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# Thermopower of two-dimensional channels and quantum point contacts in a magnetic field

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#### Abstract

The thermopower of two-dimensional parabolic quantum wires and quantum contacts in magnetic field is investigated. We obtain a convenient analytic formula for the thermopower of these structures. The temperature dependence of the thermopower is studied and the influence of the magnetic field on the thermopower is examined. Oscillations in the thermopower are investigated.

#### 1. Introduction

The purpose of the present work is to analyse thermoelectric transport in two-dimensional (2D) quantum channels and contacts placed in a magnetic field. Investigation of the thermoelectric properties of nanodevices is of utmost importance for providing fundamental information about electron properties which is not available from ballistic transport measurements alone. In connection with this, studies of the thermopower in quantum channels and quantum point contacts have received considerable attention in recent years. In particular, the thermopower of a quantum point contact was theoretically investigated in [1–3]. Measurements of the thermopower in quantum contacts were recently made in [4–6]. It was shown that experimental results are in good agreement with theoretical ones obtained using equation (1) (below). Indirect confirmation of equation (1) for a 2D quantum channel was made in [7]. A general formalism for thermoelectric transport in the case of microstructures with any number of terminals was developed in [8].

We consider a system which consists of two bulk reservoirs connected by a 2D channel or quantum contact. A bias voltage is applied between the reservoirs, which are kept at different temperatures. In this case the relationship between the thermopower and the ballistic conductance G is given in the linear-response approximation by the Cutler–Mott formula [9] which for ballistic transport has the form [10, 11]

$$S = -\frac{\pi^2 k_B^2 T}{3e} \frac{\partial \ln G}{\partial \mu} \tag{1}$$

where  $\mu$  is the chemical potential.

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It is well known that the conductance of the two-dimensional quantum channels and point contacts is a step-like function of the chemical potential. The steps in the conductance between the quantized value lead to peaks in the thermopower. As a rule, this phenomenon has been investigated using numerical methods. Equation (1) is inconvenient for the analysis because it contains a logarithm of a series. In view of this, it is quite important to obtain convenient formulae for analytic and numerical investigations of the thermopower. In this work we derive analytic expressions for the thermopower of quantum channels and quantum point contacts in a perpendicular magnetic field using an expansion the thermopower into a Fourier series and extracting the monotonic and oscillating parts of S. This allows us obtain convenient formulae for analytic investigation of the thermopower. We show that the thermopower has an oscillatory dependence on the magnetic field and the chemical potential. Periods of the oscillations are found and the temperature dependence is investigated in detail.

#### 2. Conductance of a 2D quantum channel

We model the confinement of the quantum channel with the help of a parabolic potential. This potential is widely used for studying the physical properties of quantum channels [12, 13]. The spectrum of electrons in a 2D quantum channel in a perpendicular magnetic field is [12]

$$\varepsilon_{np} = \hbar\omega \left( n + \frac{1}{2} \right) + \frac{p^2}{2m^*},\tag{2}$$

where  $\omega = \sqrt{\omega_0^2 + \omega_c^2}$ ,  $\omega_0$  is the characteristic frequency of the parabolic potential,  $\omega_c$  is the cyclotron frequency, p is the momentum in the direction of the channel axis,  $m^*$  is the effective electron mass and n = 0, 1, 2, ...

In order to calculate the thermopower (1) it is necessary, first of all, to obtain a convenient formula for the conductance of the quantum channel. Using the Landauer–Büttiker formalism for ballistic transport [14, 15] we can write the following equation for the conductance of the 2D quantum channel

$$\frac{G}{G_0} = \int_0^\infty G(\varepsilon, 0) \frac{\partial f}{\partial \mu} \,\mathrm{d}\varepsilon,\tag{3}$$

where  $G_0$  is the conductance quantum, f is the Fermi function and  $G(\varepsilon, 0)$  is the conductance of the quantum channel (in units of  $G_0$ ) at the temperature T = 0. Note that at T = 0 the conductance (in units of  $G_0$ ) is equal to the number of states  $\nu(\varepsilon)$  with an energy less than or equal to  $\varepsilon$ . Then we can express the number of states  $\nu(\varepsilon)$  in terms of the classical partition function Z [16]

$$\nu(\varepsilon) = \frac{1}{2\pi i} \int_{\alpha - i\infty}^{\alpha + i\infty} Z(\xi) e^{\varepsilon \xi} \frac{d\xi}{\xi}.$$
(4)

Here  $\alpha > 0, \xi = 1/T$ , and the function Z has the form

$$Z^{-1} = 2\sinh\left(\frac{\hbar\omega}{2T}\right).$$
(5)

