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Thermopower of three-dimensional quantum wires and constrictions

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Abstract
The thermopower of asymmetrical quantum wires and constrictions in an arbitrarily directed magnetic field is investigated. An analytic expression convenient for analysing the thermopower is obtained. The oscillations in the thermopower are studied. It is shown that the thermopower as a function of a magnetic field can undergo Aharonov–Bohm and Shubnikov–de Haas oscillations.

1. Introduction

The physical properties of quantum constrictions and wires have attracted growing attention in view of their unique physical properties. In particular, in these structures the quantization of conductance is widely studied [1–3]. However, the observation of conductance is possible only for low temperatures because of temperature smoothing of the thresholds of the conductance steps. The study of thermopower can provide additional scope for studying physical properties of quantum wires and constrictions. This is connected with the following factors. First, the thermopower can provide more information than the study of conductance [4]. Second, quantum wires and constrictions can be used as elements for low-temperature thermometers [5].

The thermopower of quantum contacts and wires is widely experimentally studied. For example, the thermopower of quantum GaAs contacts was investigated in [5, 6], the thermopower of Au contacts was studied in [7], AuFe wires were investigated in [8]. These experiments have shown that the thermopower is very sensitive to the form of the contacts and wires.

The theoretical studies of the thermopower [9–11], as a rule, are based on the numerical analysis of the Cutler–Mott formula (5). A general formalism for thermoelectric transport in the case of microstructures with any number of terminals was developed in [12].

We study the thermoelectric properties of a quantum wire placed in an arbitrarily directed magnetic field $\boldsymbol{B}(B_x, B_y, B_z)$ using the parabolic confinement potential

$$U(x, y) = \frac{m^*}{2}(\Omega_x^2 x^2 + \Omega_y^2 y^2). \tag{1}$$

Here m^* is the effective electron mass, and the characteristic frequencies Ω_j ($j = x, y$) determine the semi-axes of the elliptic cross-section of the wire $l_j = \sqrt{\hbar/4m^*\Omega_j}$.

In this case the discrete part of the spectrum of the one-electron states is given by the formula [13]

$$\varepsilon_{mn} = \hbar\omega_1(m + 1/2) + \hbar\omega_2(n + 1/2) \tag{2}$$

where $n, m = 0, 1, 2, \ldots$, and

$$\omega_{1,2} = \frac{1}{2}\left\{\left[\Omega_x^2 + \Omega_y^2 + \omega_c^2 + 2\Omega_x\Omega_y\sqrt{1 + (\omega_x/\Omega_y)^2 + (\omega_y/\Omega_x)^2}\right]^{1/2} \pm \left[\Omega_x^2 + \Omega_y^2 + \omega_c^2 - 2\Omega_x\Omega_y\sqrt{1 + (\omega_x/\Omega_y)^2 + (\omega_y/\Omega_x)^2}\right]^{1/2}\right\}, \tag{3}$$

where $\omega_c = |e|B/m^*c$ is the cyclotron frequency, and $\omega_j = |e|B_j/m^*c$ ($j = x, y, z$) are the components of the cyclotron frequency.

We use the saddle point potential to model the geometric confinement potential of a quantum constriction [14]

$$V(x, y, z) = V_0 + \tfrac{1}{2}m^*(\Omega_x^2 x^2 + \Omega_y^2 y^2 - \Omega_z^2 z^2). \tag{4}$$

Here V_0 is the potential at the saddle point. The frequency $\Omega_z = \hbar/m^* l^2$ is determined by the characteristic length of the constriction l. The characteristic frequencies Ω_j ($j = x, y$) determine the semi-axes of the elliptic cross-section of the constriction $l_j = \sqrt{\hbar/4m^*\Omega_j}$.

The discrete part of the spectrum of electrons placed in an arbitrarily directed magnetic field has a form analogous to (2) but with other frequencies $\omega_{1,2}$ which can be obtained from the sixth-order algebraic equation [15].

2. Oscillations of the thermopower

In the case when a system consists of two bulk reservoirs connected by a 3D quantum wire or constriction, there exists a simple relationship between the thermopower S and the ballistic conductance G (the Cutler–Mott formula [16–18]):

$$S = -\frac{\pi^2 k_B^2 T}{3e}\frac{\partial \ln G}{\partial\mu}, \tag{5}$$

where μ is the chemical potential.

