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The influence of the nanostructure geometry on the thermoelectric properties

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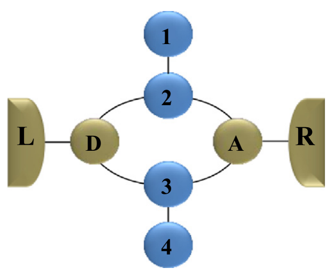
HIGHLIGHTS

- Thermoelectric properties are studied for three configurations.
- ZT enhanced in asymmetry configuration.
- Amplitude, frequency, and phase of the conductance tuned by varying magnetic flux.
- Magnetic flux suppresses antiresonance states.

GRAPHICAL ABSTRACT



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ABSTRACT

We discuss the influence of nanostructure geometry on the thermoelectric properties in quantum ring consists of one QD in each arm, each QD connects with side QD. The calculations are based on the time-dependent Hamiltonian model, 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. We investigate thermoelectric properties through three configurations of this nanostructure. Figure of merit enhanced in configuration (II) when side QD connected to upper arm of quantum ring. The magnetic flux threads quantum ring. The effect of magnetic flux on the thermoelectric properties is examined.

1. Introduction

In the last decade, thermoelectric properties of nanostructures have been attracting an increasing interest due to the potential application of the energy-conversion devices. These properties investigated both experimentally [1–4] and theoretically [5–8]. The usage the thermoelectric devices in the potential applications demanded large thermoelectric efficiency. However, the current difficulty in potential application of thermoelectric materials is due to their relatively low conversion efficiency [9].

The thermoelectric efficiency of devices is measured by the dimensionless figure of merit $ZT = GS^2T/(\kappa_{el}+\kappa_{ph})$, where G is the electrical conductance, S is the thermopower, $\kappa_{el}(\kappa_{ph})$ is the electronic (phonon) thermal conductance, and T is the system temperature [9,10].

A high increase of ZT is necessary, in order to TE materials compete conventional refrigerators and generators [10]. Optimizing thermoelectric efficiency in bulk materials is a big challenge because the interdependence among the three thermoelectric properties (G, S, κ) [11]. This the interdependence is as follows: when electrical conductance increases the thermal conductance increases, which it is accompanied by decreasing the thermopower [2]. Fortunately, recent progresses in nanotechnology have provided the possibilities to enhancement the thermoelectric efficiency in nanomaterials [12–14]. The value of Figure of merit in nanomaterials or nanostructures may exceed 3, due to enhance the thermopower because high electronic density of states near

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Fermi level, and reduce the thermal conductance caused by the boundary scattering [10].

Solid-state thermoelectric devices have many attractive features, such as no emission of toxic gases, the quietness, high reliability, and low maintenance cost, and long -term stability [15]. In parallel, extensive theoretical works were performed in order to understand how thermoelectric properties are affected in different nanostructures as a double quantum dot [12], a triple-arm Aharonov–Bohm interferometer [13], laterally coupled double-quantum-dot structure [14], and an Aharonov-Bohm ring with an embedded quantum dot [16]. Moreover, an increase of the figure of merit due to Coulomb blockade has been reported [12]. Furthermore, the influence of the quantum dot levels and spin polarization on thermoelectric transport properties in a double-dot Aharonov-Bohm interferometer coupled to ferromagnetic leads has been investigated [17].

Quantum dots, especially, the coupled multiple QD structures, available multiple channels for electron transport. In the appropriate parameter region, one or a few channels serve as the resonant paths for electron tunneling and the others are anti-resonant. Quantum interference of electron waves passing through these different paths cause the occurrence of Fano effect in the electron transport through QD structures [18]. Therefore, the ring-electrodes interface structure significantly adjusts the transmission probability of an electron in the ring [19].

Quantum ring structures lead to the Aharonov-Bohm interferometer which can be controlled by applying vertically a magnetic flux through the area enclosed by the quantum ring. Therefore, the phase of the wavefunction on the quantum ring depends on the magnetic flux [20]. In Aharonov-Bohm ring, the spin thermoelectric effect can be adjusted effectively by the magnetic flux [21,22]. Liu and Yang found the value of figure of merit can exceed 1 at room temperature in molecular junction consists of double-coupled- quantum dot by tuning the magnetic flux [5]. Furthermore, Zheng et al. [16] have studied thermoelectric effect in an AB ring with an embedded quantum dot, and found that ZT can highly improved due to the Fano effect resulted from the quantum interference effect. Maiti further studied the mesoscopic rings which threaded by magnetic flux as logical gates [19,23–26].

In this paper, we study how the interplay of nanostructure geometry and magnetic flux influences on the thermoelectric properties in quantum ring consists of one QD in each arm, each QD connects with side QD. It is found the interplay of nanostructure geometry induces quantum interference phenomena. In the presence of the interplay of magnetic flux the figure of merit is clearly increasing.