It follows that  $v(\varepsilon)$  is determined by the simple poles  $\xi = 2\pi ni/\hbar\omega$  of the integrand in equation (4), lying on the imaginary axis, and by a double pole at zero. Closing the contour in the left half-plane we reduce the considered integral to the sum of the residues in the poles

$$G(\varepsilon, 0) = \nu(\varepsilon) = \frac{\varepsilon}{\hbar\omega} + \frac{1}{\pi} \sum_{n=1}^{\infty} (-1)^n \frac{\sin(2\pi n\varepsilon/\hbar\omega)}{n}.$$
 (6)

Substituting equation (6) into equation (3) and using a formula that is similar to equation (4) [17]

$$\frac{1}{1 + \exp(x)} = \frac{1}{2i} \int_{\alpha - i\infty}^{\alpha + i\infty} \frac{\exp(-qx) \,\mathrm{d}q}{\sin(\pi q)},\tag{7}$$

we obtain the formula for the conductance at  $T \neq 0$  extracting the monotonic  $G_{mon}$  and oscillating  $G_{osc}$  parts

$$G = G_{mon} + G_{osc}.$$
 (8)

Here

$$\frac{G_{mon}}{G_0} = \frac{\mu}{\hbar\omega} \tag{9}$$

and

$$\frac{G_{osc}}{G_0} = \frac{2\pi T}{\hbar\omega} \sum_{n=1}^{\infty} (-1)^n \frac{\sin(2\pi n\mu/\hbar\omega)}{\sinh(2\pi^2 nT/\hbar\omega)}.$$
(10)

Note that we have obtained equation (8) integrating in (3) with respect to  $\varepsilon$  and then with respect to q reducing the last integral to the sum of residues in the simple poles q = -n, and  $\pm i2\pi nT/\hbar\omega$ .

It follows from equation (8) that the height of the conductance steps is equal to the conductance quantum  $G_0$ . The width of a conductance plateau is  $\hbar\omega$ . As one can see, the monotonic part of the conductance is a linear function of the chemical potential. The Fourier series in equation (10) gives the oscillating part of the conductance. It is clear that the Fourier series depends on the fractional part of the expression  $\mu/\varepsilon$ . Therefore, the oscillating part of the conductance as a function of  $\mu$  has the period  $\hbar\omega$ . The conductance steps are stipulated by the sum of a linear monotonic function and a saw-tooth oscillator function. Note that at  $T \neq 0$  the contribution of higher harmonics in  $G_{osc}$  is suppressed by factors  $\sinh(2\pi^2 n T/\hbar\omega)$ . This leads to a substantial smearing of the saw-tooth oscillations on the plot  $G_{osc}$  and, in its turn, to a substantial smearing of steps of the conductance quantization and to an inclination of plateaus on the plot of  $G(\mu)$  even at relatively low temperature. Using equations (9) and (10), it is possible to estimate the ratio of the monotonic part of the conductance to the oscillating one:

$$\frac{G_{osc}}{G_{mon}} \simeq \frac{\hbar\omega}{\mu}.$$
(11)

This circumstance allows us to simplify formula (1) for the thermopower.

#### 3. Thermopower of a 2D quantum channel

Taking into account the estimation  $G_{osc}/G_{mon} \ll 1$  we can rewrite the initial formula (1) for the thermopower in the form

$$S = \frac{k_B^2 \pi^2 T}{3e} \frac{1}{G_{mon}} \left( \frac{\partial G_{mon}}{\partial \mu} + \frac{\partial G_{osc}}{\partial \mu} \right) + O\left(\frac{\hbar\omega}{\mu}\right).$$
(12)

We stress that formula (12) is more convenient for studying the thermopower than the starting expression (1). Equation (12) lets us study the oscillation and temperature dependence of the thermopower in detail.

Calculating the partial derivatives in (12), we get S in the form

$$S = S_{mon} + S_{osc}.$$
(13)



Figure 1. Oscillations of thermopower as a function of the chemical potential:  $T = 4 \text{ K}, B = 1.2 \text{ T}, \omega_0 = 5.1 \times 10^{12} \text{ s}^{-1}.$ 

Here

$$S_{mon} = \frac{k_B^2 \pi^2}{3e} \frac{T}{\mu} \tag{14}$$

and

$$S_{osc} = \frac{k_B^2 \pi^2}{3e} \frac{2\pi^2 T^2}{\mu \hbar \omega} \sum_{n=1}^{\infty} (-1)^n \frac{n \cos(2\pi n \mu/\hbar \omega)}{\sinh(2\pi^2 n T/\hbar \omega)}.$$
(15)

Thus, the expression for the thermopower splits into two terms: monotonic and oscillating. The first of them has an inverse dependence and the second an oscillatory dependence on the chemical potential with a period  $\hbar\omega$ . The onset of each oscillation in the thermopower is due to the opening of a new channel for conduction. Hence, positions of resonance peaks correspond to thresholds of conductance quantization, namely the peaks arise at the points in which  $\mu/\hbar\omega - 1/2$  is the integer. Note that the peak value varies with  $1/\mu$  (figure 1).

