Enhancement of Thermoelectric Efficiency in Double Quantum Ring Structure

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Citation

Abstract
In this paper, we present our theoretical treatment for electron transport through double quantum ring attached to the donor and left lead on the left side, while on the right side, it is attached to the acceptor and right lead, with the magnetic flux threading both two rings. Our treatment is based on the time-dependent Hamiltonian model. The equations of motion are derived for all subsystems, then the steady state is considered to obtain an analytical expression for the transmission probability as a function of system energies. We employed the transmission probability to calculate the thermoelectric properties for this structure and investigate the temperature effect on the thermoelectric properties. It is found that the thermoelectric efficiency of the double quantum ring may be high due to the Fano effect at temperature \( T=100 \text{K} \).

1. Introduction

Demanding to advances in the nanotechnology, understanding, and controlling electron transport through the quantum dot structures are one of the most important works in nanoscale systems [1].

Among nanostructures, ring shaped devices [2] (often called quantum rings [3]) are intensely studied due to their electronic, magnetic and optical properties. Also due to their ability to show various types of quantum interference phenomena, such as the well-known Aharonov-Bohm effect [4-7], when the wave function of electron passing around a magnetic flux experiences a phase shift as a result of the enclosed magnetic flux. The quantum interference is produced by electrons which travel coherently along the two arms of the ring [8].

The thermoelectric properties of nanostructures benefit increasing interest in last years. This interest is expected to be useful in construction high-efficiency energy conversion devices [9]. The main purpose is to enhance the thermoelectric efficiency by controlling the energy transport on nanoscale [10]. The waste heat can turn into electricity or to provide refrigeration by using thermoelectric devices. Until now, one of the significant challenges of thermoelectricity has been the problem of thermoelectric efficiency of electronic devices. The efficiency is described by the quantity of figure of merit \( ZT \) [11].

Since a large figure of merit \( ZT = GS^2T/\kappa \) indicates that the material could be a good thermoelectric, one should therefore try to enhance the thermopower \( S \) and the electrical conductance \( G \) and at the same time reduce the thermal conductance \( \kappa \) [12]. These properties are interdependent, therefore \( ZT \) in bulk materials, have value slightly above 1 at room temperature or more, while the highest \( ZT \) for a thermoelectric materials is
measured at the nanoscale, Wiedemann-Franz law can be violated in nanostructures due to the quantum effects [13,14].

In this paper, we investigate the thermoelectric properties of the double quantum ring which is attached to donor and left lead on the left side, while on the right side it is attached to acceptor and right lead.

2. Theory

In this work, the considered system is left lead-donor-double quantum ring -acceptor-right lead, where the double quantum ring structure consists of five quantum dots, the left and right ring are connected together with third quantum dot. The general formula for the transmission probability for the double quantum ring will be derived from the system shown in Fig.1, this system is described by using time-dependent and spinless Anderson – Newns Hamiltonian[13], which neglects correlation interactions in all subsystems. This Hamiltonian is given by

\[ H(t) = H_E(t) + H_{DBA}(t) + H_B(t) + H_{int}(t) + H_{LR}(t) \]  

where

\[ H_E(t) = \sum_{\alpha=D,A} E_{\alpha} n_{\alpha}(t) + \sum_{m=1}^{5} E_{m} n_{m}(t) + \sum_{\beta=L,R} E_{k_\beta} n_{k_\beta}(t) \]

describes energy levels of donor($\alpha = D$), acceptor($\alpha = A$), quantum dots ($m = 1, ..., 5$), left lead ($\beta = L$), and right lead ($\beta = R$). The index $k_\beta$ being a set of quantum numbers of the lead. The occupation number is $n_{\alpha}(t) = c_{\alpha}^\dagger(t)c_{\alpha}(t)$ and the $c_{\alpha}^\dagger(t)c_{\alpha}(t)$ denotes annihilation (creation) operators. $H_{DBA}(t)$ represents the coupling interaction between the donor with first and second quantum dot $V_{Dm}$, and the coupling interaction between the acceptor with the fourth and fifth quantum dot $V_{Am}$, respectively,

