Thermal conductance of a weakly coupled quantum dot

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Abstract. We calculate the heat current through a quantum dot, weakly coupled to two electron reservoirs, when small temperature and voltage differences are applied between the reservoirs. The electronic contribution to the thermal conductance, κ_e, is then readily obtained. We restrict our interest in the regime where $\Delta\varepsilon >> k_B T$, where $\Delta\varepsilon$ is the level spacing, and we show that for a dot with equidistant energy levels κ_e exhibits periodical resonance peaks as a function of the Fermi energy in the reservoirs. The periodicity of these peaks is the same as the Coulomb blockade peaks in the conductance. The resonance values of κ_e tend rapidly to zero as $exp(-\Delta\varepsilon/k_B T)(\Delta\varepsilon/k_B T)^2$. This finding underlies a clear violation of the Wiedemann-Franz law. We point out the consequence of this violation in achieving large values of the figure of merit ZT.

Keywords: thermal conductance, thermoelectric properties, zero-dimensional nanostructures, Coulomb blockade, resonant tunneling
PACS: 73.23.Hk, 73.63.Kv

We describe a theoretical model for the calculation of the electronic contribution to the thermal conductance, κ_e, of a quantum dot weakly coupled to two electron reservoirs in the Coulomb blockade regime (CB). Our analysis is based on a master equation approach [1, 2]. We consider a quantum dot with equidistant energy levels ε_p ($p = 1, 2, \ldots$). Each level in the dot contains 0 or 1 electrons. The charging energy $E_C = e^2/2C$, where C is the capacitance between the dot and the reservoirs, is larger than the level spacing $\Delta\varepsilon$. The tunnel rate from level p to the left (right) reservoir is denoted as Γ^L (Γ^R). Here we ignore the energy dependence of the tunnel rates. Moreover, we assume $k_B T, \Delta\varepsilon >> h(\Gamma^R + \Gamma^L)$ [1] and consider only sequential-tunneling processes.

Beenakker [1] and Beenakker and Staring [2] have calculated the electron current I passes through the dot when small ΔT and ΔV are applied between the two reservoirs by using a linear response theory. Here we calculate the heat current Q. Following the linearization procedure described in Refs. [1, 2] we obtain

$$Q = -\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}\left(s_1\frac{e\Delta V}{k_B T} + s_2\frac{\Delta T}{k_B T^2}\right), \qquad (1)$$

where s_m for the integers $m = 0, 1, 2$ is given by

$$s_m = \sum_{p=1}^{\infty}\sum_{N=1}^{\infty} P_{eq}(N)P_{eq}(\varepsilon_p|N)[1-f(E)](E-E_F)^m. \quad (2)$$

In Eq.(2) $f(E) = 1/\{1+exp[\beta(E-E_F)]\}$, with $\beta = 1/k_B T$; $E = \varepsilon_p + U(N) - U(N-1)$ where $U(N) = N^2E_C - Ne\phi_{ext}$ is the electrostatic energy for a dot with N electrons and $Ne\phi_{ext}$ in the contribution from external charges; $P_{eq}(N)$ is the probability that the dot contains N electrons in equilibrium and $P_{eq}(\varepsilon_p|N)$ is the conditional probability that in equilibrium the p state is occupied given that the dot has N electrons.

The heat current is related to ΔV and ΔT by the constitutive equation $Q = M\Delta V + K\Delta T$ [3]. Inspection of Eq. (1) shows that $M = -\frac{e}{k_B T}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}s_1$ and $K = -\frac{1}{k_B T^2}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}s_2$. The thermoelectric coefficient M is related to the thermopower, S, by the Onsager's symmetry relation $M = SGT$, where $G = \frac{e^2}{k_B T}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}s_0$ is the electron conductance [1]. Finally, κ_e is obtained by the standard relationship

$$\kappa_e = -K - S^2GT. \qquad (3)$$

In what follows we restrict our interest in the regime where $\beta\Delta\varepsilon >> 1$ (quantum limit). We performed numerical calculations of K as a function of E_F for a three level dot (not shown here) and we find that K shows a double peak structure with the same periodicity, $\Delta E_F = \Delta\varepsilon + (e^2/C)$, of the CB oscillations of G [1]. Most interestingly we find that $-K \approx S^2GT$. Inspection of Eq. (3) implies that $\kappa_e \rightarrow 0$.

In order to reveal the exact way that κ_e tends to zero at low T we explore the non-zero terms. The dominant contribution to s_m in Eq.(2) is made for $N = p = N_{min}$, where N_{min} is the integer that minimizes the absolute value of $\Delta_N = E_N - E_F$ with $E_N = \varepsilon_N + U(N) - U(N-1)$ [1, 2]. In this case, $P_{eq}(N_{min}) \approx f(E_{N_{min}})$ and $P_{eq}(\varepsilon_p|N_{min}) \approx 1$. Then, $s_m \approx -k_B T f'(E_{N_{min}})(\Delta_{N_{min}})^m$, where $f'(E_{N_{min}})$ is the derivative of $f(E_{N_{min}})$ with respect to $E_{N_{min}}$. These expressions for s_m describe accurately the CB oscillations of M, K and G (not shown here) and they produce $\kappa_e = 0$ when they are substituted in Eq. (3). The non-zero terms in κ_e are due to small corrections of the order of $exp(-\beta\Delta\varepsilon)$ that are related to the energy difference between the level $p = N_{min}$ and the levels $p = N_{min} \pm 1$. By taking into account the corrections due to terms $p = N_{min} + 1$ and $p = N_{min} - 1$ we find that the electronic con-

