Thermopower oscillations of a quantum-point contact

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(Received 30 October 1990; revised manuscript received 25 March 1991)

Oscillations in the thermopower of a quantum-point constriction in the absence and presence of a magnetic field are discussed.

In addition to the quantized conductance steps discovered by van Wees *et al.*[1] and Wharam *et al.*[2] in split-gate constrictions of a two-dimensional electron gas (2DEG), Molenkamp *et al.*[3] reported very recently on oscillations in the transverse voltage of a conducting channel in a high-mobility 2DEG. They related these oscillations to the thermopower of a quantum-point contact.

On the theoretical side, while the electrical properties of quantum-point contacts have received wide interest,[4–14] much less attention has been paid so far to the analysis of the thermal and thermoelectric properties of such systems.[15–17]

Streda,[16] using an approach that goes back to work by Sivan and Imry,[15] outlines a calculation of the thermopower oscillations of a ballistic quantum-point contact as the number of one-dimensional subbands at the point contact is changed. He assumes a transverse parabolic confining potential, a longitudinal transmission coefficient through the constriction that is a step function of energy, and zero magnetic field.

However, as pointed out by Büttiker,[14] since constrictions in the experiments are usually electrostatically induced, with a pair of split gates, the confining potential must be a smooth function of the coordinates in every direction, and consequently the bottleneck of the constriction forms a saddle.

The aim of the present work is to analyze the thermopower of a quantum-point contact for the realistic case of a saddle-point constriction, give simple criteria for its observability, and study the effect of a magnetic field perpendicular to the 2DEG.

The linear response expressions for the chemical potential (μ) and temperature (Θ) dependent two-terminal conductance $G(\mu,\Theta)$ and thermopower $S(\mu,\Theta)$ for transport from one equilibrium electron reservoir to another, along a multichannel lead are given by[15]

$$G(\mu,\Theta)=\frac{2e^2}{h}\sum_i\int_0^\infty dE\left[-\frac{df}{dE}\right]T_i(E)\ , \tag{1}$$

$$\begin{aligned}S(\mu,\Theta)&=\frac{1}{e\Theta}\frac{L_1(\mu,\Theta)}{L_0(\mu,\Theta)}\\&=\frac{k_B}{e}\frac{\sum_i\int_0^\infty dE\left[-\frac{df}{dE}\right]T_i(E)\left[\frac{E-\mu}{k_B\Theta}\right]}{\sum_i\int_0^\infty dE\left[-\frac{df}{dE}\right]T_i(E)}\ ,\end{aligned} \tag{2}$$

with E_i^T being the transverse energy associated with the ith channel in the lead, T_i the transmission probability from all channels into channel i,

$$T_i=\sum_j T_{ij}\ , \tag{3}$$

f the Fermi-Dirac distribution function, and e the electronic charge ($e=-|e|$). The sum over i runs over all occupied channels. The model used for the derivation of Eqs. (1) and (2) assumes that the thermalization of electrons, by inelastic scattering, and the corresponding Joule heating occurs only in the outside reservoirs and not in the system itself.

It is already possible to make a few qualitative considerations about $G(\mu,\Theta)$ and $S(\mu,\Theta)$ from the general expressions (1) and (2), for the case of transmission about a quantum-point contact. In the case of a lead which is nonuniform along the direction of current flow (as is the case for a realistic constriction) the transmission coefficient T_i is changed by unity within a finite energy range E^L.

Accordingly a schematic drawing of the different contributions to the integrand of Eq. (2) is shown in Fig. 1.

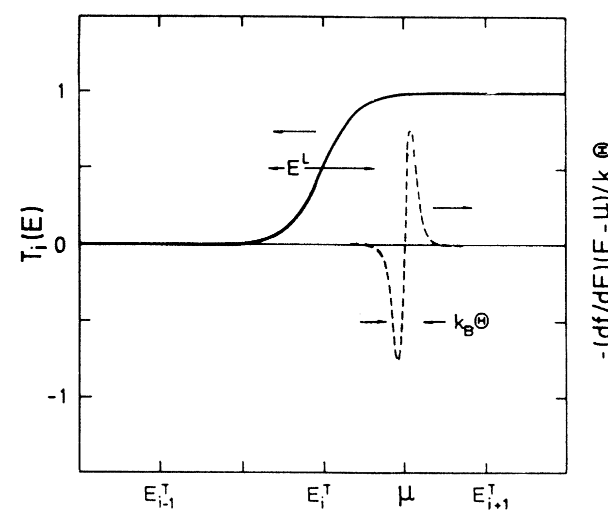

FIG. 1. Schematic drawing of the integrand in Eq. (2) which defines the thermopower.