Equation (5) is inconvenient for analysis because it contains a logarithm of a series. However, in our previous paper [19] it was shown that if the monotonic part of the conductance G_{mon} is much more than the oscillating one G_{osc}, the formula (5) can be rewritten in the form

$$S = \frac{k_B^2\pi^2 T}{3e}\frac{1}{G_{\mathrm{mon}}}\left(\frac{\partial G_{\mathrm{mon}}}{\partial\mu} + \frac{\partial G_{\mathrm{osc}}}{\partial\mu}\right) + \mathrm{O}\left(\frac{\hbar^2\omega_1\omega_2}{\mu^2}\right). \tag{6}$$

This estimate holds for a 3D quantum wire and constriction, too. Note that the monotonic and oscillating parts of the conductance of the wire and constriction were obtained in [20] and in [15], respectively.

Calculating the corresponding partial derivatives for cases of the quantum wire and constriction, we get S in the form

$$S = S_{\mathrm{mon}} + S_{\mathrm{osc}}. \tag{7}$$

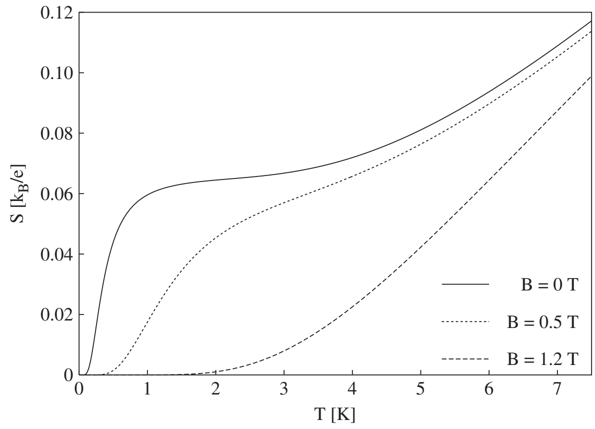

Figure 1. Thermopower as a function of the temperature: $\Omega_x = 1.10 \times 10^{13}$ s^{-1}, $\Omega_y = 0.80 \times 10^{13}$ s^{-1}, $\mu = 5 \times 10^{-14}$ erg, $\theta = \pi/3$, $\varphi = \pi/4$.

In the case of a quantum wire the monotonic and oscillating parts are

$$S_{\text{mon}}^{\text{wire}} = \frac{2\pi^2 k_B^2 T}{3e\mu}, \tag{8}$$

$$S_{\text{osc}}^{\text{wire}} = \frac{4\pi^4 k_B^3 T^2}{3e\mu^2} \sum_{n=1}^{\infty} (-1)^n n \left[\frac{\omega_2}{\omega_1} \frac{\sin(2\pi n\mu/\hbar\omega_1)}{\sinh(2\pi^2 n k_B T/\hbar\omega_1)\sin(\pi n\omega_2/\omega_1)} + \frac{\omega_1}{\omega_2} \frac{\sin(2\pi n\mu/\hbar\omega_2)}{\sinh(2\pi^2 n k_B T/\hbar\omega_2)\sin(\pi n\omega_1/\omega_2)} \right]. \tag{9}$$

In the case of a quantum constriction, we have

$$S_{\text{mon}}^{\text{cons}} = \frac{2\pi^2 k_B^2 T}{3e(\mu - V_0)} \tag{10}$$

$$S_{\text{osc}}^{\text{cons}} = \frac{4\pi^5 k_B^3 T^2 \omega_3}{3e(\mu - V_0)^2} \sum_{n=1}^{\infty} (-1)^n n^2 \times \left[\frac{\omega_2}{\omega_1^2} \frac{\sin[2\pi n(\mu - V_0)/\hbar\omega_1]}{\sinh(2\pi^2 n k_B T/\hbar\omega_1)\sinh(\pi n\omega_3/\omega_1)\sin(\pi n\omega_2/\omega_1)} + \frac{\omega_1}{\omega_2^2} \frac{\sin[2\pi n(\mu - V_0)/\hbar\omega_2]}{\sinh(2\pi^2 n k_B T/\hbar\omega_2)\sinh(\pi n\omega_3/\omega_2)\sin(\pi n\omega_1/\omega_2)} \right]; \tag{11}$$

here, the characteristic frequency ω_3 was found in [15]. It is clear from (10) and (11) that there exists a limiting transition from a quantum constriction to a quantum wire if we assume $V_0 = 0$ and $\omega_3 \to 0$.

