On the Mott formula for the thermopower of non-interacting electrons in quantum point contacts

2005 J. Phys.: Condens. Matter 17 3879

(http://iopscience.iop.org/0953-8984/17/25/014)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **17** (2005) 3879–3884 doi:10.1088/0953-8984/17/25/014

On the Mott formula for the thermopower of non-interacting electrons in quantum point contacts

Anders Mathias Lunde and Karsten Flensberg

Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

E-mail: lunan@fys.ku.dk

Received 12 April 2005
Published 10 June 2005
Online at stacks.iop.org/JPhysCM/17/3879

Abstract
We calculate the linear response thermopower S of a quantum point contact using the Landauer formula and therefore assume non-interacting electrons. The purpose of the paper is to compare analytically and numerically the linear thermopower S of non-interacting electrons to the low-temperature approximation, $S^{(1)} = (\pi^2/3e)k_B^2 T\partial_\mu[\ln G(\mu, T = 0)]$, and the so-called Mott expression, $S^M = (\pi^2/3e)k_B^2 T\partial_\mu[\ln G(\mu, T)]$, where $G(\mu, T)$ is the (temperature-dependent) conductance. This comparison is important, since the Mott formula is often used to detect deviations from single-particle behaviour in the thermopower of a point contact.

1. Introduction

A narrow constriction in for example a two-dimensional electron gas makes a small channel between two electron reservoirs. This constriction is called a quantum point contact [1]. The width of the channel can be controlled by a gate voltage, and by applying a small bias the phenomenon of quantized conductance as a function of the width (i.e. gate voltage) is observed at low temperatures [2]. This quantization is due to the wave nature of the electronic transport through the short ballistic point contact. Experimentally [3–7], it is also possible to heat up one of the sides of the point contact, thereby producing a temperature difference ΔT across the contact, which in turn gives an electric current (and a heat current) though the point contact. By applying a bias V in the opposite direction to the temperature difference ΔT, the two contributions to the electric current I can be made to cancel, which defines the thermopower S as

$$S = - \lim_{\Delta T \to 0} \frac{V}{\Delta T}\bigg|_{I=0}. \tag{1}$$

For a quantum point contact, the thermopower as a function of gate voltage has a peak every time the conductance plateau changes from one subband of the transverse quantization to the next [5, 8].

In order to compare experiment and theory for the thermopower of a point contact, the so-called Mott formula,

$$S^{\mathrm{M}} \propto \partial_{V_{\mathrm{g}}}[\ln G(V_{\mathrm{g}}, T)], \tag{2}$$

is often a valuable tool, because by differentiating the experimentally found conductance $G(V_{\mathrm{g}}, T)$ with respect to the gate voltage V_{g} one can see if there is more information in the thermopower that in the conductance. This additional information could for example be many-body effects [7], since S^{M} is an approximation to the single-particle thermopower. Note that this approximation is independent of the specific form of the transmission $\mathcal{T}(\varepsilon)$ through the point contact. It is the purpose of this paper to determine the validity of the Mott approximation S^{M}, and thereby decide if it is really deviations from single-particle behaviour the experiments [6, 7, 9] reveal or rather artefacts of this approximation.

2. Thermopower from the Landauer formula

For the sake of completeness, we begin by deriving the single-particle thermopower formula in linear response to the applied bias V and temperature difference ΔT. The current though a ballistic point contact is found from the Landauer formula [10, p 111, equation (7.30)]:

$$I = \frac{2e}{h}\int_0^\infty \mathrm{d}\varepsilon\, \mathcal{T}(\varepsilon)[f_{\mathrm{L}}^0(\varepsilon) - f_{\mathrm{R}}^0(\varepsilon)], \tag{3}$$

where $\mathcal{T}(\varepsilon)$ is the transmission and $f_i^0(\varepsilon)$ is the Fermi function for the right/left ($i = \mathrm{R}, \mathrm{L}$) lead. The Landauer formula assumes non-interacting electrons and therefore so will the derived thermopower formula. When a small bias $V = (\mu_{\mathrm{L}} - \mu_{\mathrm{R}})/(-e)$ and temperature difference $\Delta T = T_{\mathrm{L}} - T_{\mathrm{R}}$ are applied, we can expand the distribution functions around μ, T as ($|\Delta T|/T \ll 1$ and $|eV| \ll \mu$):