The parameters were chosen such that $\Delta E^T > E^L > k_B\Theta$ where ΔE^T is the transverse subband splitting.

Taking into account the odd-parity character of the factor $-(df/dE)(E-\mu)/k_B\Theta$ (with respect to μ), clearly the result is essentially zero if $|\mu - E_i^T| > E^L/2$, with a maximum contribution when $\mu \simeq E_i^T$. It should be expected as a consequence that the thermopower of a quantum-point constriction will have oscillations as function of μ, with peak values when $\mu \simeq E_i^T$ and a width of E^L.

A similar analysis for the case $\Delta E^T > k_B\Theta > E^L$ gives again an oscillating thermopower as function of μ, with peak values when $\mu \simeq E_i^T$ but a width of a few $k_B\Theta$.[16]

In accordance with these considerations the condition for the observation of well-pronounced oscillations in the thermopower of a quantum-point contact is approximately given by

$$\Delta E^T > \max(E^L, k_B\Theta) . \tag{4}$$

These qualitative arguments can be put on a more firm basis in the low-limit temperature $k_B\Theta \ll E^L$. It is then permissible to expand the transmission coefficient T_i around μ, in Eqs. (1) and (2), with the following result:

$$G(\mu,0) = \frac{2e^2}{h}\sum_i T_i(\mu) , \tag{5}$$

$$S(\mu,\Theta) = \frac{k_B}{e}\frac{\pi^2}{3}(k_B\Theta)\frac{\sum_i \left.\frac{dT_i(E)}{dE}\right|_{E=\mu}}{\sum_i T_i(\mu)} \tag{6a}$$

$$= \frac{k_B}{e}\frac{\pi^2}{3}(k_B\Theta)\frac{d}{dE}[\ln G(E,0)]_{E=\mu} . \tag{6b}$$

As it is clear from Eqs. (6a) and (6b), in order to obtain a large thermopower, one needs a transmission coefficient [and consequently, according to (5), a zero-temperature electrical conductance] which varies rapidly with energy. For a transmission coefficient as represented in Fig. 1, $S(\mu,\Theta)$ will have oscillations as function of μ, with peak values when $\mu \simeq E_i^T$ given by

$$S(\mu \simeq E_i^T, \Theta) \simeq \frac{k_B}{e}\frac{\pi^2}{3}(k_B\Theta)\frac{\left.\frac{dT_i(E)}{dE}\right|_{E=E_i^T}}{i + T_i(E_i^T)} . \tag{7}$$

Two remarks are in order concerning the result given by (7).

(i) The peak value of the thermopower is linear-temperature dependent. This should be contrasted with the temperature-independent peak value obtained using a transmission coefficient that is a step-dependent function of energy.[16]

(ii) Because the thermopower is different from zero only in the transition regions between two plateaus of the transmission coefficient (see Fig. 1), and this region is particularly sensitive to the real shape of the constriction potential, no "universal" (that is, sample-independent) peak values of the thermopower should be expected.

While the discussion until now has been completely general, with no assumptions about the particular geometry of the quantum-point contact, in order to make a quantitative calculation of the thermopower of a quantum-point constriction, a model should be adopted for the transmission coefficient T_i [or equivalently, for the constriction potential $V(x,y)$].

As mentioned above, a realistic quantum-point contact may be modeled by a constriction that close to its bottleneck forms a saddle; expanding the constriction potential around its saddle point,[14]

$$V(x,y) = V_0 - \tfrac{1}{2}m\omega_x^2x^2 + \tfrac{1}{2}m\omega_y^2y^2 , \tag{8}$$

where x and y correspond to the longitudinal and transverse directions, respectively, ω_x and ω_y are convenient parametrizations of the respective curvatures, and V_0 refers to the value of the constriction potential at the saddle point.

Fortunately the quantum-mechanical problem of transmission and reflection at the constriction potential described by Eq. (8) can be exactly solved without[18] and with[19] a magnetic field (perpendicular to the x-y plane).