We can see from figure 1 that the thermopower of a quantum wire is a monotonic function of the temperature and depends strongly on the magnetic field. However, the thermopower is linearly temperature dependent at higher temperatures (more than 5 K). There is an analogous dependence in the case of a 2D quantum channel [19] and a 3D quantum constriction.

It follows from (9) and (11) that the oscillating part of the thermopower is a sum of two terms with periods $\Delta\mu = \hbar\omega_1$ and $\Delta\mu = \hbar\omega_2$, (figure 2). In the case of quantum constrictions, the periods of oscillations are the same as in the case of the wire. Note here that the positions of resonance peaks correspond to thresholds of conductance quantization. This is due to the opening of a new channel for conduction.

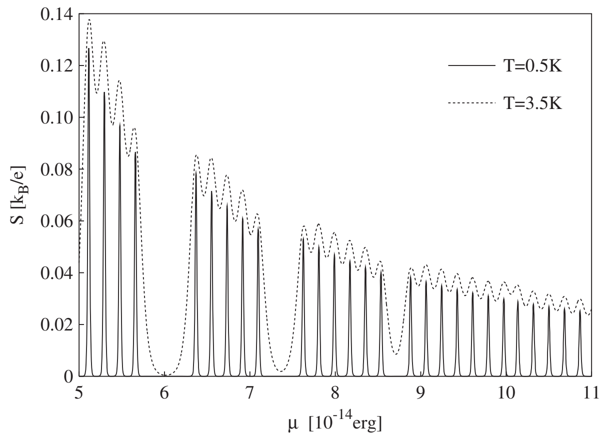

Figure 2. Oscillations of the thermopower as a function of the chemical potential: $\Omega_x = 1.35 \times 10^{13}$ s^{-1}, $\Omega_y = 1.20 \times 10^{13}$ s^{-1}, $B = 0.4$ T, $\theta = \pi/4$, $\varphi = \pi/3$.

Below, we consider only the case of the quantum wire because the behaviour of the thermopower of the quantum constriction as a function of a magnetic field is analogous to the behaviour of the thermopower of the quantum wire.

The dependence of the thermopower on the magnetic field is stipulated by the relationship between magnetic and size quantization. Let us consider below two most important cases: the magnetic field parallel to the wire symmetry axis and the magnetic field perpendicular to the wire symmetry axis.

2.1. Parallel field

In this case the frequencies $\omega_{1,2}$ are determined by the formulae

$$\omega_{1,2} = \frac{1}{2}\left\{\left[(\Omega_x + \Omega_y)^2 + \omega_c^2\right]^{1/2} \pm \left[(\Omega_x - \Omega_y)^2 + \omega_c^2\right]^{1/2}\right\}. \tag{12}$$

It is interesting to consider two cases: strong size quantization $\omega_c \ll \Omega_{x,y}$ and strong magnetic quantization $\omega_c \gg \Omega_{x,y}$.

In the first case we will study the two significant points: a symmetrical cross-section ($\Omega_x = \Omega_y = \Omega$) and a strongly asymmetrical cross-section.

