# Thermopower of quantum nanowires in a magnetic field

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Thermoelectric properties of nanowires in a magnetic field are studied. Magnetic splitting of thermopower peaks associated with electronic energy levels that are degenerate at zero field, leading to the development of separate thermopower peaks at larger fields, are predicted. A scheme is described for measuring thermopower in a circuit containing a nanowire and leads made from the same material. [S0163-1829(96)52740-2]

## I. INTRODUCTION

Ballistic transport properties through microconstrictions (or wires) connecting bulk reservoirs exhibit new behavior when the transverse size of the microconstriction junction becomes comparable to the electron Fermi wavelength, $\lambda_F$. Under such conditions quantum effects result in the appearance of new features, such as stepwise (rather than continuous) variation of the conductance[1] and sharp maxima in the thermopower,[2] as the transverse size of the constriction is varied. Both phenomena originate from the discrete character of the change in the number of conducting modes (channels) transmitted through the constriction upon variation of its transverse size. Such behavior occurs in two-dimensional (2D) constrictions[3] as well as in three-dimensional (3D) ones.[4]

Early investigations of ballistic electronic conductance and thermopower focused on 2D mesoscopic semiconductor structures (such as GaAs-$Al_xGa_{1-x}As$ heterojunctions) where $\lambda_F$ is large ($\sim$400 Å) and consequently the pertinent transverse dimension of the constriction is of submicrometer size.[3] More recently it has been shown, first through molecular-dynamics simulations[5] and then experimentally, that crystalline ordered metallic nanowires can be formed by retracting a tip from contact with a surface,[6–10] through breaking of junctions,[11] and in the process of separation of contacting wires[12] or in pin-surface experiments[13] (i.e., the separation of even macroscopic contacts results in the ultimate elongation stages in the generation of nanometer scale wires, irrespective of the initial size of the contact).[5,14] Quantized electronic transport in such nonowires has been anticipated[5] and indeed measured (see Refs. 6–13; including observation[11(c)] of conductance steps near one, three, five, and six times $2e^2/h$, as predicted in Ref. 4), since $\lambda_F$ in metals is of the order of several angstroms. These investigations include measurements of mechanical[9,10,15] and electronic conductance properties at cryogenic[11,15] and room temperatures,[6–10,12,13] current-voltage characteristics,[8] a transition to a localization regime in long nanowires,[8] studies of the effect of the shape of the transverse cross section of the wire on the quantized conductance characteristics,[16] investigation of thermoelectric properties,[17] magnetic field splitting of the conductance steps,[18] and predictions of magnetic switching, blockade, and thermal enhancement of quantum transport through nanowires.[19]

In this paper we investigate quantum thermotransport in nanowires in a longitudinal magnetic field. We show that the magnetic field splits the thermopower peaks associated with degenerate energy levels. Additionally, we demonstrate that the thermopower dependence on the magnetic field in such wires has a spectrum of peaks, and we describe a scheme for measuring thermopower in a circuit containing a nanowire (ballistic element), with both the nanowire and the leads made of the same material.

## II. RESULTS

We consider ballistic transport through a 3D nanowire connecting two bulk reservoirs. A bias voltage $V$ is applied between the reservoirs, which are kept at different temperatures $\theta_1$ and $\theta_2$ (see inset to Fig. 1). A distinctive feature of the ballistic transport regime in this case is the existence of electrons of different temperatures in the wire. Moreover, an average temperature corresponding to thermal equilibrium cannot be established in the constriction. The electric current through the nanowire is expressed in this case in terms of equilibrium Fermi functions, $f_0$, of the bulk reservoirs, and has the Landauer-type form[20,21]

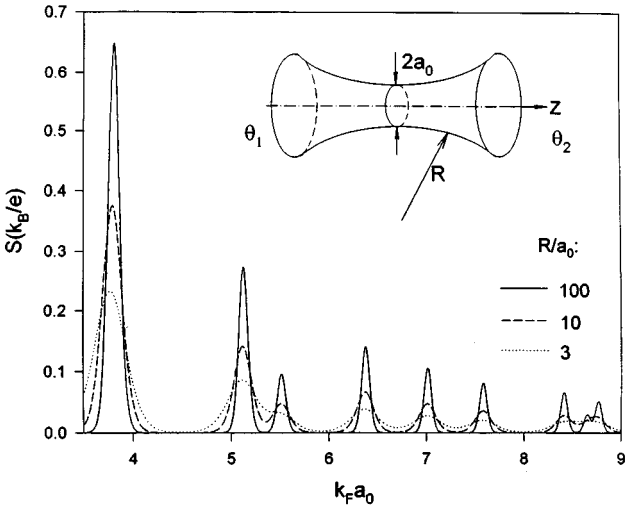


FIG. 1. Thermopower coefficient ($S$, in units of $k_B/e$, where $k_B$ is the Boltzmann constant) of a 3D wire plotted versus $k_F a_0$, with $H=0$ and $\theta=0.05$ [in units of $2\hbar^2/(m^* a_0^2 k_B)$], plotted for three values of $R/a_0$. Inset: geometry of a nanowire; $a_0$ is the radius of the narrowest cross section and $R$ is the radius of curvature.