Let us consider the temperature dependence of the thermopower. It follows from figure 2 that the behaviour of the thermopower as a function of the temperature depends strongly on the magnetic field. It is interesting to analyse the temperature dependence of the peak value of the thermopower. This was obtained by Streda [11] for the case of a 2D quantum channel in the absence of a magnetic field that the peak value of the thermopower is temperature independent at very low temperatures and acquires the value

$$S^{max} = \frac{k_B}{e} \frac{\ln 2}{i+1/2} \simeq -\frac{60}{i+1/2},\tag{16}$$

where i is the number of the occupied subbands. Note that equation (16) holds true for our case, too.

However, the peak value of the thermopower is linearly temperature dependent at higher temperatures (figure 3). Note that in contrast to the conductance quantization the temperature has a weak influence on the thermopower. This circumstance gives more favourable experimental conditions for studying the quantum channels.

The dependence of the thermopower on the magnetic filed is conditioned by the relationship between magnetic and size quantization. In the case of strong size quantization  $(\omega_0 \gg \omega_c)$  the thermopower is a monotonic function of *B* (figure 4). In the opposite case



Figure 2. Thermopower as a function of the temperature:  $\mu = 1.2 \times 10^{-13}$  erg,  $\omega = 3.4 \times 10^{12}$  s<sup>-1</sup>. (1) B = 1.497 T, (2) B = 1.61 T, (3) B = 2.1 T.



Figure 3. Thermopower as a function of the temperature:  $\mu = 1.1 \times 10^{-13}$  erg,  $\mu/\hbar\omega - 1/2 = 94$ .

 $(\omega_0 \ll \omega_c)$  the thermopower undergoes Shubnikov–de Haas oscillations (figure 5) with the period

$$\Delta \frac{1}{B} = \frac{e\hbar}{m^* c\mu}.\tag{17}$$

Note that the amplitude of the oscillation peaks is a linear function of magnetic field (figure 5).

The width of the channel has an important effect on the thermopower. In particular, the period of oscillations of the thermopower  $\hbar\omega$  grows less with increasing effective width of the channel, in proportion to  $l_{eff}^2$  ( $l_{eff} = \sqrt{\hbar/m^*\omega}$ ). Note that the thermopower undergoes oscillations as a function of the effective width of the channel (figure 6). The period of the oscillations depends strongly on the relation between the size and magnetic quantization.

### 4. Thermopower of a 2D quantum point contact

In this section we shall consider the thermoelectric properties of a 2D quantum point contact placed in a perpendicular magnetic field. In the saddle point model [18, 19], the geometric confinement potential is expressed in the form

$$V(x, y) = V_0 + \frac{m^* \omega_y^2}{2} y^2 - \frac{m^* \omega_x^2}{2} x^2,$$
(18)



Figure 4. Thermopower as a function of the magnetic field: T = 2 K,  $\mu = 4.2 \times 10^{-13}$  erg,  $\omega_0 = 5.3 \times 10^{13}$  s<sup>-1</sup> (strong size quantization case).



**Figure 5.** Thermopower as a function of the magnetic field: T = 4 K,  $\mu = 1.235 \times 10^{-13}$  erg,  $\omega_0 = 1.1 \times 10^{12}$  s<sup>-1</sup> (strong magnetic quantization case).



Figure 6. Thermopower as a function of the effective length: T=2 K, B=10 T,  $\mu=4\times 10^{-13}$  erg.

where  $V_0$  is the potential at the saddle point. In distinction from the case of the quantum channel considered in the preceding section, the conductance of a quantum point contact is

given by the generalized Landauer–Büttiker formula

$$\frac{G(T=0)}{G_0} = \sum_{n=0}^{\infty} [1 + \exp(-2\pi\varepsilon_n)]^{-1}.$$
(19)

Here  $\varepsilon_n = (E - V_0 - E_n)/\hbar\omega_2$ , *E* is the total electron energy,  $E_n = \hbar\omega_1(n + 1/2)$  is the discrete component of the electron spectrum and  $\omega_x$ ,  $\omega_y$  are the characteristic frequencies of the saddle point potential [18]:

$$\omega_1^2 = \frac{1}{2} \left( \Omega^2 + \sqrt{4\omega_x^2 \omega_y^2 + \Omega^4} \right),\tag{20}$$

$$\omega_2^2 = \frac{1}{2} \left( -\Omega^2 + \sqrt{4\omega_x^2 \omega_y^2 + \Omega^4} \right),\tag{21}$$

where  $\Omega = \sqrt{\omega_c^2 + \omega_y^2 - \omega_x^2}$ .

