Thermoelectric Properties of a T-Shaped Quantum Dot with Relatively Strong On-Site Coulomb Interaction

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The thermoelectric properties of a correlated T-shaped quantum dot system symmetrically coupled to two metallic leads are studied. This system is described by a generalized Anderson model and an approximation of correlation dynamics is employed to derive the corresponding Green’s functions. The properties are investigated by calculating the electrical conductance \( G \), thermal conductance \( \kappa \), thermopower \( S \) and figure of merit \( ZT \) for different gate voltages and temperatures. At last but not least, our numerical calculation results show that the thermoelectric properties of the T-shaped quantum dot with relatively strong on-site Coulomb interaction are mainly influenced by the bipolar effect, which is consistent with some theoretical and experimental results. [doi:10.2320/matertrans.M2013460]

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1. Introduction

Quantum dot systems (QDs) have attracted much more attention in the past few decades. The systems not only include various complex many-body effects (e.g., Coulomb blockade & Kondo effect), but also have many promising applications.\(^1,2\) The thermoelectric effects of QDs have been concerned due to their high efficiency of converting heat into electricity or vise versa. As we know, the QD thermoelectric effect is a long standing issue in condensed matter and material physics. Beenakker and Staring\(^1\) first studied the thermoelectric related properties of quantum dots theoretically and experimentally.\(^2,3\) Recently, it has received renewed special attention because of the technological progress in nanostructures and mesoscopic devices such as QDs and nanotubes.\(^4\)–\(^12\)

Nevertheless, the figure of merit (FOM) \( ZT = S^2 GT/\kappa \) depends on the Seebeck coefficient \( S \), electrical conductance \( G \), and thermal conductance \( \kappa \) of the material. In order to optimize the thermoelectric properties of materials, several possible structures have been proposed, (e.g., different quantum dot structures coupled to leads symmetrically or asymmetrically).\(^13\)–\(^16\) To our best knowledge, using the approximation of correlation dynamics and the nonequilibrium Green’s function techniques, only a small amount of theoretical work has been done on the thermoelectric properties of the T-shaped QD with just one side dot.\(^17\)–\(^20\) The other noteworthy observation is the thermo-electric properties of T-shaped QD in the relatively strong Coulomb interaction.

This paper is organized as follows. The model employed and the thermoelectric related concepts in terms of nonequilibrium Green’s functions would be introduced first in Section 2. Also in this section, the Green’s functions are calculated with the equation of motion (EOM) method using the approximation of correlation dynamics. And Section 3 will present numerical results and discussions of the thermoelectric properties. The conclusions will be drawn in Section 4.

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![Diagram of T-shaped quantum dot](image)

Fig. 1 Schematic of the T-shaped quantum dot coupled to metallic leads with just one side dot. Here \( L \) and \( R \) represent two leads, and quantum dot \( 1 \) and \( 2 \) represent the detector and side dot, respectively. \( V_L \) and \( V_R \) represent the tunneling interaction constants between the detector dot and the leads. The constant \( t \) is the coupling constant between the detector dot and the side dot.

2. Model and Methods

Our model is based on a system with an interacting central region connected to two noninteracting metallic leads. The interacting central region consists of a detector quantum dot and just one side quantum dot. This is the so-called T-shaped quantum dot system (Fig. 1). Thus the total Hamiltonian of this structure could be described by Anderson model\(^23\)–\(^27\) which has the following form:

\[
H = H_L + H_R + H_D + H_T, \tag{1}
\]

where \( H_\alpha \) is the kinetic energy of the free electron in the metallic lead \( \alpha (\alpha = L \text{ (left)}, R \text{ (right)}) \), \( H_D \) gives the energy of the localized electron of the two dots, and the last term \( H_T \) describes the electron hybridization effect between the leads and the detector quantum dot. The first two terms describing the kinetic energy of the free electrons in the leads are given by

