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Thermoelectric effects in a double quantum dot system weakly coupled to ferromagnetic leads

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ABSTRACT

Thermoelectric effects through a serial double quantum dot system weakly coupled to ferromagnetic leads are analyzed. Formal expressions of electrical conductance, thermal conductance, and thermal coefficient are obtained by means of Hubbard operators. The results show that although the thermopower is independent of the polarization of the leads, the figure of merit is reduced by an increase of polarization. The influences of temperature and interdot tunneling on the figure of merit are also investigated, and it is observed that increase of the interdot tunneling strength results in reduction of the figure of merit. The effect of temperature on the thermal conductance is also analyzed.

1. Introduction

The thermopower through devices fabricated using nanotechnology has been increasingly studied in recent years [1–11]. Recent advances in the fabrication of nanodevices and the information showing that nanodevices can work as thermal generators with high efficiency [12–14] have increased the importance of such studies. Indeed, violation of the Wiedemann–Franz law [15,16], that the ratio of the electrical conductance to the thermal conductance is proportional to the operating temperature, in nanodevices results in increase of the thermal efficiency and the figure of merit, $ZT = \frac{S^2 G_V T}{\kappa}$, where S is the thermopower, and G_V and T denote the electrical conductance and the temperature, respectively. $\kappa = \kappa_c + \kappa_{ph}$ is composed of the electrical and phonon thermal conductances, respectively. Discreteness of energy levels [17], Coulomb interactions [15,18], interference effects [19], and so on lead to the fact that nanodevices have more thermal efficiency than bulky samples.

In recent years, investigation of thermoelectrical devices fabricated from quantum dots (QDs) has attracted a lot of attention theoretically and experimentally [1,2,18–26]. However, thermoelectric effects through double quantum dots (DQDs) results in novel phenomena needing more studies. A few articles have analyzed the thermopower through a DQD just recently [27–29]. Chi et al. [28] showed that ZT has two huge peaks in the vicinity of the electron–hole symmetry points. Trocha and Barnaś [29] reported that ZT in DQD systems is enhanced due to Coulomb interactions and interference effects. We have recently studied [30] the effects of Coulomb interactions and interdot tunneling on the thermopower of a DQD system weakly coupled to metallic electrodes.

In this article, the influences of polarization of the leads, temperature, and interdot tunneling on the figure of merit and the thermoelectric conductances of a serial DQD weakly coupled to ferromagnetic leads are analyzed. The many-body representation introduced in Ref. [31] is used to obtain formal expressions for the electrical and thermal conductances, thermopower, and figure of merit. The Hamiltonian and the model used for the calculations are described in Section 2. Section 3 is devoted to numerical results and, at the end, Section 4 presents our conclusions.

2. Model and method

We consider two single-level quantum dots coupled to ferromagnetic leads. The Hamiltonian describing the system is given as

$$H = \sum_{\alpha k\sigma} \varepsilon_{\alpha k\sigma} c^{\dagger}_{\alpha k\sigma} c_{\alpha k\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + U_{12} \sum_{\sigma\sigma'} n_{L\sigma} n_{R\sigma'} + t \sum_{\sigma} [d^{\dagger}_{L\sigma} d_{R\sigma} + H.C] + \sum_{\alpha k\sigma} [V_{\alpha k\sigma} c^{\dagger}_{\alpha k\sigma} d_{\alpha\sigma} + H.C] \quad (1)$$

where $c_{\alpha k\sigma}$ ($c^{\dagger}_{\alpha k\sigma}$) destroys (creates) an electron with spin σ and wave vector k in lead $\alpha = L, R$. The energy levels of the leads are

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spin-dependent because the leads are ferromagnetic. The second and third terms in the above equation describe each dot. $d_{i\sigma}$ ($d_{i\sigma}^\dagger$) is the annihilation (creation) operator of the ith ($i = L, R$) dot and $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$. The energy levels of each dot are assumed to be degenerate. U_i and U_{12} denote, respectively, on-site and interdot Coulomb repulsions. t is the interdot tunneling strength, whereas $V_{\alpha k\sigma}$ denotes the dot–lead coupling strength. In order to study the system, the Hubbard operators have been used. In this model, the Hamiltonian of the isolated DQD system is diagonalized and the creation and annihilation operators are expanded in terms of the obtained eigenstates. It is obvious that the system has 16 different states shown as $|N, n\rangle$ where $N = 0, \ldots, 4$ is the number of electrons, whereas n denotes the nth state of the N-electron configuration. By expanding the annihilation operator as