 

$$I=\frac{2e}{h}\int dE\left[f_0\left(\frac{E-eV/2-\mu_1}{\theta_1}\right)-f_0\left(\frac{E+eV/2-\mu_2}{\theta_2}\right)\right]\sum T_{mn;m'n'}(E). \quad (1)$$

Here the chemical potentials $\mu_{1,2}=\mu(\theta_{1,2})$ are determined by the temperatures of the reservoirs $\theta_{1,2}$, and $T_{mn;m'n'}$ is the transmission probability for the incident $mn$ channel. The sum in Eq. (1) runs over all incident and transmitted channels.

In the linear response approximation the thermopower coefficient of the nanowire

$$S=\frac{V^*}{\theta_1-\theta_2} \quad (2)$$

is given by

$$S=\frac{1}{e\theta}\frac{\int dE\frac{\partial f_0}{\partial E}(E-\mu)\sum T_{mn;m'n'}(E)}{\int dE\frac{\partial f_0}{\partial E}\sum T_{mn;m'n'}(E)}. \quad (3)$$

Here, $V^*=V+1/e(\mu_1-\mu_2)$ is the electrochemical potential difference between the two reservoirs, and $\mu=(\mu_1+\mu_2)/2$ and $\theta=(\theta_1+\theta_2)/2$ are the average chemical potential and temperature, respectively. From the definition of the conductance

$$G=\frac{2e^2}{h}\int dE\left(-\frac{\partial f_0}{\partial E}\right)\sum T_{mn;m'n'}(E), \quad (4)$$

we can express the thermopower coefficient of the 3D nanowire in the Mott-type form,

$$S=\frac{\pi^2T}{3e}\frac{\partial \ln G}{\partial \mu}. \quad (5)$$

The nanowire is modeled for convenience as a constriction whose cross sections perpendicular to its axis $z$ are taken to be circles of radii $a(z)$ (see inset to Fig. 1). The magnetic field $H$ is parallel to the constriction axis. We assume that the function $a(z)$ describing the constriction shape is smooth on the scale of $k_F^{-1}$ ($k_F$ is the Fermi wave vector) so that $a'(z),a(z)a''(z)\ll 1$. Under such assumptions the electronic transmission probability through the constriction may be calculated in the adiabatic approximation, allowing separation of the transverse and longitudinal variables.[22]

Calculations, similar to those made in Ref. 19, lead to the following diagonal form (no mode mixing) of the transmission coefficient $T$:

$$T^{-1}_{mn;mn}(E)=1+\exp\{-2\pi[E-E_{mn}(a_0)]/[(-\hbar^2/m^*)\times\partial^2E_{mn}(a_0)/\partial z^2]^{1/2}\}. \quad (6)$$

Here $a_0\equiv a(0)$ is the radius at the narrowest part of the constriction, $E_{mn}$ are the electronic transverse energy levels, and $m^*$ is the electron effective mass. In the absence of tunneling effects the transmission coefficient transforms to a step function $\theta[E-E_{mn}(a_0)]$.