\[
H_L + H_R = \sum_{k\sigma\alpha=\ell L,R} \epsilon_k c_{k\sigma\alpha}^\dagger c_{k\sigma\alpha}, \tag{2}
\]

where \( c_{k\sigma\alpha}^\dagger \) (\( c_{k\sigma\alpha} \)) is the fermionic operator which creates (annihilates) a noninteracting electron with momentum \( k \),
spin $\sigma$ and corresponding energy level $\varepsilon_i$ of the lead $\alpha$. The third term $H_D$ for the interacting central quantum dot region can be treated as
\[
H_D = \sum_{i=1}^{2} \varepsilon_i d_{\alpha i}^{\dagger}d_{\alpha i} + \sum_{i=1}^{2} U n_{\alpha i}n_{\beta i} + t \sum_{\sigma}(d_{\alpha i}^{\dagger}d_{\sigma 2} + d_{\sigma 2}^{\dagger}d_{\alpha i}).
\] (3)

The first term of eq. (3) is the kinetic energy of quantum dot 1 and 2, and the second term is Coulomb interactions of the two dots on-site, and the last term is hybridization effect between dot 1 and dot 2. $d_{\alpha i}^{\dagger}$ $(d_{\alpha i})$ is the fermionic operator which creates (annihilates) a localized electron with spin $\sigma$ in the corresponding quantum dot ($i=1$, detector dot; $i=2$, side dot). In the above equation $n_{\alpha i} = d_{\alpha i}^{\dagger}d_{\alpha i}$ is the occupation number operator of the localized electron with energy level $\varepsilon_i$ and spin $\sigma$. The second term of eq. (3) is related to finite on-site Coulomb interaction described by $U_i$ for each dot. The last term involving coupling constant $t$ describes the electron tunneling between these two dots.

The tunneling interaction between the free electron in the lead $\alpha$ and the localized electron in the detector dot is given by
\[
H_T = \sum_{k,\sigma} V_{k\alpha i}(d_{k\sigma}^{\dagger}d_{i\sigma} + d_{i\sigma}^{\dagger}d_{k\sigma \alpha}).
\] (4)

Generally the constants $V_{k\alpha L}$ and $V_{k\alpha R}$ could be different for these two leads. For the sake of simplicity of computation, in this paper we only account for the symmetric coupling case.

The nonequilibrium Green’s function method and the linear response theory have been used to study the thermo-electric properties, including the electrical conductance $G$, the thermocalcium $\kappa$, the thermopower $S$, and the thermo-electric figure of merit $ZT$. The electronic and the heat current through the quantum dot could respectively be expressed as
\[
J = \frac{e}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega [f_L(\omega) - f_R(\omega)] \Gamma_{\sigma}(\omega) \rho_{\sigma}(\omega),
\] (5)

\[
J_Q = \frac{1}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega [f_L(\omega) - f_R(\omega)] \Gamma_{\sigma}(\omega)(\omega - eV) \rho_{\sigma}(\omega),
\] (6)

where $f_\omega(\omega) = [\exp(\omega - \mu_\omega)/k_B T]^{-1}$ is the Fermi distribution function of the lead $\alpha$, which has different chemical potential $\mu_\alpha = E_F + V_\alpha$ with a voltage bias $\mu_L - \mu_R = eV$. Here $k_B$ is the Boltzmann constant, $E_F$ is the Fermi energy level, $e$ is the electron charge and $\rho_{\sigma}(\omega)$ is the local density of states. $\Gamma_{\sigma}(\omega)$ is the transmission coefficient which could be expressed as $\Gamma_{\sigma}(\omega) = T^{\alpha}_{\sigma}(\omega)T^{\beta}_{\sigma}(\omega) [\Gamma^{\alpha}_{\sigma}(\omega) + \Gamma^{\beta}_{\sigma}(\omega)]$, where $T^{\alpha}_{\sigma}(\omega) = 2\pi \sum_{k} |V_{k\sigma}|^2 \delta(\omega - \varepsilon_k)$ is the so-called line-width function. This function can also describe the coupling strength between the detector dot and the lead $\alpha$.\(^\text{28}\)