$$f_i^0(\varepsilon) \simeq f^0(\varepsilon) - \partial_\varepsilon f^0(\varepsilon)(\mu - \mu_i) - (\varepsilon - \mu)\partial_\varepsilon f^0(\varepsilon)\frac{T - T_i}{T}, \tag{4}$$

where $f^0(\varepsilon)$ is the Fermi function with the equilibrium chemical potential μ and temperature T and $i = \mathrm{L}, \mathrm{R}$. To obtain the thermopower equation (1) we insert the distribution functions in equation (3), set it equal to zero and obtain

$$S(\mu, T) = \frac{1}{eT}\frac{\int_0^\infty \mathrm{d}\varepsilon\, \mathcal{T}(\varepsilon)(\varepsilon - \mu)[-\partial_\varepsilon f^0(\varepsilon)]}{\int_0^\infty \mathrm{d}\varepsilon\, \mathcal{T}(\varepsilon)[-\partial_\varepsilon f^0(\varepsilon)]}, \tag{5}$$

which is our exact single-particle formula.

3. Approximations to the thermopower and their validity

3.1. The low-temperature (first-order) approximation

For $T = 0$ we have $-\partial_\varepsilon f^0(\varepsilon) = \delta(\varepsilon - \mu)$, so the numerator in equation (5) is zero, i.e. $S(\mu, T = 0) = 0$. For temperatures $k_{\mathrm{B}}T$ much lower than the scale of variation of $\mathcal{T}(\varepsilon)$ and $k_{\mathrm{B}}T \ll \mu$, we can expand $\mathcal{T}(\varepsilon)$ around μ to first order (i.e. a Sommerfeld expansion) to obtain

$$S^{(1)}(\mu, T) = \frac{\pi^2}{3}\frac{k_{\mathrm{B}}}{e}k_{\mathrm{B}}T\frac{1}{\mathcal{T}(\mu)}\frac{\partial \mathcal{T}(\mu)}{\partial \varepsilon} = \frac{\pi^2}{3}\frac{k_{\mathrm{B}}}{e}k_{\mathrm{B}}T\frac{1}{G(\mu, T = 0)}\frac{\partial G(\mu, T = 0)}{\partial \mu}, \tag{6}$$

where $G(\mu, T = 0)$ is the conductance for zero temperature, i.e. $G(\mu, T = 0) = \frac{2e^2}{h}\mathcal{T}(\mu)$.

3.2. *The Mott approximation and analytical considerations of its validity*

The Mott approximation[1] [6, 7] is

$$S^{\mathrm{M}}(\mu,T)=\frac{\pi^2}{3}\frac{k_{\mathrm{B}}}{e}k_{\mathrm{B}}T\frac{1}{G(\mu,T)}\frac{\partial G(\mu,T)}{\partial\mu},\tag{7}$$

where $G(\mu,T)$ is the *temperature-dependent* conductance

$$G(\mu,T)=\frac{2e^2}{h}\int_0^\infty \mathrm{d}\varepsilon\,\mathcal{T}(\varepsilon)[-\partial_\varepsilon f^0(\varepsilon)].\tag{8}$$

The form of S^{M} stated in equation (2) assumes that the chemical potential and gate voltage are linear dependent. The Mott approximation to the single-particle thermopower equation (5) and its range of validity are not so obvious compared to the approximation of the first-order Sommerfeld expansion equation (6).

One way of comparing S from equation (5) and S^{M} is to differentiate equation (8) to obtain (assuming that $\mathcal{T}(\varepsilon)$ is independent of μ):

$$S^{\mathrm{M}}(\mu,T)=\frac{\pi^2}{3}\frac{k_{\mathrm{B}}}{e}\frac{1}{G(\mu,T)}\int_0^\infty \mathrm{d}\varepsilon\,\mathcal{T}(\varepsilon)\tanh\left(\frac{\varepsilon-\mu}{2k_{\mathrm{B}}T}\right)[-\partial_\varepsilon f^0(\varepsilon)],\tag{9}$$

i.e. by using the Mott formula we approximate $(\varepsilon-\mu)/k_{\mathrm{B}}T$ in the integral by $(\pi^2/3)\tanh[(\varepsilon-\mu)/(2k_{\mathrm{B}}T)]$.

