force as a function of length for $B = 1$ T for different g factors: $g =$ 0, 2, 20, and 200. For $g = 0$ there is no spin splitting, but we still see more structure than for $B = 0$ (cf. Fig. 1). This is due to the breaking of the degeneracy into the Landau levels. With increasing g factor the spin splitting becomes larger and larger; however, whatever the size of the spin splitting, more structure appears in the force with an applied magnetic field.

The Fermi energy of the bulk will also be affected by the magnetic field, due to the de Haas-van Alphen effect. In the case when an effective Fermi energy $\tilde{E}_F$ is used, this does not affect the results, since the bulk Fermi energy does not enter into the calculations. When adjusting the bulk Fermi energy for de Haas-van Alphen effect, in the simpler case shown in Fig. 3, there is no significant change of the force. We have also studied the influence of a moderate applied voltage (in the mV range) but have seen no significant effect.

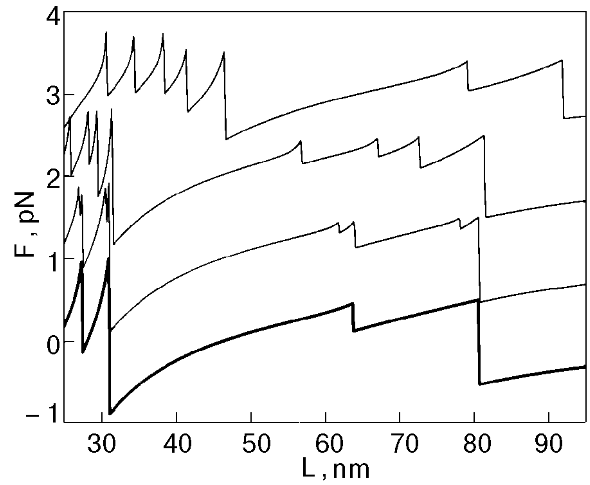

Fig. 5. Force as a function of length for $B = 1$ T for different g-factors. The lowest curve is for $g = 0$, and the following curves, each displaced by 1 pN, for $g = 2$, 20, and 200, respectively. We see that no matter what the g-factor is, an external magnetic field will give the force curves more structure than for $B = 0$ (cf. Fig. 1).

For metals the Fermi energy is in the eV range, demanding much higher magnetic fields to resolve results similar to those for bismuth above. Since the size of the splitting is proportional to the number of open channels, having more channels will decrease the magnetic field needed. Therefore, if we design the circumstances to be more favorable, i.e., having more open channels and being close to a conduction step, a moderate magnetic field will be enough to make an eigenenergy go through the Fermi level, thus giving an effect in the force and in the conductance.

IV. Conclusion

Using a free-electron model, we have shown that the force in a mesoscopic wire can be affected by an external magnetic field parallel to the wire. With a magnetic field present the degenerate eigenenergies of the conduction modes split and become conducting (open) at different elongations, resulting in more force fluctuations with increasing wire length. At fixed wire length we propose that an external magnetic field is an equilibrium method that can be used to affect the force as well as the conductance in mesoscopic wires. Since no atomic rearrangement is required (contrary to elongation experiments) in an experiment along these lines, it may give new insight into the nature of the intrinsic mechanical properties of these wires.

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