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Enhanced heat rectification effect in a quantum dot connected to ferromagnetic leads

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ABSTRACT

We study theoretically the heat generation by electric current in an interacting single level quantum-dot connected to ferromagnetic leads. The heat is transferred between the dot and the lattice vibration of its host material (phonon reservoir). Particular attention is paid on the heat's rectification effect achieved by properly arranging the dot level and the bias voltage. We find that this effect is remarkably enhanced when the two leads' magnetic moments are in antiparallel configuration, i.e., the magnitude of the heat generation is reduced (amplified) in the negative (positive) bias regime as compared to the cases of parallel configuration and nonmagnetic leads. The rectification effect is even enhanced when one of the lead's spin polarization approaches to unit, during which the negative differential of the heat generation is weakened due to the change of the spin-dependent electron occupation numbers on the dot. The found results may be used for thermal transistor in the newly emerged research subject of phononics.

1. Introduction

Advancements in the fabrication and characterization of nanostructures have greatly promoted the development of phonon engineering and phononics, a research subject devoted to use phonons to carry heat flow and information instead of electrons or photons [1,2]. Analogous to electronics, the building blocks of phononics are the realization and operation of a thermal diode and a thermal memory device. The thermal diode is used for rectifying heat current to switch and amplify heat flow [3–6], and the thermal memory device is designed to build a quantum computer using phonons [7,8]. Until now, although many hard efforts have been made repeatedly, this research subject is still at an initial stage because the flow of phonons is much more difficult to be controlled as compared to that of the electrons in a solid. The reason is that, unlike electrons, the phonons are quasiparticles in the form of energy that have neither a bare mass nor a bare charge. Moreover, isolated phonons do not interact with each other, and then the dominant electron-phonon interaction(EPI) [2,9–19] has become an effective means for investigating and manipulating heat flow in nanoscale systems.

In 2007, Sun and Xie studied the heat current flowing through a nanostructure within the framework of non-equilibrium Keldysh Green's function technique [13]. In their work, the heat is generated due to the EPI, through which the energy associated with the electric current in central region is transferred to the phonon bath in the form of heat. They demonstrated that the law of the heat generation in macroscopic system, i.e., the Joule law, breaks down in zero-dimensional quantum-dot (QD) system and some unique behaviors of the heat current were predicted [13,14,20–27]. For example, resonant phonon emitting occurs when the modified intradot Coulomb interaction is equal to the phonon energy, giving rise to a huge peak in heat generation despite a very weak electric current [14]. By properly adjusting the dot level, the magnitude of the heat current will decrease with increasing bias voltage due to the phonon emission processes, and thus a negative differential of the heat generation emerges [14]. In the presence of external ac bias voltage, finite heat current can be driven out from the phonon bath without the accompany of electric current [20]. If the system is subjected to a thermal bias, we have found that the resonant tunneling electrons can drive heat out from the phonon bath to the central region that are held at the same temperature, and thus can be used as a nano-refrigerator [21]. A thermal rectifier or diode was also proposed by us with the help of the thermal bias [26]. As compared to the one- or two-dimensional heterostructures [28], the advantage of the zero-dimensional QD structures relies on the precise manipulation of its various parameters by gate voltages.

In phononics, thermal diode works under a thermal bias, i.e., when one end of the diode is at a higher temperature as compared