\[ H_{DBA}(t) = \sum_{m=1}^{5} V_{Dm} e^{(-1)^{m+1}i\phi/4} c_{D}^\dagger(t) c_{m}(t) + \sum_{m=1}^{5} V_{Am} e^{(-1)^{m+1}i\phi/4} c_{A}^\dagger(t) c_{m}(t) + H.C. \]  

while Hamiltonian part that describes interdot tunneling coupling is

\[ H_B(t) = \sum_{m=1}^{5} V_{m3} e^{(-1)^{m+1}i\phi/4} c_{m}^\dagger(t) c_{3}(t) + \sum_{m=1}^{5} V_{m4} e^{(-1)^{m+1}i\phi/4} c_{4}^\dagger(t) c_{m}(t) + \sum_{m=1}^{5} V_{m5} e^{(-1)^{m+1}i\phi/4} c_{5}^\dagger(t) c_{m}(t) + H.C. \]  

\[ H_{LR}(t) \text{ describes the tunneling between donor and left lead from side } V_{Dk_\beta}, \text{ and the tunneling between acceptor and right lead from other side } V_{Ak_\beta}. \]

\[ H_{LR}(t) = \sum_{k_\beta} V_{Dk_\beta} c_{D}^\dagger(t) c_{k_\beta}(t) + \sum_{k_\beta} V_{Ak_\beta} c_{A}^\dagger(t) c_{k_\beta}(t) + H.C. \]  

The equations of motion for $c_{\alpha}(t)$ can be obtained by

\[ \dot{c}_{D}(t) = -iE_{D} c_{D}(t) - i \sum_{m=1}^{5} V_{Dm} e^{(-1)^{m+1}i\phi/4} c_{m}(t) - i \sum_{k_\beta} V_{Dk_\beta} c_{k_\beta}(t) \]  

\[ \dot{c}_{A}(t) = -iE_{A} c_{A}(t) - i \sum_{m=4}^{5} V_{Am} e^{(-1)^{m+1}i\phi/4} c_{m}(t) - i \sum_{k_\beta} V_{Ak_\beta} c_{k_\beta}(t) \]

\[ \dot{c}_{m}(t) = -iE_{m} c_{m}(t) - iV_{m3} e^{(-1)^{m+1}i\phi/4} c_{3}(t) - iV_{m4} e^{(-1)^{m+1}i\phi/4} c_{4}(t) - iV_{m5} e^{(-1)^{m+1}i\phi/4} c_{5}(t) \]  

\[ \text{form } \neq 1,2 \]

\[ \dot{c}_{3}(t) = -iE_{3} c_{3}(t) - iV_{3m} e^{(-1)^{m+1}i\phi/4} c_{m}(t) \]  

\[ \text{form } 1,2,4,5 \]

\[ \dot{c}_{4}(t) = -iE_{4} c_{4}(t) - iV_{4m} e^{(-1)^{m+1}i\phi/4} c_{m}(t) \]  

\[ \text{form } \neq 4,5 \]

\[ \dot{c}_{5}(t) = -iE_{5} c_{5}(t) - iV_{5m} e^{(-1)^{m+1}i\phi/4} c_{m}(t) \]  

\[ \text{form } \neq 4,5 \]

\[ \dot{c}_{k_\beta}(t) = -iE_{k_\beta} c_{k_\beta}(t) - iV_{k_\beta D} c_{D}(t) \]

\[ \dot{c}_{k_\beta}(t) = -iE_{k_\beta} c_{k_\beta}(t) - iV_{k_\beta A} c_{A}(t) \]

Fig. 1. Shows the double quantum ring structure
Eq. (9) be related to left quantum ring, while Eq. (11) be related to the right quantum ring. For steady state we define $C_j(t)$ by the following

$$C_j(t) = \tilde{C}_j(E) e^{-iEt}$$

where $E$ denotes the system eigenvalues, then accordingly, $\tilde{C}_j(E) = 0$. So we get

$$C_D(E) = \sum_{m=1}^{2} V_{Dm} e^{-(1)^{m+1}i/4}\tau_m(E) + \sum_{kI} V_{DkI} \tilde{C}_{kI}(E)$$