2. Theory

The considered system is shown in Fig. 1. This the system consists of left lead (L)-donor (D)-quantum ring-acceptor (A)-right lead (R), where the quantum ring contains one quantum dot in each arm, every quantum dot in the quantum ring connected to side quantum dot. The general formula for the transmission probability of this system will be derived, which is described by using time-dependent and spin less Anderson-Newns Hamiltonian [27] neglecting the correlation interactions in all subsystems.

This Hamiltonian is given as,

$$H(t)=H_{dot}+H_{\alpha}+H_{\beta}, \tag{1}$$

where the first term describes the electron in the four QDs, which takes a form as,

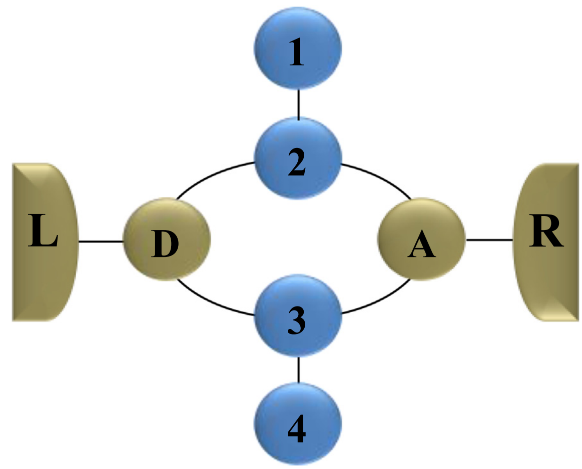

Fig. 1. Shows quantum ring consists of one quantum dot in each arm (two and three), every quantum dot of quantum ring connected to side quantum dot (one and four).

$$H_{dot}=\sum_{m=1}^{4} E_m n_m(t)+(t_{12}+H.\,C.)+(t_{34}+H.\,C.). \tag{2}$$

The second term is the Hamiltonian for electrons in the donor and the acceptor,

$$H_{\alpha}(t)=\sum_{\alpha=D,A} E_{\alpha} n_{\alpha}(t)+\left(V_{D2}e^{i\phi/4}+H.\,C.\right)+\left(V_{D3}e^{-i\phi/4}+H.\,C.\right) \\ +\left(V_{A2}e^{-i\phi/4}+H.\,C.\right)+\left(V_{A3}e^{i\phi/4}+H.\,C.\right). \tag{3}$$

The last term in the Hamiltonian describes electron in the two leads. It is given by,

$$H_{\beta}(t)=\sum_{k_\beta} E_{k_\beta} n_{k_\beta}(t)+\sum_{k_L}(V_{Dk_L}C_D^{\dagger}(t)C_{k_L}(t)+H.\,C.) \\ +\sum_{k_R}\left(V_{Ak_R}C_A^{\dagger}(t)C_{k_R}(t)+H.\,C.\right), \tag{4}$$

where, $n_j(t)=C_j^{\dagger}(t)C_j(t)$ and $C_j^{\dagger}(t)(C_j(t))$ denotes annihilation (creation) operators, with $j=D, A, m, k_L$ and k_R. The index k_β being a set of quantum numbers, where $\beta=L, R$. Notably, the summation in the first term in Eq. (1) is over all quantum dots (each one with one effective energy level E_m). t_{12} and t_{34} describe the interdot interactions. $V_{\alpha 2}$ and $V_{\alpha 3}$ are concerning the coupling interaction between the donor ($\alpha=D$) from left side and the acceptor ($\alpha=A$) from right side with quantum dot of number 2 and number 3, respectively. The donor and the acceptor with one effective energy level E_D and E_A. The energy levels of leads described by E_{k_β}, V_{Dk_L} represents coupling interaction between donor and left lead, V_{Ak_R} represents coupling interaction between acceptor and right lead. The phase shift ϕ is related with the magnetic flux Φ threading the system by a formula $\phi=2\pi\Phi/\Phi_0$,in which $\Phi_0=h/e$ is the flux quantum.

In order to get to the transmission probability, we following the same method in paper [28], we get,

$$\begin{vmatrix} E-E_1 & -t_{12} & 0 & 0 \\ -t_{21} & E-E_2 & 0 & 0 \\ 0 & 0 & E-E_3 & -t_{34} \\ 0 & 0 & -t_{43} & E-E_4 \end{vmatrix} \begin{vmatrix} \bar{C}_1 \\ \bar{C}_2 \\ \bar{C}_3 \\ \bar{C}_4 \end{vmatrix} = \begin{vmatrix} 0 \\ V_{2D}e^{-i\phi/4}\bar{C}_D+V_{2A}e^{i\phi/4}\bar{C}_A \\ V_{3D}e^{i\phi/4}\bar{C}_D+V_{3A}e^{-i\phi/4}\bar{C}_A \\ 0 \end{vmatrix}, \tag{5}$$

from matrix Eq. (5), the transmission probability amplitude $t(E)=\bar{C}_A(E)/\bar{C}_D(E)$ can be calculated by,