For the symmetrical wire

$$\omega_{1,2} = \frac{1}{2}\left[\left(4\Omega^2 + \omega_c^2\right)^{1/2} \pm \omega_c\right]; \tag{13}$$

it is convenient to expand $\omega_{1,2}$ in terms of ω_c/Ω:

$$\omega_{1,2} \simeq \Omega \pm \frac{\omega_c}{2}. \tag{14}$$

This gives the following simple expression for S_{osc}^{wire}:

$$S_{osc}^{wire} = \frac{8k_B^3\pi^4T^2}{3e\mu^2}\sum_{n=1}^{\infty}\frac{n\cos(2\pi n\mu/\hbar\Omega)\sin(\pi n\mu\omega_c/\hbar\Omega^2)}{\sinh(2\pi^2 nk_BT/\hbar\Omega)\sin(\pi n\omega_c/\Omega)}. \tag{15}$$

It can be seen from relation (15) that in the symmetrical case the thermopower is periodic in the magnetic field (Aharonov–Bohm oscillations) with period

$$\Delta B = \frac{2m^*c\hbar\Omega^2}{e\mu}. \tag{16}$$

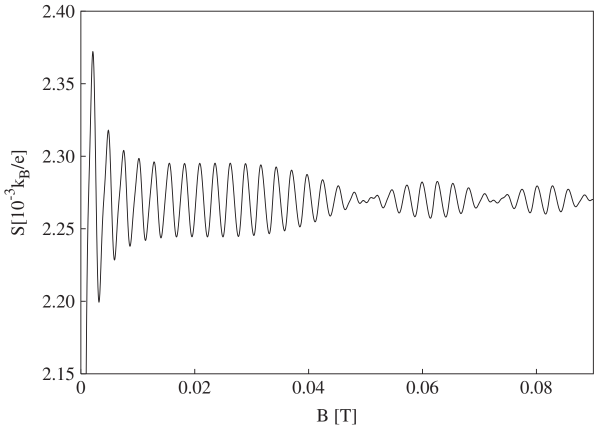

Figure 3. Thermopower of a symmetrical wire as a function of a magnetic field B: $\Omega = 1.5 \times 10^{12}$ s^{-1}, $\theta = 0$, $\mu = 6 \times 10^{-13}$ erg, $T = 1.5$ K.

Note that the weak dependence of the Fourier coefficients on the magnetic field does not destroy the oscillations; it only modulates their amplitude (figure 3).

In the strongly asymmetrical case ($\omega_c \ll \Omega_{x,y}$ and $\omega_c \ll \Omega_x - \Omega_y$, $\Omega_x > \Omega_y$),

$$\omega_1 \simeq \Omega_x \left[1 + \frac{\omega_c^2}{2(\Omega_x^2 - \Omega_y^2)}\right], \qquad \omega_2 \simeq \Omega_y \left[1 - \frac{\omega_c^2}{2(\Omega_x^2 - \Omega_y^2)}\right]. \tag{17}$$

In this case, the expression for the oscillating part of the thermopower is the sum of two terms periodic in B^2 with periods

$$\Delta_j(B^2) = \frac{2m^{*2}c^2\hbar\Omega_j(\Omega_x^2 - \Omega_y^2)}{e^2\mu}, \qquad j = x, y. \tag{18}$$

It should be noted that, in the case $\Omega_x \gg \Omega_y$, the first oscillating term in equation (9) is considerably larger then the second term, and $\Delta_x(B^2) \gg \Delta_y(B^2)$. If the frequencies Ω_x and Ω_y are close, the magnetic-field-induced oscillations of the thermopower have the form of beats (figure 4).

In the case of a strong magnetic quantization, the frequencies ω_1 and ω_2 can be presented in the form

$$\omega_1 = \omega_c \left[1 + \mathrm{o}\left(\frac{\Omega_x^2 + \Omega_y^2}{\omega_c^2}\right)\right], \qquad \omega_2 = \frac{\Omega_x \Omega_y}{\omega_c} + \omega_c \mathrm{o}\left(\frac{\Omega_x\Omega_y}{\omega_c^2}\right)^2. \tag{19}$$

In this case the major contribution in the thermopower gives the first term (9) (figure 5) with a period

$$\Delta\left(\frac{1}{B}\right) = \frac{e\hbar}{m^* c\mu}. \tag{20}$$

That is because of the large denominator $\sinh(2\pi^2 n k_B T \omega_c / \hbar\Omega_x\Omega_y)$ in the second term. The second term (9) creates a fine structure of oscillations of the thermopower in strong fields with the period of the Aharonov–Bohm oscillations

$$\Delta B = \frac{m^* c\hbar\Omega_x\Omega_y}{e\mu}. \tag{21}$$

The fine structure of the Shubnikov–de Haas oscillations depicted in figure 5 is plotted in figure 6. The Aharonov–Bohm oscillations can be observed only at the very low temperatures