According to these results, the transmission probability at the saddle is given by

$$T_{ij} = \delta_{ij}\frac{1}{1+e^{-\pi\varepsilon_i}} , \tag{9}$$

where

$$\varepsilon_i = \frac{E - \Delta E^T(i+\frac{1}{2}) - V_0}{E^L} = \frac{E - E_i^T - V_0}{E^L} \tag{10}$$

and

$$\Delta E^T = \frac{\hbar}{\sqrt{2}}[(\Omega^4 + 4\omega_x^2\omega_y^2)^{1/2} + \Omega^2]^{1/2} , \tag{11}$$

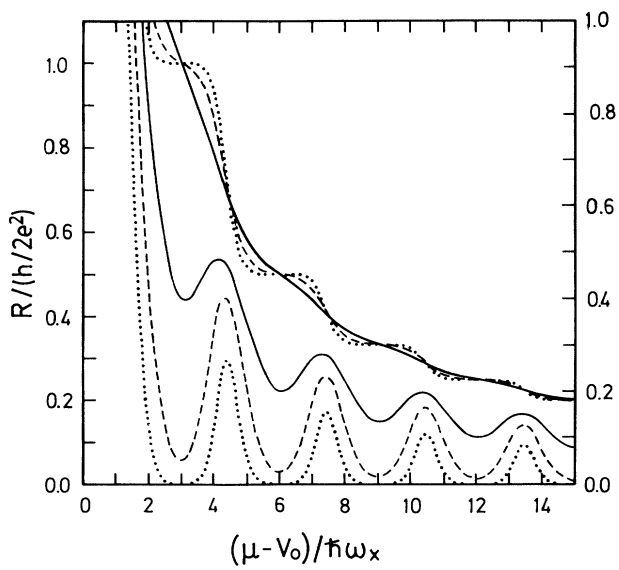

FIG. 2. Resistence (left scale) and thermopower (right scale) as function of chemical potential μ for a ratio of $\omega_y/\omega_x = 3$. Full line, $k_B\Theta/\hbar\omega_x = 0.5$; dashed line, $k_B\Theta/\hbar\omega_x = 0.25$; dotted line, $k_B\Theta/\hbar\omega_x = 0.1$.

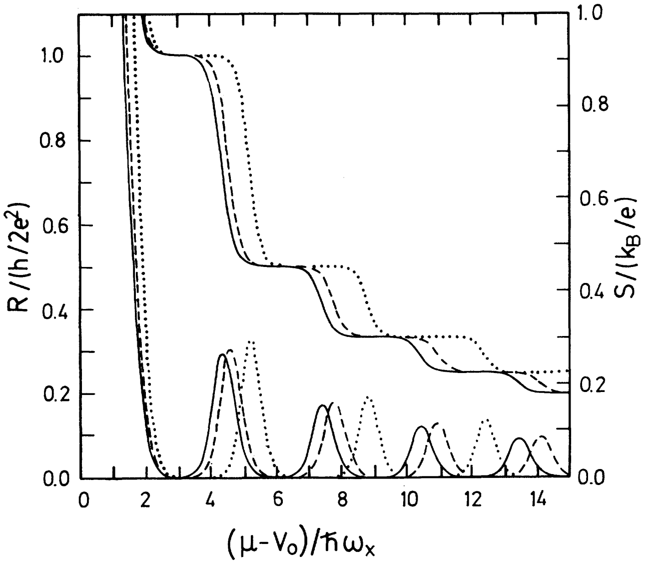

FIG. 3. Resistence (left scale) and thermopower (right scale) as function of μ, in presence of magnetic field: full line, $\omega_c/\omega_x=0$; dashed line, $\omega_c/\omega_x=1$; dotted line, $\omega_c/\omega_x=2$. The ratio $\omega_y/\omega_x=3$ and $k_B\Theta/\hbar\omega_x=0.1$.