To compare S and S^{M} in another way, we observe that for low temperatures $k_{\mathrm{B}}T\ll\mu$ the Mott approximation S^{M} simplifies to the $S^{(1)}$ equation (6), because $G(\mu,T)\to\frac{2e^2}{h}\mathcal{T}(\mu)$ for $T\to 0$, i.e. $S(\mu,T)=S^{(1)}(\mu,T)=S^{\mathrm{M}}(\mu,T)$ for $k_{\mathrm{B}}T/\mu\to 0$. Therefore, we compare S and S^{M} by expanding both quantities in orders of $k_{\mathrm{B}}T$ and comparing order by order. Using

$$\mathcal{T}(\varepsilon)=\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n\mathcal{T}(\mu)}{\partial\varepsilon^n}(\varepsilon-\mu)^n,\tag{10}$$

we can exactly rewrite equation (8):

$$\begin{aligned}G&=\frac{2e^2}{h}\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n\mathcal{T}(\mu)}{\partial\varepsilon^n}\int_0^\infty \mathrm{d}\varepsilon\,(\varepsilon-\mu)^n[-\partial_\varepsilon f^0(\varepsilon)]\\&=\frac{2e^2}{h}\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n\mathcal{T}(\mu)}{\partial\varepsilon^n}(k_{\mathrm{B}}T)^n\mathfrak{B}_n\left(\frac{\mu}{k_{\mathrm{B}}T}\right),\end{aligned}\tag{11}$$

where $(y=(\varepsilon-\mu)/k_{\mathrm{B}}T)$

$$\mathfrak{B}_n\left(\frac{\mu}{k_{\mathrm{B}}T}\right)\equiv\int_{-\frac{\mu}{k_{\mathrm{B}}T}}^{\infty}\mathrm{d}y\,\frac{y^n}{4\cosh^2(y/2)}\to I_n\equiv\int_{-\infty}^{\infty}\mathrm{d}y\,\frac{y^n}{4\cosh^2(y/2)}\qquad\text{for } k_{\mathrm{B}}T\ll\mu,\tag{12}$$

where we note that $I_{2n+1}=0$ for all integer n. Numerically, it turns out that $\mathfrak{B}_n(\mu/k_{\mathrm{B}}T)/\mathfrak{B}_n(0)\simeq 0$ for $\mu\gtrsim(10+n)k_{\mathrm{B}}T$ as seen in figure 1. The integral I_n can be calculated, and the first values are

$$I_0=1,\ I_2=\frac{\pi^2}{3},\ I_4=\frac{7\pi^4}{15},\ I_6=\frac{31\pi^6}{21},\ I_8=\frac{127\pi^8}{15},\ \ldots.\tag{13}$$

Using the approximation equation (12) we get

$$G(\mu,T)\simeq\frac{2e^2}{h}\sum_{n=0}^{\infty}\frac{1}{(2n)!}\frac{\partial^{2n}\mathcal{T}(\mu)}{\partial\varepsilon^{2n}}I_{2n}(k_{\mathrm{B}}T)^{2n}.\tag{14}$$

[1] In the early works by Mott and co-workers [11, 12] it was actually the first-order approximation equation (6) which was referred to as the Mott formula.

