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 to control the number of transporting channels. Under the least favorable circumstances (on the middle of a low conduction step) one needs about 1.3 T, for a mesoscopic Bismuth wire, to see an abrupt change in the force, at fixed wire length.

I. INTRODUCTION

The 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].

Most nanowire experiments have been performed on metals, however conductance quantization have been seen [4] in Bismuth at 4K. Since Bismuth has a Fermi wavelength \( \lambda_F = 26 \text{ nm} \), these semi-metal “nanowires” are larger than the metallic nanowires.

The stepwise variation of conductance in such a mesoscopic wire is accompanied by an abrupt change of the force in the wire [4]. Using a free electron model, neglecting all atomic structure of the wire, it has been shown [5] 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 \( \alpha \) of energy \( E_\alpha \). In the simplest version of the Landauer formalism, a mode is considered fully transmitting, open, if \( E_F > E_\alpha \) and closed otherwise [6]. 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 [7] and in three dimensions [8].

It has been suggested [9] 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. A relatively large applied voltage is needed so 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 in the conductance and in the force as a function of \( B \). The effect of a magnetic field on the conductance has been considered in ref. [10]. To use an external magnetic field is an equilibrium method to control 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 in the wire, \( E_F \). Assuming that the number of electrons (per unit volume) is constant, \( E_F \) can be determined selfconsistently 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 semi-metals. 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 semi-metal. For Bismuth also the spin splitting is 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,

\[
\omega(r) = \frac{\omega_0^2 m^* r^2}{2} \equiv E_F \frac{r^2}{R^2},
\]

using cylindrical coordinates \((r, \phi, z)\) and where \( m^* \) is the effective electron mass. The wire is along the \( z \)-direction. The last equality in Eq. 1 defines \( \omega_0 \). 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\[2\]. If also spin is included the eigenenergies are

$$E_\alpha = \hbar \left( \frac{\omega_c^2}{4} + \omega_0^2 \right)^{1/2} n + \frac{1}{2} \hbar \omega_c + s g \mu_B B \tag{2}$$

where $\omega_c = eB/m^*$ is the cyclotron frequency, $\mu_B$ is the Bohr magnetron and $sg\mu_B$ 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, $\mu$ the chemical potential and $N$ 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

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

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

$$F = -\frac{\delta \Omega}{\delta L}. \tag{4}$$

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 a function 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 we do not adjust the Fermi energy for band bending, but use the bulk Fermi energy for zero magnetic field, one can analytically calculate the $B$-field needed, when keeping the wire at a specific 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 semi-metal with $E_F = 25$ meV\[\text{[4]}\]. Bismuth has an anisotropic Fermi surface resulting in different effective masses in different directions, between 0.009$m_e - 1.8m_e$. The cyclotron effective mass is in the range 0.009$m_e - 0.13m_e$. Assuming an isotropic Fermi surface and an quadratic dispersion relation, both effective masses are the same, for $E_F = 25$ meV $m^* = 0.07m_e$. The spectroscopic splitting factor, $g$, can be as high as 260, or one order of magnitude smaller depending on the direction of the magnetic field\[2\]. 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 30000 nm$^3$.

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 $10^{-4}\%$.

![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 $B = 0.5$ T, $B = 1$ T 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 $E_F$.](image-url)
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 $E_F$-case than in the more simple case when the wire is elongated. The reason for this is that the effective Fermi energy, as a function of wire length, follows the eigenenergies before intercepting it and closing the channel.

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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, 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 $l$, whos absolute maximum is equal to $n$.

In Fig. 2 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 the length corresponds to the middle of the second conduction step. In the lower part of the same figure we also see the effective Fermi energy (thick line) and 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.

In Fig. 3 we see the spectroscopic splitting factor $g = 20$. In Fig. 4 we see 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 is: more structure in the force appears with an applied magnetic field.

Also the Fermi energy of the bulk will be affected by the magnetic field, due to the de Haas-van Alphen effect. In the case when an effective Fermi energy, $E_F$, 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 more simple case shown in Fig. 3 there is

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.

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.

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no significant change on the force. We have also studied the influence of a moderate applied voltage (in the mV-range) but have seen no significant effect.

![Graph showing force as a function of length for different g-factors.](image)

**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 $g = 2$, $g = 20$ and $g = 200$ 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 a 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. So if we design the circumstances to be more favorable, i.e., more open channels and 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.

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