In the linear regime, for infinitesimally small voltage biases and temperature gradients, the two current expressions can be approximated in the terms of three linear coefficients $L_{ij}$ ($i, j=1, 2$) which could be directly written as:
\[
L_{11} = \frac{T}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \Gamma_{\sigma}(\omega) \text{Im} \left[ G^{\prime}_{\sigma}(\omega) \left( -\frac{\partial f_L(\omega)}{\partial \omega} \right) \right],
\] (7)

\[
L_{12} = \frac{T^2}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \Gamma_{\sigma}(\omega) \text{Im} \left[ G^{\prime}_{\sigma}(\omega) \left( -\frac{\partial f_R(\omega)}{\partial \omega} \right) \right],
\] (8)

\[
L_{22} = \frac{T^2}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \Gamma_{\sigma}(\omega) \text{Im} \left[ G^{\prime}_{\sigma}(\omega) \left( -\frac{\partial f_L(\omega)}{\partial \omega} \right) \right].
\] (9)

Accordingly, the electrical conductance is given by $G = e^2 L_{11}/T$, the thermal conductance by $k = (L_{22} - L_{11})/L_{22}$, the thermopower (Seebeck coefficient)$S = -L_{12}/(eTL_{11})$, and the figure of merit by $ZT = S^2 GT/k$.\(^\text{28}\)

The EOM method is used to derive the Green’s functions. It is well-known that this method would lead to an infinite hierarchy of higher-order Green’s functions and these functions can not be solved exactly due to the existence of the on-site Coulomb interaction. So an appropriate self-consistent approximation procedure should be employed to decouple the hierarchy. The quantum many-body correlation dynamics approximation method is widely used.\(^\text{17-19}\)

Following the procedure of Wang et al., we could obtain the Hubbard-I approximation of the Green’s functions of the detector and side dot, respectively,

\[
G_{1\sigma}(\omega) = \frac{1}{(\omega - \varepsilon_1)(\omega - \varepsilon_1 - U_1)} - \frac{t^2}{(\omega - \varepsilon_2)(\omega - \varepsilon_2 - U_2)} - \sum_{k} \frac{V_{k1}^2}{(\omega - \varepsilon_k)},
\] (10)

\[
G_{2\sigma}(\omega) = \frac{1}{(\omega - \varepsilon_2)(\omega - \varepsilon_2 - U_2)} - \frac{t^2}{(\omega - \varepsilon_1)(\omega - \varepsilon_1 - U_1)} - \sum_{k} \frac{V_{k1}^2}{(\omega - \varepsilon_k)}.
\] (11)

Now, we could self-consistently calculate the Green’s functions accordingly with the Fig. 2. And then the thermo-electric quantities also could be easily calculated.

3. Numerical Results and Discussions

In the following numerical calculations, we choose the coupling interaction constant $t$ between the detector dot and the side dot as the energy unit, i.e., $t = 1$. As we are only interested in the linear-response regime the temperatures of the two leads are set to be $T_L = T_R = T$. And we have $G_L = G_R = G$ corresponding to the case that the detector dot is coupled to the two leads symmetrically. We also set $E_F = 0$. In principle the localized energy levels of the dots
(including the detector dot and the side dot) could be tuned by the gate voltage, \( \frac{1}{U_1} = \frac{1}{U_2} = \frac{1}{U} \). Table 1 lists some parameters used in the simulations.

Firstly, the electron occupation number per spin orientation for each dot versus applied gate voltage is calculated for different temperatures (the figure is not listed here). It is worth emphasizing once again that the distribution function used to calculate the occupation number is the "pseudoequilibrium" Fermi distribution function.22 The overall trend of the electron occupation number can be roughly divided into three parts. When the applied gate voltage is lower than \(-U\), the occupation number for each dot nearly remains stable, equal to one. As the gate voltage is between \(-U\) and \(E_F\), the occupation number is almost 0.5. Finally the occupation number tends to zero when the voltage is higher than \(E_F\).