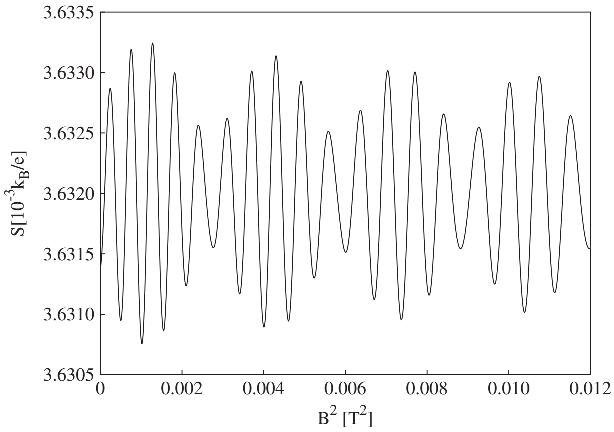

Figure 4. Thermopower as a function of B^2: $\Omega_x = 2.00 \times 10^{12}$ s^{-1}, $\Omega_y = 1.71 \times 10^{12}$ s^{-1}, $\theta = 0$, $\mu = 1 \times 10^{-12}$ erg, $T = 4$ K.

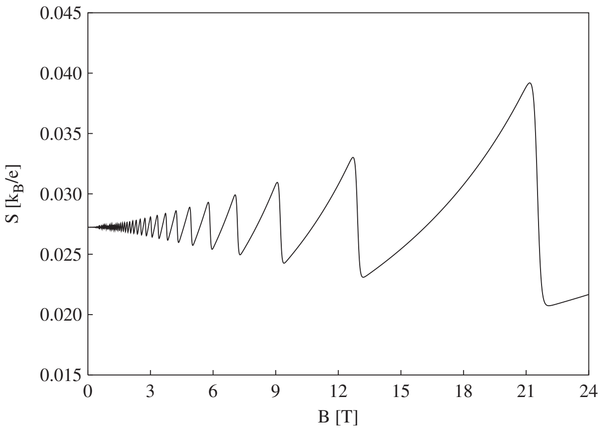

Figure 5. Thermopower as a function of a magnetic field B: $\Omega_x = 1.2 \times 10^{12}$ s^{-1}, $\Omega_y = 0.8 \times 10^{12}$ s^{-1}, $\theta = 0$, $\mu = 1 \times 10^{-13}$ erg, $T = 3$ K.

($<$1 K) because the amplitude of the Aharonov–Bohm oscillations is much less than the amplitude of the Shubnikov–de Haas oscillations and decreases rapidly upon heating.

2.2. Perpendicular field

In this case the frequencies $\omega_{1,2}$ are determined by the formulae ($\boldsymbol{B} \parallel \mathrm{O}x$)

$$\omega_1 = \sqrt{\Omega_y^2 + \omega_c^2}, \qquad \omega_2 = \Omega_x. \tag{22}$$

It follows from (22) that ω_2 does not depend on a magnetic field. Hence the second term (9) practically does not oscillate as the magnetic field varies because of the weak dependence of the Fourier coefficients on the magnetic field.

Let us consider two cases: strong size quantization $\omega_c \ll \Omega_{x,y}$ and strong magnetic quantization $\omega_c \gg \Omega_{x,y}$.

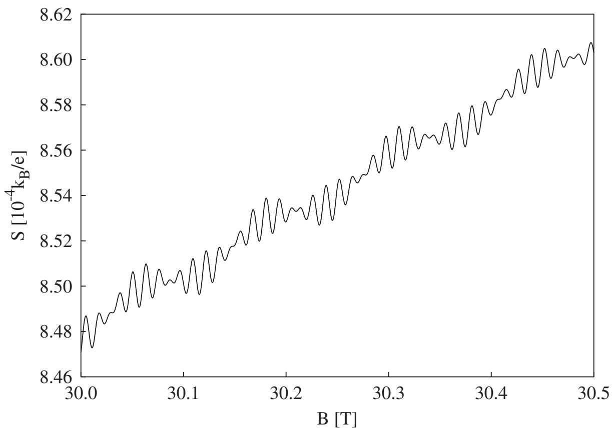

Figure 6. Thermopower as a function of a magnetic field B: $\Omega_x = 3.90 \times 10^{12}\ \mathrm{s}^{-1}$, $\Omega_y = 1.73 \times 10^{12}\ \mathrm{s}^{-1}$, $\mu = 3 \times 10^{-13}$ erg, $\theta = 0$, $T = 0.3$ K.