(15)

$$C_A(E) = \sum_{m=4}^{5} V_{Am} e^{-(1)^{m+1}i/4}\tau_m(E) + \sum_{kR} V_{AkR} \tilde{C}_{kR}(E)$$

(16)

$$\tilde{C}_m(E) = V_{m0} e^{-(1)^{m+1}i/4}\tau_m(E) + t_{m0} \tilde{C}_n(E)$$

(17)

$$\tilde{C}_A(E) = V_{A0} e^{-(1)^{m+1}i/4}\tau_m(E) + t_{A0} \tilde{C}_n(E)$$

(18)

$$C_{kI}(E) = V_{kI}^R \tilde{C}_D(E)$$

(20)

$$C_{kR}(E) = V_{kR}^R \tilde{C}_D(E)$$

(21)

Then the transmission probability amplitude can be calculated respectively by using the following relation

$$t(E) = \frac{C_+(E)}{C_D(E)}$$

(22)

$$\Delta = \sum_{n=1}^{4} \tau_n(E)$$

(23)

$$K_n(\mu, T) = \int \left( \frac{\partial f}{\partial E} \right)(E - \mu)^n T(E) dE$$

(29)

$$G = \frac{2e^2}{h} K_0$$

(30)

$$S = -\frac{1}{eT} K_1$$

(31)

$$\kappa_{el} = -\frac{I_e}{\Delta T}$$

(32)
$ZT = \frac{1}{K} \frac{\kappa \Delta S}{\Delta T}$

(33)

where we neglect the phonon thermal conductance, which often disregarded in theoretical studies of thermal transport through quantum dots and molecules at low temperatures. While electron thermal conductance remains predominant comparatively[9].

3. Results and Discussion

We perform our calculation to investigate the thermoelectric properties of the double-quantum ring structure.

Firstly, we present the results for the case in the absence of magnetic flux for different system temperatures. Typical experimental values of coupling interactions among the subsystems may vary from a few μeV to a few meV [16]. All energies measured by units $\Gamma$, where $\Gamma$ is constant. We choose the parameter values $V_{12} = V_{23} = V_{34} = V_{25} = \Gamma$, $V_{D1} = V_{D2} = V_{AA} = V_{AB} = 0.5\Gamma$, and $V_{D1} = V_{AR} = 1.5\Gamma$. The quantum dot energy levels are taken to be $E_1 = \Gamma, E_2 = 0.5\Gamma, E_3 = 0.0, E_4 = -0.5\Gamma$, and $E_5 = -\Gamma$. We consider interdot tunneling coupling $t_{23} = t_{34} = t_{45} = 0.0, 0.5\Gamma, \Gamma$.

Experimentally, the quantum dots level positions can shift with respect to the energy zero point by tuning the gate voltage. In Fig. 2a, we plot the spectra of the electrical conductance, thermopower, electron thermal conductance and the figure of merit as a function of gate voltage, respectively, in case of interdot tunneling coupling $t_c = 0$.

In Fig. 2a the resonance type and the resonance number in electrical conductance spectrum are determined by the unlined values of energy levels. Where we found three Breit-Wigner resonances and two Fano resonances in the electrical conductance spectrum. The electrical conductance is insignificantly sensitive to temperature, which decreases when temperature increases. As shown in the inset of Fig. (2a), Fano resonance is suppressed when the temperature increases, this may be attributed to rising the temperature which may attenuate the quantum interference effect.

Fig. 2b clearly shows that the thermopower changes its' sign from positive to negative when the gate voltage moves across each resonance of the electrical conductance spectrum, where the thermopower approaches to zero. This because the voltage drop induced by the electrons are balanced by that induced by the holes[5]. Consequently, the charge current vanishes resulting in zero value of thermopower. Fano resonances in electrical conductance give rise to maxima in the absolute value of thermopower occurring at the same values of the gate voltage. And the smallest value of the thermopower is obtained at Breit-Wigner resonances. We also note that the absolute value of the thermopower increases when temperature increases at Breit-Wigner resonance, while at Fano resonance it decreases with increasing temperature.

In Fig. 2c, the behavior of electron thermal conductance is similar to that of electrical conductance. But the difference between them are the electron thermal conductance clearly enhanced when temperature increases, and significantly sensitive to temperature. Since the average electron tunneling probability decreases and the transferred heat increases when the system temperature increases.