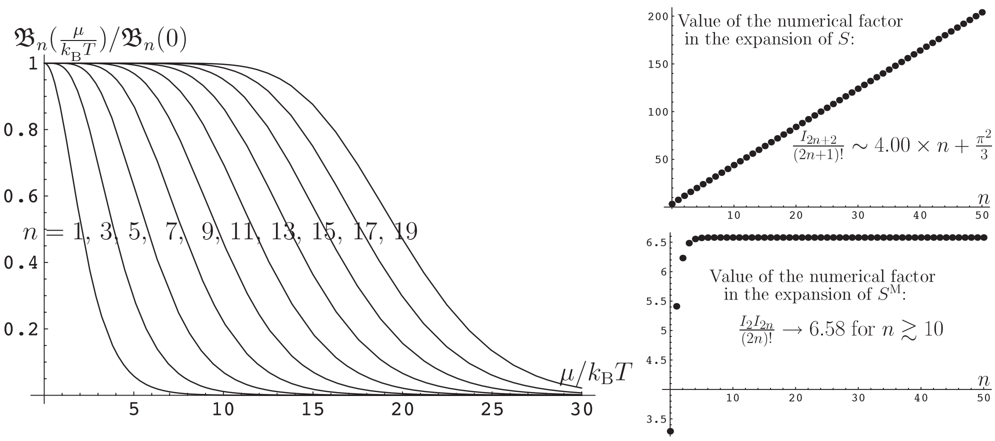

Figure 1. Left: the approximation in equation (12) is pictured for odd integer values of n from 1 (left) to 19 (right) in $\mathfrak{B}_n(\mu/k_B T)$. We note that $\mathfrak{B}_n(\mu/k_B T)/\mathfrak{B}_n(0) \simeq 0$ for $\mu \gtrsim (10+n)k_B T$. Right: the numerical values of the factors in the series expansions of the Mott approximation equation (15) (lower) and the exact linear single-particle series expansion equation (16) (upper).

This leads to a Mott approximation to the thermopower for low temperatures as

$$S^M(\mu, T) \simeq \frac{k_B}{e}\frac{1}{G(\mu, T)}\frac{2e^2}{h}\left[\sum_{n=0}^{\infty}\frac{I_2 I_{2n}}{(2n)!}\frac{\partial^{2n+1}\mathcal{T}(\mu)}{\partial\varepsilon^{2n+1}}(k_B T)^{2n+1}\right]. \tag{15}$$

Writing the exact single-particle thermopower S equation (5) by using equation (10) and the approximation of low temperatures equation (12), we get

$$S(\mu, T) \simeq \frac{k_B}{e}\frac{1}{G(\mu, T)}\frac{2e^2}{h}\left[\sum_{n=0}^{\infty}\frac{I_{2n+2}}{(2n+1)!}\frac{\partial^{2n+1}\mathcal{T}(\mu)}{\partial\varepsilon^{2n+1}}(k_B T)^{2n+1}\right]. \tag{16}$$

We see that both formulae only have odd terms in $k_B T$, and the first-order term is the same (which is $S^{(1)}$). However, none of the higher-order terms are the same, and in figure 1(right) the different numerical factors of the two series expansions are seen to behave very differently as the power of $k_B T$ grows:

$$\frac{I_{2n+2}}{(2n+1)!} \sim 4.00 \times n + \frac{\pi^2}{3} \qquad \text{and} \qquad \frac{I_2 I_{2n}}{(2n)!} \rightarrow 6.58 \quad \text{for } n \gtrsim 10. \tag{17}$$

So the Mott approximation is better the smaller the temperature compared to μ, but it is not a bad approximation for moderate temperatures (i.e. $k_B T$ comparable to other energy scales), as we shall see numerically. Note that if the approximation equation (12) is not valid, then we have all powers of $k_B T$.

4. Comparison of the approximations to the exact single-particle thermopower from numerical integration

We need a specific model for the transmission to do a numerical comparison of S from equation (5) to S^M and $S^{(1)}$. Using a harmonic potential in the point contact, i.e. a saddle point potential, a transmission in the form of a Fermi function can be derived [13]:

$$\mathcal{T}(\varepsilon) = \sum_{n=1}^{n_{max}}\frac{1}{\exp(\frac{n\varepsilon_0-\varepsilon}{\varepsilon_s})+1}, \tag{18}$$

