Thermoelectric effects through weakly coupled double quantum dots

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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.

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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 $ZT = G_s S^2 T / k$ denoting the energy conversion efficiency is an important factor in thermoelectronic devices. $S$ and $G_s$ denote Seebeck coefficient and electrical conductance, respectively. $T$ is the temperature of the system and $k = k_c + k_{ph}$ 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 equilibrium.

Trocha and Barnas [18] reported that the figure of merit has two huge peaks in vicinity of electron-hole equilibrium. Figure of merit has two huge peaks in vicinity of electron–hole equilibrium Green function formalism. Their results show that 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 equilibrium.

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

$$H = H_{leads} + H_{DD} + H_T$$

where $H_{leads} = \sum_{\sigma} \epsilon_d d_{\sigma}^d d_{\sigma}^s$ describes the left and right leads in which $\epsilon_d$ is the energy of the electron with wave vector $k$, spin $\sigma$ in the lead $z = L,R$, and $c_{\sigma \delta \sigma}^L (c_{\sigma \delta \sigma}^R)$ is annihilation (creation) operator. $H_{DD}$ describes the isolated double quantum dot and is given as

$$H_{DD} = \sum_{\sigma \sigma'} \epsilon_d d_{\sigma}\sigma d_{\sigma' \sigma} + \sum_{\sigma \alpha = \Gamma, \delta} U_{\alpha} n_{\alpha \sigma} n_{\alpha \bar{\sigma}} + \sum_{\sigma} \left[ d_{\sigma}^d d_{\sigma}^s + d_{\sigma}^s d_{\sigma}^d \right]$$

where $\epsilon_d$ stands for the energy level of the zth dot, while $d_{\sigma\alpha}(d_{\sigma\alpha}^d)$ destroys (creates) an electron with spin $\sigma$ in the dot $z$. $U_{\alpha} = U_{\alpha L} + U_{\alpha R}$ denote, respectively, intra- and interdot Coulomb repulsions, and $n_{\alpha \sigma} = d_{\alpha \sigma}^d d_{\alpha \sigma}^s$. 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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leads as follows:

\[ H_T = \sum_{n \neq \nu} [V_{sk\nu} c_{sk}^\dagger d_{\nu} + V_{sk\nu}^* d_{\nu}^\dagger c_{sk}] \]

where \( h_{\nu \nu}^n = |N, \nu \rangle \langle N, \nu | \) are the diagonal transitions of the Hubbard operators \( X_{\nu \nu}^N = |N, \nu \rangle \langle N, \nu | \). Whereas \( d_{\nu \nu}^\dagger \) annihilates an electron with spin \( \sigma \) in the dot \( \nu \). It is straightforward to show

\[ d_{\nu \nu} = \sum_{n \neq \nu} [d_{\nu \nu}^\dagger n_{\nu}^N + \gamma_{N \nu}^{NN} n_{\nu} n_{\nu} + 1] \]

where \( (d_{\nu \nu} n_{\nu}^N) = |N, \nu \rangle \langle N, \nu | + 1 \). Using Eqs. (4) and (5), the total Hamiltonian can be written as

\[ H = \sum_{sk} h_{sk} n_{sk} + \sum_{\nu} E_{\nu} n_{\nu} + \sum_{sk \nu} [V_{sk \nu} c_{sk}^\dagger n_{\nu}^N + 1 c_{sk} n_{\nu}^N + 1 + H.C.] \]

Now, we can compute the population numbers \( P_{\nu \nu} \), probability of being in the state \( |N, \nu \rangle \), 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 \( V_{sk\nu} \). Using the Markovian limit and the wide band limit, the time evolution of the population numbers are given as [19]

\[ \frac{dP_{\nu \nu}}{dt} = \sum_{\nu'} \Gamma_{\nu \nu'}^t \langle \nu' | P_{\nu \nu} + \Gamma_{\nu \nu'}^t \langle \nu | P_{\nu \nu'} \] (7a)

\[ \frac{dP_{\nu \nu}}{dt} = \sum_{\nu'} \left( \Gamma_{\nu \nu'}^t \langle \nu' | P_{\nu \nu'} + \Gamma_{\nu \nu'}^t \langle \nu | P_{\nu \nu'} \right) \] (7b)

where the transition rates are

\[ \Gamma_{\nu \nu'}^t = \frac{1}{\hbar} \int dx f(x) \langle \nu' | \hat{H}_T | \nu \rangle \]

for the energy eigenvalues is shown in Fig. 1. Now, Eq. (2) of the contributions of the fourth order in \( \gamma_{N \nu}^{NN} \) elements of the density matrix are neglected, because they give the probability of being in the state \( |N, \nu \rangle \). Using Eqs. (4) and (5), the conductance coefficients can easily obtained from Eqs. (9) [21]. For simulation purpose, we set \( K_{Q \nu} = 3K_{Q} \) where \( K_{Q} = (\pi e_0^2/3h)T \) 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 \( \{|1, 1>, \ldots, |1, 1>, |1, 1>, |1, 1>, \sqrt{2} \rangle \) and the singlet state \( \{|1, 1>, \ldots, |1, 1>, 1/\sqrt{2} \} \) 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 QD system can be considered as a single large QD when the interdot tunneling is strong enough. There are four peaks in \( G_{\nu} \). 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 \( \mu_3 + U_{12} \geq \mu_{\nu} \), 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 \( \mu_{\nu} \), the system goes from \( |1n\rangle \) to \( |01\rangle \) and as a consequence the last
peak is observed. Indeed, each peak observed in $G_T$ denotes one of the occupied eigenstates of the DQD. In strong $t$, the eigenstates of the $N$-electron configuration are split, so that, for example, the singlet state is more accessible than the triplet states at $N=2$. The position of each peak shifts proportional to $t$. It is also observed that the peak height is decreased with increase of $t$. Fig. 2b describes the behavior of the thermal coefficient as a function of the energy level of the dots. It is observed that $G_T$ becomes zero in some energies. There are two different reasons. It is straightforward to obtain $G_T$ by expanding the Fermi function of the left lead in Eqs. (8) and substituting in Eq. (9a), so we have