Note that equations (20), (21) were obtained in [18] using the method of Bogolubov canonical transformations. However, it is easy to obtain these formulae using only simple methods of linear algebra with the help of canonical transformation of the phase space from analogy with [20].

A comparison between the terms in brackets in (19) and the Fermi distribution shows that the value  $\hbar \omega_2/2\pi$  plays the same role as the temperature in the Fermi distribution, i.e. it smears the threshold electron energy.

Using equation (7), one can obtain a convenient formula for the conductance at zero temperature:

$$G(\varepsilon, 0) = \frac{E - V_0}{\hbar\omega_1} + \frac{1}{2} \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\exp[-2\pi (E - V_0)k/\hbar\omega_2]}{\sinh(\pi k\omega_1/\omega_2)} + \frac{\omega_2}{\omega_1} \sum_{k=1}^{\infty} (-1)^k \frac{\sin[2\pi (E - V_0)k/\hbar\omega_1]}{\sinh(\pi k\omega_2/\omega_1)}.$$
(22)

In order to find the temperature dependence of the conductance we use the approach developed in the preceding section. Taking into account the estimation  $\mu \gg T$ , we obtain the formula for the conductance at  $T \neq 0$  extracting the monotonic  $G_{mon}$  and oscillating  $G_{osc}$  parts

$$G = G_{mon} + G_{osc}.$$
 (23)

Here

$$\frac{G_{mon}}{G_0} = \frac{\mu - V_0}{\hbar\omega_1} \tag{24}$$

and

$$\frac{G_{osc}}{G_0} = 2\pi^2 \frac{T}{\hbar\omega_1} \frac{\omega_2}{\omega_1} \sum_{k=1}^{\infty} (-1)^k \frac{\sin[2\pi k(\mu - V_0)/\hbar\omega_1]}{\sinh(2\pi^2 kT/\hbar\omega_1)\sinh(\pi k\omega_2/\omega_1)}.$$
 (25)

It follows from equation (25) that the oscillating component of the conductance  $G_{osc}$  has maxima at the points where  $\mu - V_0 = \hbar \omega_1 (n + 1/2)$  that correspond to the thresholds of the conductance steps. The monotonic part of the conductance is a linear function of the chemical potential. It should be noted that the smoothing of the oscillation peaks in equation (25) is determined by the product of two factors,  $\sinh(2\pi^2 kT/\hbar\omega_1)$  and  $\sinh(\pi k\omega_2/\omega_1)$ , each influencing the profile of the oscillation. As was pointed out in [17], an increase in the first factor with temperature may be compensated by the smallness of the second factor to such an extent that quantization of the conductance can also be observed at fairly high temperatures.

Using equation (12), we get the thermopower of the quantum contact S in the form

$$S = S_{mon} + S_{osc}.$$
 (26)

Here

$$S_{mon} = \frac{k_B^2 \pi^2}{3e} \frac{T}{\mu - V_0}$$
(27)

and

$$S_{osc} = \frac{k_B^2 \pi^2}{3e} \frac{4\pi^3 T^2 \omega_2}{(\mu - V_0)\hbar\omega_1^2} \sum_{k=1}^{\infty} (-1)^k \frac{k \cos[2\pi n(\mu - V_0)/\hbar\omega_1]}{\sinh(2\pi^2 k T/\hbar\omega_1) \sinh(\pi k \omega_2/\omega_1)}.$$
 (28)

It follows from equations (26)–(28) that the behaviour of the thermopower of the quantum contact as a function of the chemical potential and temperature is analogous to the behaviour of the thermopower of the quantum channel. The dependence of the thermopower on the magnetic field is more difficult in this case and is conditioned by the relationship between magnetic and size quantization.

### 5. Conclusions

We have studied the conductance and the thermopower of a 2D parabolic quantum channel and quantum point contact placed in a magnetic field. We have shown that the thermopower of the channels and contacts undergoes oscillations as a function of chemical potential and of magnetic field. The amplitudes and periods of the oscillation have been found. It is shown that the amplitude of the oscillations is temperature independent at very low temperatures and linearly temperature dependent at higher temperatures. In the case of strong size quantization the thermopower of the quantum channel is a monotonic function of the magnetic field. It is shown that in the case of quantum point contact the value  $\hbar\omega_2/2\pi$  plays exactly the same role as the temperature.

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