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to the other end, heat is allowed to flow almost freely. In contrast, when the temperatures of the two ends are interchanged, the magnitude of heat is strongly suppressed [1,3–6,26]. In the present paper, however, we propose to rectify heat flow by the usual electric bias voltage. The work mechanism of our diode is as follows: The chemical potential of the right lead is fixed as $\mu_R = 0$ as the energy zero point. The bias voltage is applied to vary the chemical potential of the left lead, i.e., $eV = \mu_L$. The dot can be in either an empty state or be occupied by a single electron at equilibrium. If the dot is in empty state, its discrete level renormalized by EPI $\tilde{\varepsilon}_d$ is above the Fermi levels of the two leads in the absence of bias voltage ($\tilde{\varepsilon}_d > \mu_L = \mu_R = 0$). Whereas if the dot is occupied by an electron, its renormalized level is below the leads' Fermi level at equilibrium, but the other level $\tilde{U} + \tilde{\varepsilon}_d$ is above the leads' Fermi level ($\tilde{U}$ is the renormalized intradot Coulomb interaction). Taking the empty dot state for an example, for positive bias voltage $eV = \mu_L > \tilde{\varepsilon}_d$, electrons can transport through the dot via $\tilde{\varepsilon}_d$ resulting in finite current. During this process, the electrons will absorb or emit phonons and the energy is exchanged between the dot and the phonon reservoir in the form of heat flow. Whereas if the bias direction is reversed, the electrons can hardly tunnel through the dot because the Fermi levels of the two leads are below the dot level. In this way, the left-right symmetry for the electron transport is broken and the heat current can be amplified or suppressed depending on the direction of the bias voltage. Furthermore, if the leads coupled to the dot is made of ferromagnetic materials, we find that the rectification effect of the heat flow is significantly enhanced. If the system is symmetrically biased, i.e., $\mu_L = -\mu_R = eV/2$, the rectification effect for the current and the heat generation vanishes accordingly. Moreover, if the dot level is shifted by the bias voltage in a form of $\epsilon_d = \epsilon_d^0 - xeV$, where x measures the difference between the lengths of the left and right barriers and $\epsilon_d{}^0$ denotes the dot level in equilibrium, the current is $J(V) = -J(-V)$ in a symmetric device [29]. Under this condition, the rectification effect also vanishes. Even in an asymmetric system [30], where the QD is coupled to one normal metal lead and one ferromagnetic lead, the current is finite in both positive and negative bias regimes regardless of the varying of the dot level with the bias as in Ref. [29]. It should be noted that the electron spin degree of freedom has not attracted much attention in those previous works concerning heat generation or thermal diode [13,14,20–27]. Recently, we studied the heat generation in a system composed of a QD connected to ferromagnetic leads, and found that the ferromagnetism of the external leads will influence the heat generation and the electric current in different ways. For example, the heat generation can vary non-monotonously with the spin-polarization of the leads. The magnitude of the negative differential of the heat generation that was previously found in a QD connected to metal leads may be weakened at large leads' ferromagnetism due to the spin-blockade effect [27].

2. Model and method

The studied system with a QD coupled to the left and right ferromagnetic leads can be modeled by the following Hamiltonian [13,14,31,32]:

$$H = \sum_{k,\beta,\sigma} \varepsilon_{k\beta\sigma} a^\dagger_{k\beta\sigma} a_{k\beta\sigma} + \sum_\sigma [\varepsilon_d + \lambda_q(a_q^\dagger + a_q)] c_\sigma^\dagger c_\sigma + U c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow + \hbar\omega_q a_q^\dagger a_q + \sum_{k,\beta,\sigma} (T_{k\beta\sigma} a^\dagger_{k\beta\sigma} c_\sigma + H.c), \tag{1}$$

where the first term describes the left ($\beta = L$) and right ($\beta = R$) electron reservoir (lead) in the non-interacting quasi-particle approximation with $a^\dagger_{k\beta\sigma}$ ($a_{k\beta\sigma}$) being the creation (annihilation) operator of an electron with momentum k, energy $\varepsilon_{k\beta\sigma}$ and spin σ. The second and the third terms are for the electron on the QD, and $c_\sigma^\dagger$ (c_σ) creates (annihilates) an electron with energy ε_d and intradot Coulomb interaction U. $a_q^\dagger(a_q)$ is the creation (annihilation) operator of a single-mode phonon having frequency ω_q and wave vector q; the quantity λ_q is the electron-phonon coupling strength. The fourth term accounts for the phonon mode, and the last term describes the conduction electron hopping between the QD and the leads with $T_{k\beta\sigma}$ being the spin-dependent tunneling matrix element. To decouple the EPI, one usually make a canonical transformation, i.e., [13,14,18,33–35], $\tilde{H} = \hat{X} H \hat{X}^\dagger$ with $\hat{X} = \exp[(\lambda_q/\hbar\omega_q)\sum_\sigma (a_q^\dagger - a_q) c_\sigma^\dagger c_\sigma]$. The transformed Hamiltonian reads

$$\tilde{H} = \sum_{k,\beta} \varepsilon_{k\beta} a^\dagger_{k\beta\sigma} a_{k\beta\sigma} + \hbar\omega_q a_q^\dagger a_q + \sum_\sigma \tilde{\varepsilon}_d c_\sigma^\dagger c_\sigma + \tilde{U} c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow + \sum_{k,\alpha} (\tilde{T}_{k\beta\sigma} a^\dagger_{k\alpha\sigma} c_\sigma + H.c), \tag{2}$$