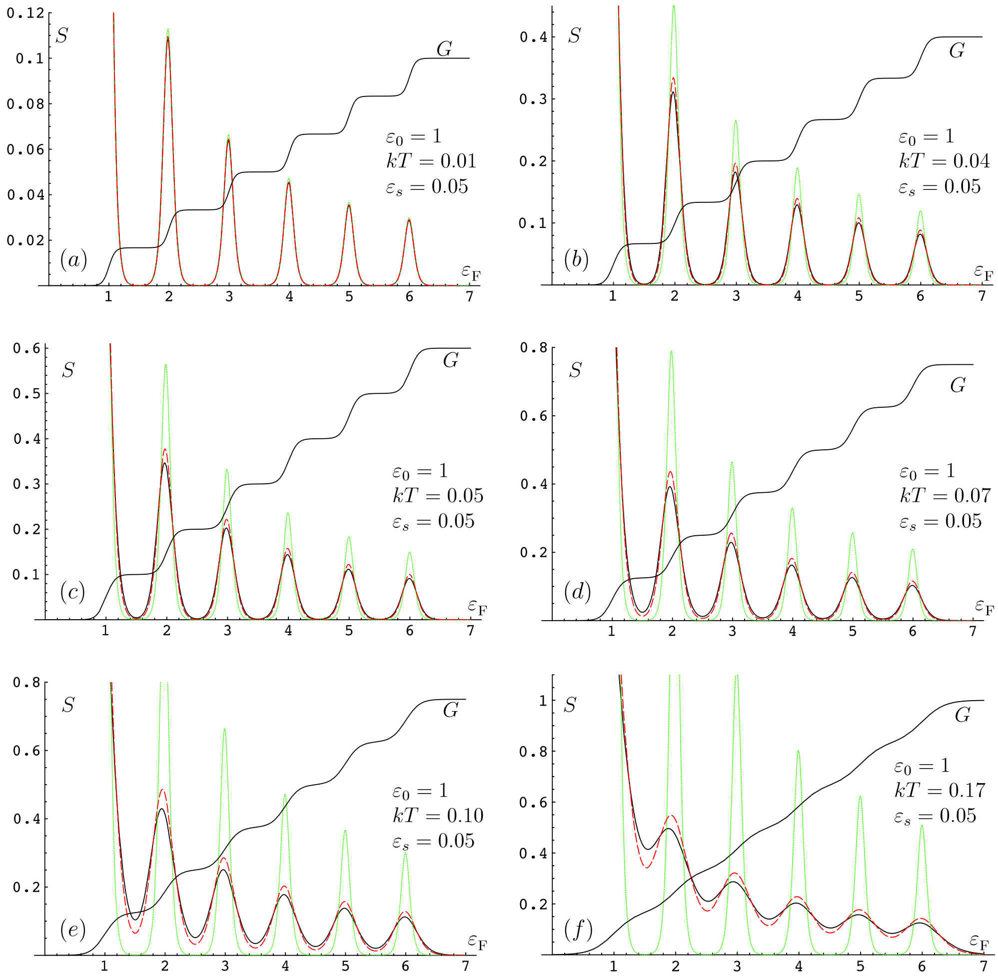

Figure 2. Thermopower S from numerical integration of equation (5) (black solid line), the Mott formula S^{M} equation (7) (red dashed line) and the first-order approximation $S^{(1)}$ equation (6) (green dotted line). From (a) to (f) the temperature is changed from the low-temperature regime $k_{\mathrm{B}}T < \varepsilon_s$ to $k_{\mathrm{B}}T > \varepsilon_s$ in small steps. The smearing of the transmission ε_s is kept constant, and note that $\varepsilon_s, k_{\mathrm{B}}T \ll \varepsilon_0$ and $\varepsilon_s, k_{\mathrm{B}}T \ll \varepsilon_{\mathrm{F}}$ in all the graphs. The thermopowers are all in units of k_{B}/e, but note the different magnitudes of the thermopower from (a) to (f). The conductance G is shown (in arbitrary units) for comparison.

(This figure is in colour only in the electronic version)

where ε_s is the smearing of the transmission between the steps and ε_0 is the length of the steps (often called the subband spacing). In terms of the harmonic potential $V(x, y) = \text{const} - m\omega_x^2 x^2/2 + m\omega_y^2 y^2/2$, where x is along the channel, we have $\varepsilon_0 = \hbar\omega_y$ and $\varepsilon_s = \hbar\omega_x/(2\pi)$. Other functional forms of $\mathcal{T}$ have also been tested, but provided they have the same graphical structure (such as for example a tanh dependence) the same conclusions are obtained.

