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Nonequilibrium spin-polarized thermal transport in ferromagnetic–quantum dot–metal system

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ABSTRACT

We use nonequilibrium Green function to analyze the nonequilibrium spin-polarized thermal transport through the ferromagnetic–quantum dot–metal system, in which a quantum dot (QD) is coupled to the ferromagnetic and metal electrodes with the voltage bias and the temperature shift. The differential thermoelectric conductance $L(\theta)$ is always zero and has no relation with the temperature shift when ε is equal to the Fermi level. The positive and negative values of $L(\theta)$ manifest the thermoelectric characteristic of electron-like (or hole-like) carrier when the temperature shift is nonzero. The electrostatic potential U becomes spin-dependent, and makes the dot level renormalization when the ferromagnetic–quantum dot–metal system is driven by the voltage bias and the temperature shift. We define that the spin polarization of the currents between the spin current I_s and the electric current I_c is denoted as I_s/I_c. The spin polarization I_s/I_c shows novel and unique physical phenomenon when the voltage bias and the temperature shift are changed in the nonequilibrium state. Another interesting phenomenon is that we can obtain the pure spin current and a zero point of the thermocurrent I_{th} by adjusting the voltage bias and the temperature shift.

1. Introduction

With the development of nanotechnology, many researchers have raised great interest in fundamental questions on electron transport and energy storage of the hybrid mesoscopic structure in recent years [1–9]. Electron transport and thermal-to-electric conversion through the hybrid mesoscopic structure, such as carbon nanotubes [10], molecular junctions [11,12], quantum dots [13,14], exhibit novel physical phenomenon and potential device applications in spintronics [15–18]. The hybrid mesoscopic structure becomes promising candidate for the potential applications in thermoelectric devices. The thermoelectric efficiency η of the heat engine increases with the increasing of the effective thermoelectric figure of merit $Y = \frac{GS^2T}{K}$ (G, S and K are the electrical conductance, the thermopower and the thermal conductance) when the system is time-reversal symmetry and situates in the linear regime [19–21]. Whereas, Y is not suitable for describing the thermodynamic efficiency in the nonlinear regime [24,25]. The nonlinear thermodynamic efficiency depends not only on the magnitude of the thermal bias and the voltage bias, but also on the geometrical capacitance [22]. The electron transport can be operated and detected by adjusting the temperature and voltage of the electrode in the nonlinear regime. When the mesoscopic structure is simultaneously driven by the thermal and electric forces, the thermovoltage V_{th} and the thermocurrent I_{th} appear. The emergence of V_{th} and I_{th} indicates the energy conversion in the nonlinear regime [27]. M. Leijnse, M.R. Wegewijs and K. Flensberg analyzed the efficiency and output power of a nonlinear molecular thermoelectric device operated as a power converter by adjusting the voltage and the temperature [23]. Kacper Wrześniewski and Ireneusz Weymann studied the spin-resolved transport property of a triangular quantum dot coupled to external ferromagnetic electrodes in both the linear and nonlinear response regime [26]. Electron transport through a quantum dot coupled to two electrodes was theoretically researched by nonequilibrium Green function in the Coulomb blockade regime [27]. The spin-polarized transport was analyzed in the Kondo regime when the system is driven by an external voltage [28].

Thermoelectric effect considers the influence of electrostatic potential using a scattering theory of transport in the nonlinear regime [9]. The self-consistent electrostatic potential [9,24,25] makes the dot level renormalization due to the electrical and thermal driving forces within a mean-field approximation. The char-

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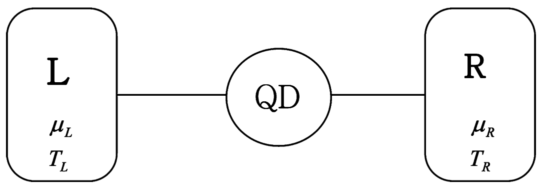