CP893, *Physics of Semiconductors, 28th International Conference*
edited by W. Jantsch and F. Schäffler

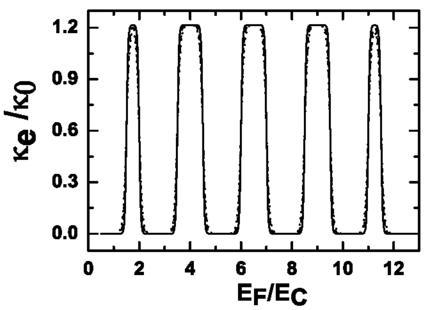

FIGURE 1. The calculated κ_e as a function of E_F in a five level quantum dot. The results for $\beta\Delta\varepsilon = 16$, 10 and 8 are shown as solid, dashed and doted lines, respectively. The three curves are hardly distinguishable. $\Delta\varepsilon = 0.5E_C$ and $\kappa_0 = L_0 T G^{max}(\beta\Delta\varepsilon)^2 e^{-\beta\Delta\varepsilon}$.

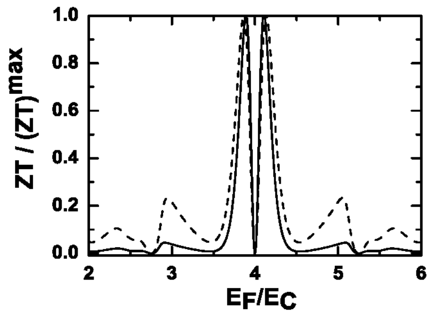

FIGURE 2. The calculated ZT in a three level quantum dot, around $\Delta_{N_{min}} = 0$, for $\beta\Delta\varepsilon = 11$ (solid line) and 9 (dashed line). $\Delta\varepsilon = 0.5E_C$ and $(ZT)^{max} = 0.44 e^{\beta\Delta\varepsilon}/(\beta\Delta\varepsilon)^2$.

tribution to the thermal conductance is given by

$$\kappa_e = k_B \frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}(\beta\Delta\varepsilon)^2 \times \frac{(1+e^{\beta\Delta\varepsilon})e^{\beta\Delta_{N_{min}}}}{e^{\beta\Delta\varepsilon}(e^{2\beta\Delta_{N_{min}}}+1)+e^{\beta\Delta_{N_{min}}}(e^{2\beta\Delta\varepsilon}+1)}. \quad (4)$$

The magnitude of the peak values of κ_e around $\Delta_{N_{min}} = 0$ ($\Delta_{N_{min}}$ becomes zero each time an electron enters the dot) is given by the simple expression

$$\kappa_e = k_B \frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}(\beta\Delta\varepsilon)^2 e^{-\beta\Delta\varepsilon}. \quad (5)$$

Equation (4) is in excellent agreement with the calculated values of κ_e obtained from Eqs.(2) and (3).

In Fig.2 we show the calculated κ_e for a five level dot with $\Delta\varepsilon = 0.5E_C$. The calculations are made for $\beta\Delta\varepsilon =$ 8, 10, and 16. We see that κ_e exhibits resonance peaks with the periodicity of the CB oscillations in G. For a dot with non-equidistant energy levels the behavior of κ_e (not shown here) is different than that depicted in Fig.1.

Inspection of Eq. (5) shows that the Wiedemann-Franz (W-F) law according to which $\kappa_e/G = L_0 T$, where L_0 is the Lorentz number, fails in the quantum limit. The ratio of the peak values of κ_e and G for $\Delta_{N_{min}} = 0$ is

$$\frac{k_e^{max}}{G^{max}} = \frac{12}{\pi^2} L_0 T (\beta\Delta\varepsilon)^2 e^{-\beta\Delta\varepsilon} \quad (6)$$

where $G^{max} = (e^2/4k_BT)[\Gamma^L\Gamma^R/(\Gamma^L+\Gamma^R)]$. The violation of the W-F law leads to a significant enhancement of the figure of merit $ZT = S^2GT/\kappa_e$ when the phononic contribution is ignored. The calculated values of ZT for a three level dot, around $\Delta_{N_{min}} = 0$, appear in Fig.2. ZT follows closely the structure of $-K$ and the magnitude of the two strong peaks increases exponentially with $\beta\Delta\varepsilon$.

Also, very recently, it has been reported that deviations from the W-F law result to large calculated values of ZT in nanocontacts made of two-capped single wall nanotubes [4]. We should remark that, the contribution of phonons could suppress ZT. However, the phonon confinement in nanostructures could decrease dramatically the phononic contribution to the thermal conductance [5]. Our findings suggest that the mutual control of the electron and phonon confinement effects in nanostructures can improve significantly their thermoelectric properties.

In conclusion, we have calculated the thermal conductance of spin-less electrons in a weakly coupled quantum dot in the quantum limit. We show that the W-F law fails in this regime. Due to this failure the calculated values of ZT are found to be significantly large when the phononic contribution to the thermal conductance is neglected.

ACKNOWLEDGMENTS

The authors wish to thank R. Fletcher for stimulating remarks and valuable suggestions. MT acknowledges X. Zianni (TEI Chalkidas, Greece) for giving the motivation through the ‘Archimedes I’ programme funded by the European Commission and by the Greek Ministry of Education (E.P.E.A.E.K.)

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