Physica B 407 (2012) 765–769

Contents lists available at SciVerse ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Thermoelectric effects through weakly coupled double quantum dots

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ARTICLE INFO

Article history:
Received 5 October 2011
Received in revised form
8 December 2011
Accepted 9 December 2011
Available online 17 December 2011

Keywords:
Double quantum dot
Rate equations
Thermopower
Thermoelectrical figure of merit

ABSTRACT

The electrical conductance, the thermal conductance, the thermopower and the thermoelectrical figure of merit are analyzed through a double quantum dot system weakly coupled to metal electrodes, by means of density matrix approach. The effects of interdot tunneling, intra- and interdot Coulomb repulsions on the figure of merit are examined. Results show that increase of interdot tunneling gives rise to a reduction in figure of merit. On the other hand, increase of Coulomb repulsion results in enhancement of figure of merit because of reduce of bipolar effect.

1. Introduction

In recent years, thermopower and spin-thermopower through nanostructures have been widely studied both experimentally and theoretically [1–14]. Indeed, deviation from Wiedmann–Franz law in nanostructures results in significant enhancement in the thermopower [15]. The quantized energy levels and Coulomb interaction in quantum dots influence on the thermopower, significantly. Figure of merit $ZT=G_VS^2T/\kappa$ denoting the energy conversion efficiency is an important factor in thermoelectronic devices. S and G_V denote Seebeck coefficient and electrical conductance, respectively. T is the temperature of the system and $\kappa=\kappa_c+\kappa_{ph}$ is composed of the electrical and the phonon thermal conductances.

Study of thermopower through multilevel quantum dots and double quantum dot systems has attracted a lot of attention in recent years. Liu et al. [16] examined the thermopower in a multilevel quantum dot and showed that Coulomb interaction can result in the enhancement of the figure of merit due to the reduction of the bipolar effect. Chi et al. [17] investigated the thermopower in a serially coupled quantum dot using nonequilibrium Green function formalism. Their results show that the figure of merit has two huge peaks in vicinity of electron–hole symmetry points. Trocha and Barnaś [18] reported that the figure of merit is enhanced through a double quantum dot because of quantum interference effects and Coulomb interactions.

In this paper, we analyze the thermopower and the figure of merit through a double quantum dot weakly coupled to the metal leads by means of density matrix approach. The many-body representation introduced in Ref. [19] is used to obtain the population numbers and the thermopower. In the next section, the model Hamiltonian and the main equations are presented. The influence of the temperature, the interdot tunneling strength, and the Coulomb interaction on the thermopower and the figure of merit are studied in the third section. In the end, some sentences are given as a conclusion.

2. Model

The system under consideration is described by the Hamiltonian

$$H=H_{Leads}+H_{DQD}+H_T \tag{1}$$

where $H_{Leads}=\sum_{\alpha k\sigma}\varepsilon_{\alpha k\sigma}c^{\dagger}_{\alpha k\sigma}c_{\alpha k\sigma}$ describes the left and right leads in which $\varepsilon_{\alpha k\sigma}$ denotes the energy of the electron with wave vector k, spin σ in the lead $\alpha=L,R$, and $c_{\alpha k\sigma}(c^{\dagger}_{\alpha k\sigma})$ is annihilation (creation) operator. H_{DQD} describes the isolated double quantum dot and is given as

$$H_{DQD}=\sum_{\alpha\sigma}\varepsilon_\alpha d^{\dagger}_{\alpha\sigma}d_{\alpha\sigma}+\sum_{\alpha=L,R}U_\alpha n_{\alpha\uparrow}n_{\alpha\downarrow}+U_{12}\sum_{\sigma\sigma'}n_{L\sigma}n_{R\sigma'}+t\sum_{\sigma}[d^{\dagger}_{L\sigma}d_{R\sigma}+d^{\dagger}_{R\sigma}d_{L\sigma}] \tag{2}$$

where ε_α stands for the energy level of the αth dot, while $d_{\alpha\sigma}(d^{\dagger}_{\alpha\sigma})$ destroys (creates) an electron with spin σ in the dot α. U_α and U_{12} denote, respectively, intra- and interdot Coulomb repulsions, and $n_{\alpha\sigma}=d^{\dagger}_{\alpha\sigma}d_{\alpha\sigma}$. The last term in above equation denotes the tunneling between two dots. H_T describes tunneling between the dots and the

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doi:10.1016/j.physb.2011.12.021