where the renormalized dot level and the intradot Coulomb interaction are respectively given by $\tilde{\varepsilon}_d = \varepsilon_d - g\omega_q$ and $\tilde{U} = U - 2g\omega_q$ with $g = (\lambda_q/\omega_q)^2$. The tunneling matrix element is also renormalized to $\tilde{T}_{k\beta\sigma} = T_{k\beta\sigma} X$, with the phonon operator $X = \exp[-g(a_q^\dagger - a_q)]$. If $T_{k\beta\sigma}$ is small compared to λ_q, X can be replaced by its expectation value $\langle X \rangle = \exp[-g(N_{ph} + 1/2)]$, where $N_{ph} = 1/[\exp(\hbar\omega_q/k_B T_{ph}) - 1]$ is the phonon distribution function with T_{ph} the temperature of the phonon bath [13,14]. Since in the above unitary transformation, the operators $a_q^\dagger a_q$ and $c_\sigma^\dagger c_\sigma$ remain unchanged, and then the heat flow between the electrons and the phonons $Q(t) = \hbar\omega_q \langle d a_q^\dagger(t) a_q(t)/dt \rangle$[13,14,22] can be calculated from the transformed Hamiltonian in Eq. (2). Following Ref. [13], the Fourier transform of $Q(t)$ can be obtained as [13,14],

$$Q = \mathrm{Re} \sum_\sigma \hbar\omega_q \lambda_q^2 \frac{d\omega}{2\pi} \{\tilde{G}_\sigma^<(\omega)\tilde{G}_\sigma^>(\bar{\omega}) - 2N_{ph}[\tilde{G}_\sigma^>(\omega)\tilde{G}_\sigma^a(\bar{\omega}) + \tilde{G}_\sigma^r(\omega)\tilde{G}_\sigma^>(\bar{\omega})]\}, \tag{3}$$

where $\bar{\omega} = \omega - \omega_q$. The dot single-electron Green's functions $\tilde{G}_\sigma^{r,a,<,>}(\omega)$ are the Fourier transforms of $\tilde{G}_\sigma^{r,a,<,>}(t)$ defined in terms of Hamiltonian (2), i.e., the retarded (advanced) one $\tilde{G}_\sigma^{r(a)}(t) = \mp i\theta(\mp t)\langle\{c_\sigma(t), c_\sigma^\dagger(0)\}\rangle$, the lesser Green's function $\tilde{G}_\sigma^<(t) = i\langle c_\sigma^\dagger(0) c_\sigma(t)\rangle$, and the greater Green's function $\tilde{G}_\sigma^>(t) = -i < c_\sigma^\dagger(t) c_\sigma(0) >$. It is worth noting that the heat generation here actually is the rate of heat generation. Moreover, since the present system is a net resistive one, the total dissipation is equal to the input power IV, where I is the current intensity and V the bias voltage. The remaining dissipation $Q_r = IV - Q$ occurs in the reservoirs [13,14]. Based on Hamiltonian (2), $\tilde{G}_\sigma^r(\omega)$ can be easily calculated by the equation of motion method as follows [37,38],

$$\tilde{G}_\sigma^r(\omega) = \frac{1}{\tilde{g}_\sigma^{r-1}(\omega) + i(\tilde{\Gamma}_{L\sigma} + \tilde{\Gamma}_{R\sigma})/2}, \tag{4}$$

where the dressed Green's function without coupling to the leads is $\tilde{g}_\sigma^r(\omega) = [\omega - \tilde{\varepsilon}_d - \tilde{U}(1 - n_{\bar{\sigma}})]/[(\omega - \tilde{\varepsilon}_d)(\omega - \tilde{\varepsilon}_d - \tilde{U})]$. Other Green's functions can be determined accordingly, $\tilde{G}_\sigma^a(\omega) = [\tilde{G}_\sigma^r(\omega)]^*$, $\tilde{G}_\sigma^{<(>)}(\omega) = \tilde{G}_\sigma^r(\omega)\tilde{\Sigma}_\sigma^{<(>)}\tilde{G}_\sigma^a(\omega)$, in which the lesser and greater self-energies are respectively given by $\tilde{\Sigma}_\sigma^< = i[\tilde{\Gamma}_{L\sigma} f_L(\omega) + \tilde{\Gamma}_{R\sigma} f_R(\omega)]$, and $\tilde{\Sigma}_\sigma^> = -i\{\tilde{\Gamma}_{L\sigma}[1 - f_L(\omega)] + \tilde{\Gamma}_{R\sigma}[1 - f_R(\omega)]\}$ [13,14]. During the calculation, we have used the Hartree–Fock scheme to truncate the higher-order Green's function. This scheme captures the main