$$G_T = \frac{1}{2N} \sum_{n=0}^{N} \sum_{\sigma} \rho_{0n} \left[ \left( \frac{d\rho_{0n}}{dn} \right)_{1^{+}} \right] \frac{2E_{N+1\sigma} - E_{0n}}{\pi^2} f(E_{N+1\sigma} - E_{0n})$$

$$+ \left( \frac{d\rho_{0n}}{dn} \right)_{1^{-}} \frac{2E_{0n} - E_{N-1\sigma}}{\pi^2} f(E_{0n} - E_{N-1\sigma})$$

(11)

At $\epsilon = -4, -3, -1, 0$, $G_T$ becomes zero because the probability of being in the $N$- and $N+1$-electron states will be equal to each other and, the energy levels are identical. In such cases, $G_T$ becomes zero because the energy difference between the occupied level and its neighbor levels is equal. Note, in these energies the system is in an individual $N$-electron state. In contrast with former case, the left side of $G_T$ is negative in these points. This is so-called bipolar effect previously reported in multilevel quantum dots. For example, the probability of finding the system in the singlet or triplet state is one at $\epsilon = -2$, and we have $E_{2\sigma T} - E_{1\sigma} = -(E_{3n} - E_{2\sigma T})$, that $S(T)$ stands for singlet (triplet). At $\epsilon = -3$, one can show that $P_{2\sigma T} = P_{3n} = 0.5$. Increasing interdot tunneling strength results in the decrease of the thermal conductance height and the shift of the zeroes of $G_T$ because the eigenvalues of the Hamiltonian are a function of the interdot coupling. In comparison with $G_T$, $\kappa_T$ has three broader peaks. It is interesting to note that if the operating temperature is much lower than $2K$, one observes that there are four peaks in the thermal conductance. Indeed, increase of temperature results in the increase of the heat of the electrons and the amplification of the bipolar effect so that peaks are now merged and there are three peaks. Increase of interdot tunneling gives rise to decrease of the peaks’ height and more broadening in the thermal conductance spectrum. One can also observe that the interdot tunneling can significantly influence on the shape of $\kappa_T$, because it is not only a function of $G_T$ and $G_T$ but also a function of the thermopower and $K$, for more discussion see Ref. [15].

The thermopower and the thermo-electrical figure of merit are described in Fig. 3. The thermopower oscillations in a sawtooth fashion as a function of the energy level. Change of the number of electrons on the system results in such oscillations. Such behavior was previously observed in single quantum dots [2,23]. The thermopower is antisymmetric because of electron–hole symmetry. The thermal difference produced between the leads results in that more electrons move above the chemical potential of the left lead which is hotter and as a result, more holes create below the chemical potential [16]. The thermopower caused by holes is positive while, negative thermopower is caused by electrons. The results show that the interdot tunneling strength does not influence on the magnitude of the thermopower. Such result was before reported [22]. The figure of merit obtained here is much smaller than results reported in Refs. [16,17] because we consider the thermal conductance of phonons. It is observed that there are huge peaks in the figure of merit in the vicinity of the electron–hole symmetry points, recently reported in Ref. [17]. The thermopower and the figure of merit are suppressed in so me energies due to bipolar effect. As we expect the thermopower becomes zero in electron–hole symmetry points.
The dependence of the figure of merit on the temperature and interdot tunneling is studied in Fig. 4. The energy level of the dots is set $e_i = -4.5$ meV, in which the figure of merit has a resonant peak in Fig. 3. It is observed that increasing temperature results in suppressing of the figure of merit because, the lattice thermal conductance ($k_0$) is linearly related to the temperature, so increase of the temperature leads to increase of $k_0$ and as a result, figure of merit will be decreased. Splittings of energy levels with increase of interdot tunneling results in reduction of the figure of merit. Results show that the figure of merit can take significant magnitude in high tunneling regime if the temperature of the system is low enough.

The influence of intra- and interdot Coulomb interactions on the figure of merit is examined in Fig. 5. Increase of Coulomb interaction results in increase of the figure of merit because, the Coulomb interaction decreases the bipolar effect. Enhancement of figure of merit due to Coulomb blockade effect in multilevel quantum dots has been recently observed [16]. Indeed, the level spacing is increased by increase of Coulomb interaction. It is interesting to note that intra- and interdot Coulomb interactions significantly influence on the figure of merit. It comes from the fact that the necessary energy for adding of an extra electron in each dot is related to both intra- and interdot Coulomb interactions. Notice, changing the single energy levels of the QDs can slightly change the color map of the figure of merit.

4. Conclusion

In this paper, we study the thermopower through double quantum dot systems weakly coupled to metal electrodes by means of density matrix approach. The many-body representation is used to compute the population numbers and the current. The effects of the interdot tunneling and temperature on the figure of merit and the thermopower are examined. It is found that the figure of merit is enhanced by the increase of Coulomb repulsion because the Coulomb interaction results in the increase of the level spacing and as a result, the bipolar effect is reduced.

References

[21] A typical deriving of the conductance coefficients from rate equations can be found, for example, in Refs. [3,15].