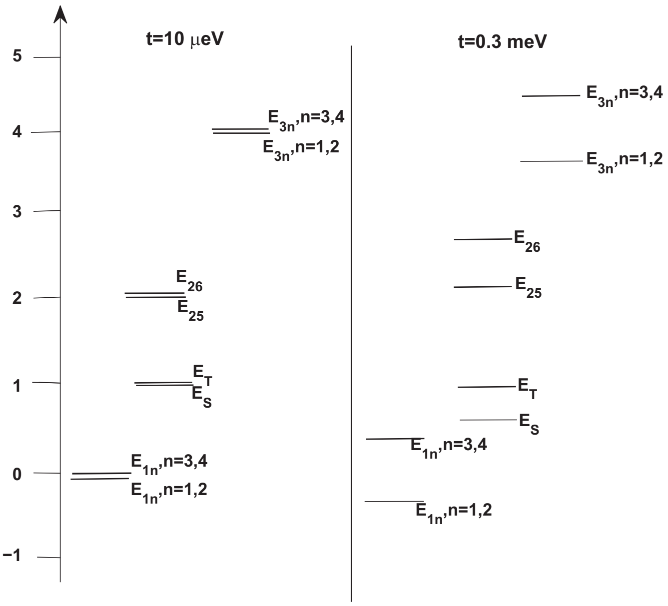

Fig. 1. Eigenenergies of the DQD for both weak and strong interdot tunneling. We set $\varepsilon_i = 0$.

leads as follows:

$$H_T = \sum_{\alpha k \sigma} [V_{\alpha k \sigma} c^{\dagger}_{\alpha k \sigma} d_{\alpha\sigma} + V^{*}_{\alpha k \sigma} d^{\dagger}_{\alpha\sigma} c_{\alpha k \sigma}] \tag{3}$$

In order to compute thermopower, we diagonalize H_{DQD}, and denote its eigenstates as $|N,n\rangle$ where n stands for the nth state of the N-electron configuration. It is obvious that there are 16 different states expressed, for example, in Ref. [19]. A generic graph for the energy eigenvalues is shown in Fig. 1. Now, Eq. (2) can be written as

$$H_{DQD} = \sum_{N=0}^{4} \sum_{n} E_{Nn} h^{n}_{N} \tag{4}$$

where $h^n_N = |N,n\rangle\langle N,n|$ are the diagonal transitions of the Hubbard operators $X^{nn'}_{NN'} = |N,n\rangle\langle N',n'|$. Whereas $d_{\alpha\sigma}$ annihilates an electron with spin σ in the dot α. It is straightforward to show

$$d_{\alpha\sigma} = \sum_{Nnn'} (d_{\alpha\sigma})^{nn'}_{NN+1} X^{nn'}_{NN+1} \tag{5}$$

where $(d_{\alpha\sigma})^{nn'}_{NN+1} = \langle Nn|d_{\alpha\sigma}|N+1,n'\rangle$. Using Eqs. (4) and (5), the total Hamiltonian can be written as

$$H = \sum_{\alpha k \sigma} \varepsilon_{\alpha k \sigma} c^{\dagger}_{\alpha k \sigma} c_{\alpha k \sigma} + \sum_{Nn} E_{Nn} h^{n}_{N} + \sum_{\alpha k N n n'} [V_{\alpha k \sigma} (d_{\alpha\sigma})^{nn'}_{NN+1} c^{\dagger}_{\alpha k \sigma} X^{nn'}_{NN+1} + H.C.] \tag{6}$$

Now, we can compute the population numbers P_{Nn}, probability of being in the state $|Nn\rangle$, by means of the density matrix approach. Coupling to the leads is so weak that off diagonal elements of the density matrix are neglected, because they give the contributions of the fourth order in $V_{\alpha k \sigma}$. Using the Markovian limit and the wide band limit, the time evolution of the population numbers are given as [19]

$$\frac{dP_{01}}{dt} = \sum_{\alpha n} [-\Gamma^{\alpha}_{|01\rangle \to |1n\rangle} P_{01} + \Gamma^{\alpha}_{|1n\rangle \to |01\rangle} P_{1n}] \tag{7a}$$

$$\frac{dP_{Nn}}{dt} = \sum_{\alpha n'} -[\Gamma^{\alpha}_{|Nn\rangle \to |N-1n'\rangle} + \Gamma^{\alpha}_{|Nn\rangle \to |N+1n'\rangle}] P_{Nn} + \Gamma^{\alpha}_{|N-1n'\rangle \to |Nn\rangle} P_{N-1n'} + \Gamma^{\alpha}_{|N+1n'\rangle \to |Nn\rangle} P_{N+1n'} \tag{7b}$$

$$\frac{dP_{41}}{dt} = \sum_{\alpha n} [-\Gamma^{\alpha}_{|41\rangle \to |3n\rangle} P_{41} + \Gamma^{\alpha}_{|3n\rangle \to |41\rangle} P_{3n}] \tag{7c}$$