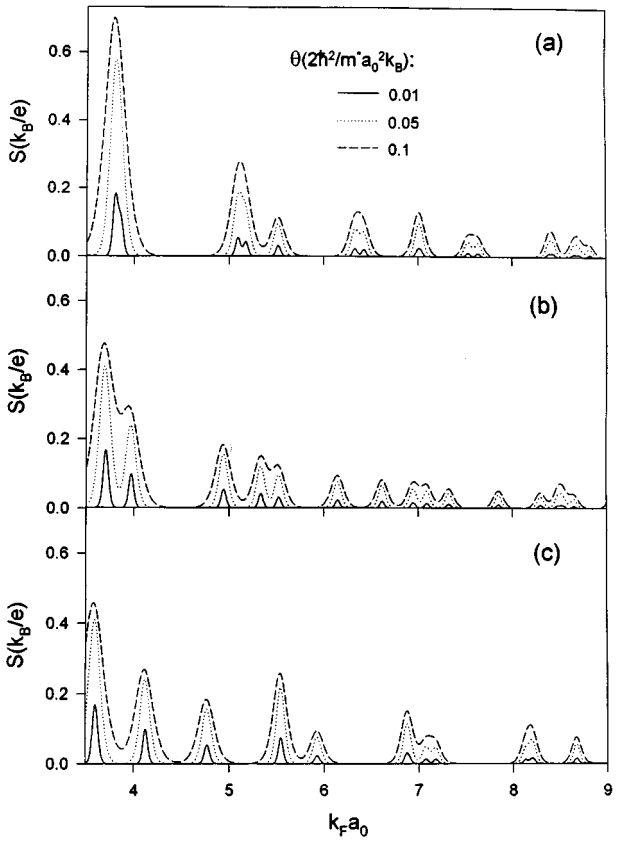


FIG. 2. Thermopower coefficient ($S$, in units of $k_B/e$) of a 3D wire with $R/a_0=100$, plotted versus $k_Fa_0$ for different values of the temperatures $\theta$ [in units $2\hbar^2/(m^*a_0^2k_B)$] and for three values of the dimensionless magnetic flux parameter $\alpha=\pi a_0^2H/\phi_0$, $\phi_0=hc/e$. In (a) $\alpha$=0.1; in (b) $\alpha$=0.5; in (c) $\alpha$=1.

In zero magnetic field the transverse energy levels $E^{(0)}_{mn}$ are given by the expression

$$E^{(0)}_{mn}=\frac{\hbar^2\gamma^2_{m.n}}{2m^*a^2(z)}, \quad (7)$$

and the zeros of Bessel functions $\gamma_{m,n}$ determine the positions of single or double steps (depending on the degeneracy of the energy levels since $\gamma_{m,n}=\gamma_{-m,n}$) of the conductance,[4,18] and of the thermopower peaks.[17] The thermopower peaks are more pronounced in long constrictions; see Fig. 1, where the thermopower coefficient is plotted versus $k_Fa_0$ for two values of the parameter $(a_0a_0'')^{-1}=R/a_0$, ($R$ is the radius of curvature which determines the effective length of the constriction). Note the increased smearing of the peaks due to the more significant role of tunneling effects in the shorter wire (dashed line).

In a magnetic field the electronic energy levels are computed from the equation for the confluent hypergeometric function[19]

$$F\left\{-\left(\frac{k^2_{mn}a_0^2}{4\alpha}-\frac{|m|+m+1}{2}\right),|m|+1,\alpha\right\}=0, \quad (8)$$

where $k^2_{mn}=2m^*E_{mn}(a_0)/\hbar^2$, and $\alpha=\pi a_0^2H/\phi_0$ is the magnetic flux through the narrowest part of the constriction in units of the flux quantum $\phi_0=hc/e$. The magnetic field shifts the transverse energy levels and removes their $m$

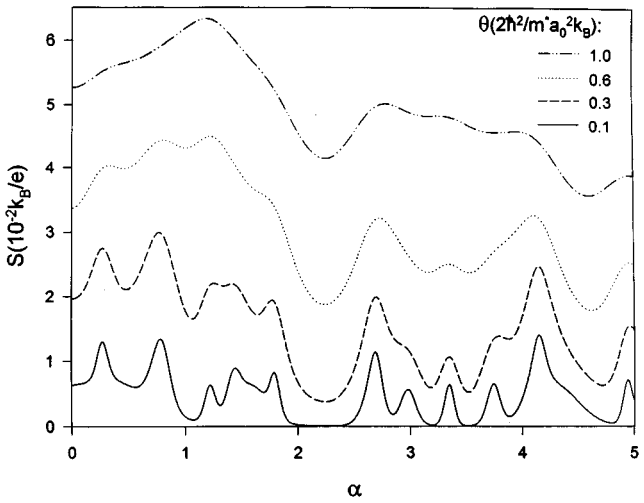


FIG. 3. Thermopower coefficient ($S$, in $10^{-2}k_B/e$ units) of a 3D wire plotted versus the dimensionless magnetic flux $\alpha=\phi/\phi_0$ for $k_Fa_0=18$, $R/a_0=100$ and different values of the temperature [in units $2\hbar^2/(m^*a_0^2k_B)$].