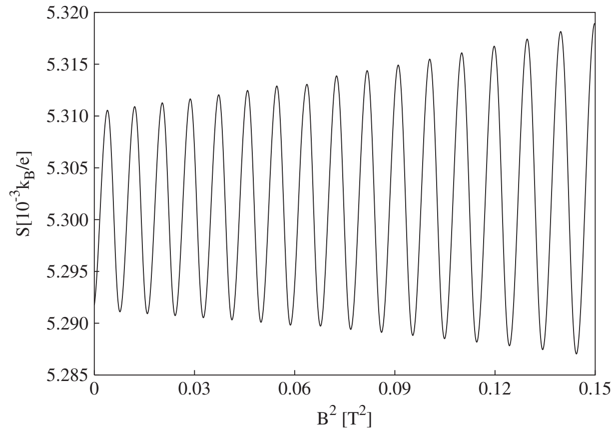

Figure 7. Thermopower as a function of B^2: $\Omega_x = 3.5 \times 10^{12}\ \mathrm{s}^{-1}$, $\Omega_y = 2.7 \times 10^{12}\ \mathrm{s}^{-1}$, $\mu = 6 \times 10^{-13}$ erg, $\theta = \pi/2$, $\varphi = 0$, $T = 3.5$ K.

In the case of strong size quantization, from (22) we get

$$\omega_1 = \Omega_y \left[1 + \frac{1}{2} \left(\frac{\omega_c}{\Omega_y} \right)^2 \right]. \tag{23}$$

It is clear that in this case the thermopower is a periodic function with respect to B^2 (figure 7) with the period

$$\Delta B^2 = \frac{2\hbar m^{*2} c^2 \Omega_y^3}{\mu e^2}. \tag{24}$$

In the case of a strong magnetic quantization $\omega_1 = \omega_c$ and the thermopower oscillates with the period of the Shubnikov–de Haas oscillations (20) but, in contrast to the case for the parallel field, without a fine structure.

Note now that in view of the complexity of the analytic dependence of the thermopower on the azimuthal θ and polar φ angles of the direction of a magnetic field (that is conditioned

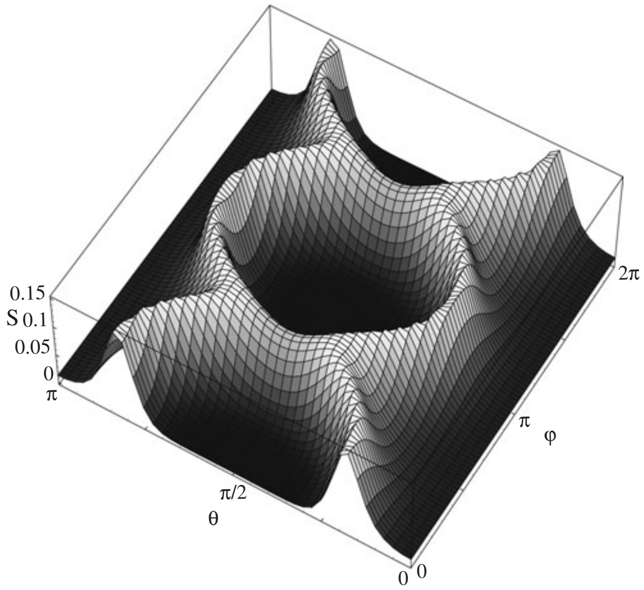

Figure 8. Thermopower of the quantum wire (in units of k_B/e) as a function of azimuthal θ and polar φ angles: $\Omega_x = 1.80 \times 10^{13}$ s^{-1}, $\Omega_y = 1.10 \times 10^{13}$ s^{-1}, $\mu = 5 \times 10^{-14}$ erg, $B = 1.7$ T, $T = 3$ K.

by the complexity of the dependence of the $\omega_{1,2}$ on θ and φ), a detailed analysis requires numerical studies. Numerical analysis shows that the thermopower strongly depends on the direction of a magnetic field (figure 8).