Three regimes of temperatures relevant to experiments are investigated numerically:

$$k_{\mathrm{B}}T < \varepsilon_s \text{ (figure 2(a))}, \qquad k_{\mathrm{B}}T \sim \varepsilon_s \text{ (figures 2(b)–(d))}$$
$$\text{and} \qquad k_{\mathrm{B}}T > \varepsilon_s \text{ (figures 2(e), (f))}. \tag{19}$$

The thermopower S for the transmission model equation (18) is found from numerical integration of equation (5) and compared to the Mott approximation S^{M} equation (7) and the first-order approximation $S^{(1)}$ equation (6). In all three regimes, we have a staircase conductance, so $k_{\mathrm{B}}T \ll \varepsilon_0$, and $G(\mu, T)$ is also shown in the figures (in arbitrary units) for comparison. Furthermore, $\mu = \varepsilon_{\mathrm{F}}$ is of order ε_0, so the approximation $k_{\mathrm{B}}T \ll \varepsilon_{\mathrm{F}}$ used for example in equation (12) is indeed very good. Note that all energies in the figures are given in units of the step length ε_0.

The information obtained from the numerical calculations is the following. Figures 2(a), (b) show that for $k_{\mathrm{B}}T$ being the lowest energy scale both approximations work very well, as expected from the analytical considerations. When the temperature becomes comparable to the smearing of the steps, $k_{\mathrm{B}}T \sim \varepsilon_s$, the Culter–Mott formula works well and is better than the first-order approximation, as seen in figures 2(b)–(d). For $k_{\mathrm{B}}T$ bigger than ε_s, the Mott approximation still works quite well, whereas $S^{(1)}$ is no longer a good approximation. The reason that the Mott approximation works well is found in the similar terms in the analytic temperature expansions equations (15) and (16). Note that as $k_{\mathrm{B}}T$ increases both $S^{(1)}$ and S^{M} show a tendency to overestimate S at the peaks and underestimate it at the valleys.

In summary, we have found that the Mott approximation to the single-particle thermopower is a fairly good approximation provided the temperature is smaller than the Fermi level, but $k_{\mathrm{B}}T$ can be both compatible and larger than the smearing of the transmission ε_s. However, to rule out any doubt one could use an experimental determination of $\mathcal{T}(\varepsilon)$ from the (very low-temperature) conductance to find the single-particle thermopower from equation (5), which could perhaps give an interesting comparison to the experimental result. Thereby one would obtain an even more convincing statement of deviations from single-particle behaviour in the thermopower.

Acknowledgment

We would like to thank James T Nicholls for sharing his experimental results with us and for discussions of the thermopower in point contacts in general.

References

[1] Houten H V and Beenakker C 1996 *Phys. Today* (July) 22 for an minor review
[2] van Wees B J *et al* 1988 *Phys. Rev. Lett.* **60** 848
[3] Molenkamp L W *et al* 1990 *Phys. Rev. Lett.* **65** 1052
[4] Molenkamp L W *et al* 1992 *Phys. Rev. Lett.* **68** 3765
[5] van Houten H, Molenkamp L W, Beenakker C W J and Foxon C T 1992 *Semicond. Sci. Technol.* **7** B215
[6] Appleyard N J *et al* 1998 *Phys. Rev. Lett.* **81** 3491
[7] Appleyard N J *et al* 2000 *Phys. Rev.* B **62** 16275(R)
[8] Streda P 1989 *J. Phys.: Condens. Matter* **1** 1025
[9] Proskuryakov Y Y *et al* 2004 unpublished
[10] Bruus H and Flensberg K 2004 Many-body quantum theory in condensed matter physics *Oxford Graduate Texts* 1st edn (New York: Oxford University Press)
[11] Mott N F and Jones H 1936 *The Theory of the Properties of Metals and Alloys* 1st edn (Oxford: Clarendon)
[12] Cutler M and Mott N F 1969 *Phys. Rev.* **181** 1336
[13] Büttiker M 1990 *Phys. Rev.* B **41** 7906(R)