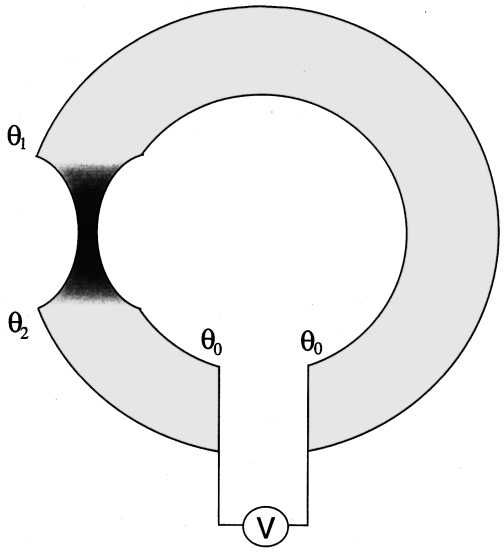


FIG. 4. Schematic of a homogeneous thermoelectric circuit incorporating a nanoconstriction. Both the nanoconstriction (dark grey) and leads (light grey) are made of the same material. $\theta_1$ and $\theta_2$ are the temperatures near the nanoconstriction, and $\theta_0$ is the temperature in the leads far from the nanoconstriction. The circled $V$ denotes a voltage measuring device.

degeneracy.[23] The latter results in splitting of the thermopower peaks associated with degenerate levels. For larger magnetic fields the separation between the split peaks increases leading to their appearance as separate peaks. In Fig. 2 the thermopower coefficient is plotted versus $k_Fa_0$ for different values of the magnetic field (i.e., the dimensionless parameter $\alpha$). Note the increase in the number of thermopower peaks for $\alpha=0.5$ [Fig. 2(b)] compared to the zero field case (Fig. 1).

Thermopower peaks may also occur when the size of the constriction is maintained as a constant and the magnetic field is varied. The magnetic-field-induced thermopower peaks are due to the monotonic dependence of the electronic energy levels obtained from Eq. (8) [see Fig. 4(c) in Ref. 19]. Unlike the conductance where magnetic field on-and-off switching of the energy levels leads to up-and-down jumps in the conductance, all the thermopower peaks are of the same sign; the latter is because of the different signs of the derivative $\partial E_{mn}/\partial H$ at the points when the number of allowed conducting channels $N=N(E-E_{mn})$ increases or decreases upon variation of the magnetic field, and $\partial N/\partial E=(-\partial N/\partial H)(\partial E_{mn}/\partial H)^{-1}$. In Fig. 3 we plotted the variation of the thermopower coefficient versus the magnetic flux $\alpha$. Note the appearance of thermopower peaks on a scale less than a flux quantum $hc/e$. Increase of the temperature leads to an increase of the ''period of oscillations'' (compare with a similar behavior of the conductance steps studied in Ref. 18). It is of interest also to compare these results with the thermopower behavior in classical microconstrictions ($a_0 \gg \lambda_F$), where the magnetic field leads to an additional term in the thermopower which varies monotonically with the field.[24]

## III. SUMMARY

The variations in the structure of the thermopower spectrum as a function of $H$ discussed by us in the preceding section (Figs. 2 and 3) are caused by shifts of the electronic energy levels in the presence of a magnetic field. To achieve such an effect the magnitude of the flux associated with the applied magnetic field should generally be of the order of the flux quantum ($hc/e$). For wires characterized by a small number of conducting channels this may be realized most easily for semimetals and semiconducting materials, where $k_F$ is relatively small. For example, magnetic fields of several teslas are required for bismuth wires ($k_F \sim 2\times10^6$ cm$^{-1}$) with $k_Fa_0=5$, corresponding to three conducting channels (see Fig. 1 in Ref. 19). In normal metallic wires much higher fields are required (for a more detailed discussion of this subject, see Ref. 19).

In experiments one normally measures the thermopower difference between two conductors made of different materials. A distinctive feature in our case is the possibility of measuring thermopower in a homogeneous circuit containing a nanoconstriction,[25] since the (ballistic) nature of transport in the nanoconstriction is different from that in the leads. Such a scheme is shown in Fig. 4. The measured voltage

$$\Delta V = V^* - \int_{\theta_2}^{\theta_1} S_{\rm bulk}\, d\theta \tag{9}$$

is the difference between the thermopowers of the quantum constriction $V^*$ [Eqs. (2) and (3)] and that of the bulk ($S_{\rm bulk}$ being the absolute differential thermopower of the bulk metal). Since the thermopower of the bulk metal (current leads) does not depend on the constriction parameters, by changing the latter one can measure thermopower quantum characteristics of nanowires using the scheme proposed in Fig. 4.

## ACKNOWLEDGMENTS

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[23] Underlying the $m$ degeneracy of the transverse energy levels is the circular cross section of the nanowire assumed in this study. In less symmetric constrictions (e.g., of ellipsoidal cross section) this degeneracy may be lifted even under field-free conditions. In such circumstances the effect of the applied manetic field is to shift the positions of the thermopower peaks. A discussion of the influence of the constriction shape on quantum transport in nanowires has been given in Ref. 16, and E. N. Bogachek, A. G. Scherbakov, and U. Landman (unpublished).

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