3. Conclusions

We have studied theoretically the thermopower of the anisotropic quantum wires and constrictions placed in an arbitrarily directed magnetic field. We have shown that the oscillating part of the thermopower as a function of a chemical potential is the sum of two terms with periods $\Delta\mu = \hbar\omega_1$ and $\hbar\omega_2$.

The behaviour of the thermopower as a function of a magnetic field strongly depends on the relation between the characteristic frequencies of the parabolic confinement potential and on the magnetic field.

In the case of a parallel field and symmetrical cross-section of the wire the thermopower undergoes Aharonov–Bohm oscillations with modulated amplitude. In the case of a strong magnetic quantization for an asymmetric wire, the magnetic field dependence of the thermopower has the form of Shubnikov–de Haas oscillations with a fine structure determined by the Aharonov–Bohm oscillations. In the opposite case of a strong size quantization, the magnetic field dependence of the thermopower is a superposition of two oscillatory terms periodic in the squared magnetic field. Note that when Ω_x is of the same order of magnitude as Ω_y, oscillations have the form of the beats. Let us remark that the period of the Aharonov–Bohm oscillations in the weak fields (16) is equal to two periods in the strong fields (21).

In the case of a perpendicular field and strong magnetic quantization the thermopower undergoes Shubnikov–de Haas oscillations. In the opposite case of strong size quantization the thermopower is a periodic function with respect to B^2.

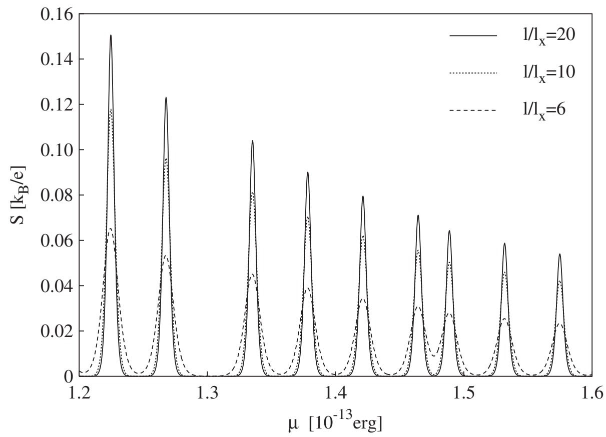

Figure 9. Oscillations of thermopower of the constriction as a function of the chemical potential: $\Omega_x = 1.8 \times 10^{13}$ s^{-1}, $\Omega_y = 1.5 \times 10^{13}$ s^{-1}, $V_0 = 0.7 \times 10^{-13}$ erg, $B = 1.2$ T, $\theta = \pi/6$, $\varphi = \pi/3$, $T = 1$ K.

In the case of a symmetrical wire the expression for the frequencies $\omega_{1,2}$ has the form

$$\omega_{1,2} = \frac{1}{2}\left[\left(\omega_c^2 + 2\Omega^2 + 2\Omega\sqrt{\Omega^2 + \omega_c^2 - \omega_z^2}\right)^{1/2} \pm \left(\omega_c^2 + 2\Omega^2 - 2\Omega\sqrt{\Omega^2 + \omega_c^2 - \omega_z^2}\right)^{1/2}\right]. \tag{25}$$

In this case $\omega_{1,2}$ does not depend on the polar angle and, consequently, the thermopower also does not depend on this angle. This can be used as a test for defining the deviation of the cross-section form from the circular one.

Note, in conclusion, that the length of the constriction has an essential effect on the thermopower (figure 9). In particular, the amplitude of the oscillations of the thermopower grows less with decreasing effective length. Note the increased smearing of the peaks due to the more significant role of tunnelling effects in the shorter constrictions.

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