After combining these three thermoelectric properties ($G, S$, and $\kappa$), we get the figure of merit (see Fig. 2d). The optimal figure of merit is found at $T=100 K$, it reaches $ZT=6$ in Fano resonance, while the value of the figure of merit decreases with increasing temperature.

In Fig. 3, we start to investigate the effect of interdot tunneling coupling $t_c = 0.5\Gamma$ on the properties of the thermoelectric spectra. The electrical conductance spectrum characterizes by shifting the quantum dot level’s position toward the bonding states and changing Fano resonance’s position (see Fig. 3a). The absolute value of thermopower increases at $t_c = 0.5\Gamma$ because of the number of electron transport pathways increases as shown in Fig. 3b, while the electron thermal conductance decreases (see Fig. 3c). Consequently, Fig. 3d shows that the magnitude of figure of merit is not changed. With increasing interdot tunneling coupling to value $t_c = \Gamma$, all the electrical conductance resonances are change in behavior except the first resonance at $V_g = -2.7\Gamma$ as shown in Fig. 4a. Height of figure of merit at Fano resonance is not changed in Fig. 4d and in all previous Figures. Therefore, this structure can be good thermoelectric device when we adjust the gate voltage at Fano resonance, thus we get a higher figure of merit value.

Secondly, we present the results for the case with a magnetic flux threading through the double quantum ring. In Fig. 5, we consider the magnetic flux $\phi = \pi/2$ and interdot tunneling coupling $t_c = 0$. The magnetic flux eliminates one resonances of the electrical conductance spectrum at $V_g = -2\Gamma$, and suppresses Fano resonance (see Fig. 5a). Suppression of Fano resonance in electrical conductance is clearly seen in thermopower spectrum, where it is not found abrupt rise in the thermopower for all values of gate voltage in Fig. 5b. Especially, electron thermal conductance is lesser sensitive to temperature in the presence of the magnetic flux $\phi = \pi/2$, in comparison with the case of $\phi = 0$ as shown in Fig. 5c. Finally, we note in Fig. 5d that the $ZT$ value is smaller for $\phi = \pi/2$ because of the disappearance of the Fano effect from electrical conductance spectrum. Figure of merit in the presence of the magnetic flux is enhanced by increasing temperature.
Fig. 2. (a) the electrical conductance, (b) the thermopower, (c) the electron thermal conductance and (d) the figure of merit as a function of gate voltage $V_g$ for different temperatures $T=100, 200$ and $300$K, with $t_c=0.0$ and $\theta = 0.0$.

Fig. 3. (a) the electrical conductance, (b) the thermopower, (c) the electron thermal conductance and (d) the figure of merit as a function of gate voltage $V_g$ for different temperatures $T=100, 200$ and $300$K, with $t_c=0.5\Gamma$ and $\theta = 0.0$. 
Fig. 4. (a) the electrical conductance, (b) the thermopower, (c) the electron thermal conductance and (d) the figure of merit as a function of gate voltage $V_g$ for different temperatures $T=100,200$ and $300\text{K}$, with $t_c=\Gamma$ and $\phi=0.0$.

Fig. 5. (a) the electrical conductance, (b) the thermopower, (c) the electron thermal conductance and (d) the figure of merit as a function of gate voltage $V_g$ for different temperatures $T=100,200$ and $300\text{K}$, with $t_c=0.0,\phi=0.5\pi$.

4. Conclusions

In summary, we have studied the thermoelectric properties of a double quantum ring structure for different temperatures. The high figure of merit can be obtained by adjusting gate voltage at Fano resonance. Moreover, the interdot tunneling coupling $t_c$ exerts significant impacts on the spectra of the thermoelectric properties. The thermoelectric efficiency will enhance when gate voltage adjusted at Fano resonance. Especially, electron thermal conductance is more sensitive to temperature in the absence of the magnetic flux $\phi = 0$, in comparison with the case of $\phi = \pi/2$. Therefore, this
structure can be a good thermoelectric device when we adjust the gate voltage at Fano resonance.

References