Moreover, the occupation number undergoes an abrupt decline when the applied voltage is around \(\frac{1}{U}\) or \(\frac{E_F}{t}\). The fall to about zero as the voltage is higher than \(E_F\) indicates that electrons will flow directly from the left lead to the right.

Figure 3 shows the dependence of the electrical conductance \(G\) on the applied gate voltage for different temperatures. The peak structure for the electrical conductance is basically similar to that reported in Refs. 14 and 26. The electrical conductance \(G\) presents an insulating band forms. Zheng et al. argued that this is attributed to the strengthening of the destructive quantum interference among infinite Feynman paths.26 Obviously several peaks as usual are shown in this figure, exhibiting the typical Coulomb blockade effect. These peaks locate at around \(\frac{1}{U}\) and \(\frac{E_F}{t}\). As the temperature rises no shift appears for the peak positions, yet each peak height has a slight decrease. This decrease can be interpreted as that the increase of temperature weakens the quantum interference effect.29

Figure 4 shows the linear thermal conductance \(\kappa\) as a function of the applied gate voltage at different temperatures. Several thermal conductance peaks similar to those of the electrical conductance can also be observed here, especially at lower temperatures. More specifically, at the lowest operating temperature considered here \((k_B T = 0.02t)\) the structure of the thermal conductance \(\kappa\) resembles that of the electrical conductance; when the operating temperature increases to \(k_B T = 0.04t\), two inner peaks begin to split; as the temperature rises to \(k_B T = 0.08t\), all the four peaks split. Liu et al. argued that this is induced by the bipolar effect.21 The peak of the thermal conductance decreases and becomes broader with the increase of temperature, which is in

<table>
<thead>
<tr>
<th>(k_B T/t)</th>
<th>(U/t)</th>
<th>(\varepsilon_d/t)</th>
<th>(I'/t)</th>
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<tr>
<td>0.02/0.04/0.08</td>
<td>5</td>
<td>—</td>
<td>0.5</td>
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results of Scheibner temperatures (Fig. 5), consistent with the experimental called bipolar effect) with respect to gate voltage at different
accordance with Ref. 24). Nie et al. argued that it is due to
the broadening of the Fermi distribution function.24)

The thermal power (S) exhibits a change of sign (the so-called bipolar effect) with respect to gate voltage at different temperatures (Fig. 5), consistent with the experimental results of Scheibner et al.30) and theoretical prediction in the metallic single-electron transistor.31,32) The sign of the thermopower S could indicate the main channel of heat transportation. When heat is mainly carried by hole channels, the sign is positive. Otherwise the sign is negative as the transportation. When heat is mainly carried by hole channels, the sign is positive. Otherwise the sign is negative as the

Figure 6 describes the figure of merit ZT at different temperatures. It is found that the figure of merit ZT increases as temperature increases, while these peaks locating at the level positions ε_{d1} = −U and ε_{d2} = E_F begin to split when the temperature rises from k_B T = 0.04r. It is supposed to be induced by the bipolar effect,21) same with the variation of the thermal conductance κ with temperature.

4. Conclusions

The thermoelectric properties of a T-shaped quantum dot with relatively strong on-site Coulomb interaction are investigated for different gate voltages and temperatures. This dot system just containing one side dot is symmetrically coupled to two metallic leads and it is described by a microscopic Anderson quantum model. The approximation method of correlation dynamics is used to deal with the hierarchy of Green’s functions. It should be noted that throughout this paper phonon’s contribution to thermal conductance has been neglected as it can be controlled to be rather small.14) At last but not least, our numerical calculation results show that the thermoelectric properties (electrical conductance G, thermal conductance κ, thermopower S, and figure of merit ZT) of the T-shaped quantum dot with relatively strong on-site Coulomb interaction, are mainly influenced by the bipolar effect, which is consistent with some theoretical and experimental results.

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REFERENCES