$$d_{\alpha\sigma} = \sum_{Nnn'} (d_{\alpha\sigma})_{NN+1}^{nn'} X_{NN+1}^{nn'} \tag{2}$$

where the Hubbard operator, $X_{NN+1}^{nn'} = |Nn\rangle\langle N+1n'|$, describes a transition in which an electron inside the DQD system is annihilated, the whole Hamiltonian is given as

$$H = \sum_{\alpha k\sigma} \varepsilon_{\alpha k\sigma} c_{\alpha k\sigma}^\dagger c_{\alpha k\sigma} + \sum_{Nn} E_{Nn} h_N^n + \sum_{\alpha k\sigma Nnn'} [V_{\alpha k\sigma} (d_{\alpha\sigma})_{NN+1}^{nn'} c_{\alpha k\sigma}^\dagger X_{NN+1}^{nn'} + H.C] \tag{3}$$

where $h_N^n = |Nn\rangle\langle Nn|$.

Now, the population number P_{Nn}, the probability of being in the state $|Nn\rangle$, is computed by means of the density matrix approach. Coupling to the leads is considered to be so weak that non-diagonal elements of the density matrix are ignored because they are proportional to $V_{\alpha k\sigma}^4$. Using the Markov approximation and the wide band limit, the time evolution of the population numbers is given as [31]

$$\frac{dP_{01}}{dt} = \sum_{\alpha n} [-\Gamma_{|01\rangle\to|1n\rangle}^\alpha P_{01} + \Gamma_{|1n\rangle\to|01\rangle}^\alpha P_{1n}] \tag{4a}$$

$$\frac{dP_{Nn}}{dt} = \sum_{\alpha n'} -[\Gamma_{|Nn\rangle\to|N-1n'\rangle}^\alpha + \Gamma_{|Nn\rangle\to|N+1n'\rangle}^\alpha] P_{Nn} + \Gamma_{|N-1n'\rangle\to|Nn\rangle}^\alpha P_{N-1n'} + \Gamma_{|N+1n'\rangle\to|Nn\rangle}^\alpha P_{N+1n'} \tag{4b}$$

$$\frac{dP_{41}}{dt} = \sum_{\alpha n} [-\Gamma_{|41\rangle\to|3n\rangle}^\alpha P_{41} + \Gamma_{|3n\rangle\to|41\rangle}^\alpha P_{3n}]. \tag{4c}$$

It is obvious that there is one configuration for zero- and four-electron states. The transition rates are

$$\Gamma_{|Nn\rangle\to|N+1n'\rangle}^\alpha = \frac{1}{\hbar} \sum_\sigma \Gamma_\sigma^\alpha |(d_{\alpha\sigma})_{NN+1}^{nn'}|^2 f_\alpha (E_{N+1n'} - E_{Nn}) \tag{5a}$$

$$\Gamma_{|N+1n'\rangle\to|Nn\rangle}^\alpha = \frac{1}{\hbar} \sum_\sigma \Gamma_\sigma^\alpha |(d_{\alpha\sigma})_{NN+1}^{nn'}|^2 f_\alpha^- (E_{N+1n'} - E_{Nn}) \tag{5b}$$

where $\Gamma_\sigma^\alpha = 2\pi \sum_{k\in\alpha} |V_{\alpha k\sigma}|^2$ is the spin-dependent tunneling rate, $f_\alpha(x) = (1 + \exp((x - \mu_\alpha)/kT_\alpha))^{-1}$ is the Fermi–Dirac distribution function in which μ_α and T_α stand for the chemical potential and the operating temperature of the lead α, respectively, and $f_\alpha^- = 1 - f_\alpha$. The charge and energy currents are computed by solving Eqs. (4) in the steady state situation ($\frac{dP_{Nn}}{dt} = 0$)

$$I^\alpha = -e \sum_{N,N',n,n'} \Gamma_{|Nn\rangle\to|N'n'\rangle}^\alpha P_{|Nn\rangle} \operatorname{sgn}(N' - N) \tag{6a}$$

$$Q^\alpha = \sum_{N,N',n,n'} \Gamma_{|Nn\rangle\to|N'n'\rangle}^\alpha (E_{|N'n'\rangle} - E_{|Nn\rangle}) P_{|Nn\rangle} \operatorname{sgn}(N' - N) \tag{6b}$$

where $\operatorname{sgn}(x)$ is a signum function.