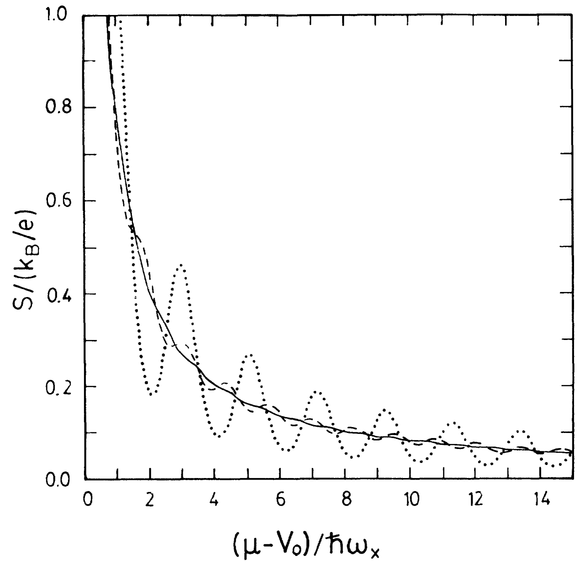

FIG. 4. Magnetic-field-induced thermopower oscillations for $\omega_y/\omega_x=1$ and $k_B\Theta/\hbar\omega_x=0.25$. Full line, $\omega_c/\omega_x=0$; dashed line, $\omega_c/\omega_x=1$; dotted line $\omega_c/\omega_x=2$.

$$E^L=\frac{1}{2}\frac{\hbar}{\sqrt{2}}[(\Omega^4+4\omega_x^2\omega_y^2)^{1/2}-\Omega^2]^{1/2}\ , \tag{12}$$

$$\Omega^2=\omega_c^2+\omega_y^2-\omega_x^2\ , \tag{13}$$

$$\omega_c=\frac{eB}{mc}\ . \tag{14}$$

In the limit of zero magnetic field $\Delta E^T\to\hbar\omega_y$ and $E^L\to\hbar\omega_x/2$, while when $\omega_c\gg\omega_x$ and ω_y, $\Delta E^T\to\hbar\omega_c$, and $E^L\to\hbar\omega_x\omega_y/2\omega_c$. Using (9)–(14) Büttiker analyzed the conditions for the occurrence of well-pronounced steps in the zero-temperature two-terminal conductance, and the accuracy of its quantization.

The numerical evaluation of Eqs. (1) and (2), with the saddle-point constriction transmission as given by (9) produces the results shown in Figs. 2–4. The two-terminal zero magnetic-field resistance (left scale) and thermopower (right scale) are shown in Fig. 2. The parameters are chosen such that condition (4) is fulfilled and consequently pronounced oscillations in the thermopower are obtained.

As already mentioned, the temperature dependence of the oscillations (width and peak value) is explained by the low-temperature expansion (6). It is interesting to point out that for the maximum temperature shown in Fig. 2 ($k_B\Theta/\hbar\omega_x=0.5$), while the resistance shows weak indication of quantization, it is still possible to have well-defined oscillations in the thermopower.

We display in Fig. 3 the dependence of the resistance and thermopower on magnetic field. As discussed previously, the onset of each oscillation in the thermopower is related to the opening of a new channel for conduction. Because ΔE^T is an increasing function of B, the oscillations spread apart for increasing values of B.

The parameters chosen in Fig. 3 correspond to a situation where already for $B=0$ the thermopower has pronounced oscillations (the essential effect of $B\neq 0$ being that of changing the distance between two successive oscillations). However, an interesting situation arises in connection with condition (4), because since ΔE^T is an increasing function of B, it is possible that $\Delta E^T(B=0)<\max(E^L,k_B\Theta)$ while $\Delta E^T(B\neq 0)>\max(E^L,k_B\Theta)$, with a crossover from a poor-oscillation regime to a well-developed oscillation regime.

Such an example of magnetic-field-induced oscillation is shown in Fig. 4. For $\omega_y=\omega_x$ and $k_B\Theta/\hbar\omega_x=0.25$ the zero-field thermopower shows only an indication of oscillatory behavior. However, when $\omega_c=\omega_y$ the oscillations begin to grow and when $\omega_c=2\omega_y$ they are clearly visible. For $\omega_c=2\omega_y$, $\Delta E^T/\hbar\omega_x\simeq 2$ and condition (4) is well fulfilled.[20]

In summary, we have calculated the thermopower of a quantum-point constriction. Our results show that the thermopower shows oscillations as a function of chemical potential μ, each time a new quantum channel is open for conduction. The amplitude of the oscillations is temperature dependent. Finally, the possibility of magnetic-field-induced oscillations is suggested.

The author would like to thank Dr. Markus Büttiker for very useful criticism of an earlier version of this paper and Professor Abdus Salam, for hospitality at the International Centre for Theoretical Physics, Trieste, where the present work was initiated.

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