where the transition rates are

$$\Gamma^{\alpha}_{|Nn\rangle \to |N+1n'\rangle} = \frac{1}{\hbar} \sum_{\sigma} \Gamma^{\alpha}_{\sigma} |(d_{\alpha\sigma})^{nn'}_{NN+1}|^2 f_{\alpha}(E_{N+1n'} - E_{Nn}) \tag{8a}$$

$$\Gamma^{\alpha}_{|N+1n'\rangle \to |Nn\rangle} = \frac{1}{\hbar} \sum_{\sigma} \Gamma^{\alpha}_{\sigma} |(d_{\alpha\sigma})^{nn'}_{NN+1}|^2 f^{-}_{\alpha}(E_{N+1n'} - E_{Nn}) \tag{8b}$$

where $\Gamma^{\alpha}_{\sigma} = 2\pi \sum_{k \in \alpha} |V_{\alpha k \sigma}|^2$ is the dot-lead coupling strength, $f_{\alpha}(x) = (1+\exp((x-\mu_{\alpha})/kT_{\alpha}))^{-1}$ is the Fermi–Dirac distribution function in which μ_{α} and T_{α} stand for the chemical potential and the temperature of the lead α, respectively, and $f^{-}_{\alpha} = 1 - f_{\alpha}$.

Solving rate equations in the steady state, the electric and heat currents crossing from the lead α are computed by

$$I^{\alpha} = -e \sum_{N,N',n,n'} \Gamma^{\alpha}_{|Nn\rangle \to |N'n'\rangle} P_{|Nn\rangle} \mathrm{sgn}(N'-N) \tag{9a}$$

$$Q^{\alpha} = \sum_{N,N',n,n'} \Gamma^{\alpha}_{|Nn\rangle \to |N'n'\rangle} (E_{|N'n'\rangle} - E_{|Nn\rangle}) P_{|Nn\rangle} \mathrm{sgn}(N'-N) \tag{9b}$$

where $\mathrm{sgn}(x)$ is a signum function. It is clear that $I^L = -I^R$. In linear response regime, the electric and heat currents are expressed as [15,20]

$$I^{\alpha} = G_V V + G_T \Delta T \tag{10a}$$

$$Q^{\alpha} = MV + K\Delta T \tag{10b}$$

where G_V and G_T are the electrical conductance and the thermal coefficient, respectively. In the limit of zero current, the thermopower is computed by $S = -V/\Delta T = G_T/G_V$. In order to compute G_V and G_T, we assume that $T_L = T_R + \Delta T$ and $\mu_L = \mu_R + e\Delta_V$. Expanding Fermi–Dirac distribution function of the left lead in Eqs. (8a) and (8b) according to $f_L(\varepsilon) = f(\varepsilon) - eVf'(\varepsilon) - \Delta T(\varepsilon - \mu_R)/Tf'(\varepsilon)$ where $f'(\varepsilon) = \partial f(\varepsilon)/\partial\varepsilon$, and setting $I^L = 1/2(I^L - I^R)$, the conductance coefficients can easily obtained from Eqs. (9) [21]. For simulation purpose, we set $\kappa_{ph} = 3\kappa_0$ where $\kappa_0 = (\pi^2 k_B^2/3h)T$ is the quantum of thermal conductance [6] and, assume that the single electron levels in the QDs are degenerate.

3. Results and discussions

The electrical conductance, the thermal coefficient, and the thermal conductance are plotted in Fig. 2 for both weak and strong interdot couplings. Interdot coupling can be controlled by applying gate voltages, therefore both regimes are accessible in experiments. It is interesting to note that the electronic states of N-electron configuration are nearly degenerate in weak interdot tunneling regime. More specifically, the triplet states ($|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$, $(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)/\sqrt{2}$) and the singlet state ($(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)/\sqrt{2}$) are degenerated under conditions that no magnetic field is applied and the interdot coupling is weak enough, see Fig. 1. On the other hand, the DQD system can be considered as a large single QD when the interdot tunneling is strong enough. There are four peaks in G_V. The first peak occurs when the system locates in the states of the three-electron configuration. The second peak appears under condition that the energy level of the dot lies halfway between E_{3n} and E_{2n}. Under this condition, the probability of being in the two-electron configuration goes toward 1 and this transition results in a peak in the conductance. When the energy levels of the dots are near to the chemical potential of the leads and $\varepsilon_{\sigma} + U_{12} > \mu_{\alpha}$, the probability of being in the one electron states increases and as a result the third peak is observed. When the energy levels of the dots are higher than μ_{α}, the system goes from $|1n\rangle$ to $|01\rangle$ and as a consequence the last