To compute the thermoelectrical characteristics of the system, the linear response regime is used. We assume that the left lead is slightly hotter than the right one ($T_L = T_R + \Delta T$), and $\mu_L = \mu_R - e\Delta V$, so that the charge and energy currents are given as follows:

$$I^\alpha = G_V \Delta V + G_T \Delta T \tag{7a}$$

$$Q^\alpha = M\Delta V + K\Delta T \tag{7b}$$

where G_V is the electrical conductance and G_T is the thermal coefficient. The thermopower is defined as minus the ratio of the induced voltage to the applied temperature gradient under the condition that the charge current is zero, so we have $S = \frac{G_T}{G_V}$. Putting $I^L = 1/2(I^L - I^R)$ and expanding the Fermi–Dirac distribution function as $f_L(x) = f_R(x) - x/Tf'(x)\Delta T + e\Delta V f'(x)$ where $f'(x) = \partial f(x)/\partial x$, one can easily obtain

$$G_V = -\frac{e^2}{2\hbar} \sum_{Nnn'} \sum_\sigma P_{Nn} \Gamma_\sigma^L [|(d_{L\sigma})_{NN+1}^{nn'}|^2 f'(E_{N+1n'} - E_{Nn}) + |(d_{L\sigma})_{N-1N}^{n'n}|^2 f'(E_{Nn} - E_{N-1n'})] \tag{8a}$$

$$G_T = \frac{e}{2\hbar} \sum_{Nnn'} \sum_\sigma P_{Nn} \Gamma_\sigma^L \left[|(d_{L\sigma})_{NN+1}^{nn'}|^2 \times \frac{(E_{N+1n'} - E_{Nn})}{T} f'(E_{N+1n'} - E_{Nn}) + |(d_{L\sigma})_{N-1N}^{n'n}|^2 \frac{(E_{Nn} - E_{N-1n'})}{T} f'(E_{Nn} - E_{N-1n'}) \right]. \tag{8b}$$

Using the above equations and the Onsager relation, the thermal conductance is computed as [17]

$$\kappa_c = [K - S^2 G_V T] \tag{9}$$

where

$$K = -\frac{1}{2\hbar} \sum_{Nnn'} \sum_\sigma P_{Nn} \Gamma_\sigma^L \left[|(d_{L\sigma})_{NN+1}^{nn'}|^2 \times \frac{(E_{N+1n'} - E_{Nn})^2}{T} f'(E_{N+1n'} - E_{Nn}) + |(d_{L\sigma})_{N-1N}^{n'n}|^2 \frac{(E_{Nn} - E_{N-1n'})^2}{T} f'(E_{Nn} - E_{N-1n'}) \right]. \tag{10}$$

For simulation purposes, we assume that $\Gamma_\uparrow^L = \Gamma_\uparrow^R = \Gamma_0$ and the spin-down tunneling rate is equal to $\Gamma_\downarrow^L = \Gamma_\downarrow^R = \alpha\Gamma_0$ where $0 \le \alpha \le 1$. It is obvious that $\alpha = 1$ denotes normal metallic electrodes whereas $\alpha = 0$ stands for half-metal leads. We also set $\kappa_{ph} = 3\kappa_0$ where $\kappa_0 = \frac{\pi^2 k_B^2}{3h} T$ is the quantum of thermal conductance [32] and assume that the single electron levels in the QDs are degenerate. In recent years, the phonon contribution in the transport through QDs has been extensively studied experimentally and theoretically [33–35].

3. Results and discussion

The figure of merit (ZT) as a function of the QDs' energy level and the temperature is plotted in Fig. 1 for different αs. A similar plot was previously presented in Ref. [18] for a QD coupled to ferromagnetic electrodes and in Ref. [29] for a DQD coupled to external electrodes. One can observe that increasing α results in the reduction of ZT. On the other hand, ZT has some peaks whose intensities decrease with increase of temperature, but become wider. The results also show that ZT approaches zero in $-3 < \varepsilon_i < 0$ and high temperature ($T > 4k$). With respect to the fact that ZT