Fig. 1. (Color online.) A schematic picture of a double-barrier junction which consists of a quantum dot (QD) and two electrodes. The left ($\alpha = L$) electrode is the ferromagnetic electrode with the temperature T_L and the chemical potential μ_L. The right ($\alpha = R$) electrode is the metal electrode with the temperature T_R and the chemical potential μ_R.

acteristic potential describes how the electrostatic potential measures charge's buildup inside the mesoscopic system when the voltage bias and the temperature shift is nonzero. Hence, the characteristic potential depends on a bare charge δq^b which is injected from the electrode and a screening charge δq^s which is generated by the charge shift [9,22]. Recently, David Sánchez and Rosa López investigated that the thermopower sensitivity would provide information to the renormalization of the dot level because the screening effect depends on the voltage and temperature difference [9,29]. The nonlinear spin-polarization effect could be generated in two-dimensional topological insulators. Interestingly, the screening potential at the dot region becomes spin-dependent due to the voltage or temperature shifts [36]. The characteristic of the spin-polarized electron transport in the nonlinear and linear regime was described by applying an external magnetic field in the Kondo regime using higher-order Green's function in the equation of motion and numerical renormalization group method [30–34]. Miguel A. Sierra and David Sánchez discussed that the crossed effects could influence the thermovoltage and heat dissipation through Coulomb-blockaded quantum dots [35].

We use nonequilibrium Green function to analyze the nonequilibrium spin-polarized transport property through the ferromagnetic-quantum dot–metal system, in which a quantum dot (QD) is coupled to the ferromagnetic and metal leads with the voltage bias V and the temperature shift θ. We neglect spin-flip effect and only consider electron tunneling between two electrodes and the QD. The positive and negative values of the differential thermoelectric conductance $L(\theta)$ manifest the thermoelectric characteristic of electron-like (or hole-like) carrier when the temperature shift θ is nonzero. The electrostatic potential becomes spin-dependent, and makes the dot level renormalization when the ferromagnetic–quantum dot–metal system is driven by the voltage bias and the temperature shift. We define that the spin polarization of the currents between the spin current I_s and the electric current I_c is denoted as I_s/I_c. The spin polarization I_s/I_c shows novel and unique physical phenomenon when the voltage bias and the temperature shift are changed in the nonequilibrium state. Another interesting phenomenon is that we can obtain the pure spin current and a zero point of thermocurrent I_{th} by adjusting the voltage bias and the temperature shift. The paper is organized as follows. In Sec. 2, we introduce the model Hamiltonian of the ferromagnetic–quantum dot–metal system. The expressions of the electric current I_c and the spin current I_s are derived by means of the nonequilibrium Green function technique. The numerical results and discussion are given in Sec. 3. In Sec. 4, we summarize the work.

2. Physical model and formula derivation

In this paper, we consider a double-barrier junction which consists of a QD and two electrodes (as shown in Fig. 1). The left ($\alpha = L$) electrode is the ferromagnetic electrode with the temperature T_L and the chemical potential μ_L. The right ($\alpha = R$) electrode is the metal electrode with the temperature T_R and the chemical potential μ_R. The chemical potential μ_α and the temperature T_α of the αth ($\alpha = L, R$) electrode are $\mu_\alpha = eV_\alpha + E_F$ (V_α is the voltage bias of the αth electrode, E_F is the Fermi level) and $T_\alpha = \theta_\alpha + T$ (θ_α is the temperature shift of the αth electrode, T is the base temperature), respectively. The excess charge is piled up inside the QD due to the presence of θ_α and V_α. Meanwhile, the electrostatic potential U [9,22,36] is generated inside the QD. For simplicity, we assume that the Fermi level E_F is zero, and the electrostatic potential is zero at the equilibrium state (eq: $V_\alpha = 0$ and $\theta_\alpha = 0$), $U_{eq} = 0$. The double-barrier junction can be described by the following Hamiltonian [35–37]:

$$H = H_D + H_\alpha + H_T \tag{1}$$

Here $H_D = \sum_\sigma (\varepsilon - eU) d_\sigma^\dagger d_\sigma$ describes the Hamiltonian of the QD ($e = 1$). Operator $d_\sigma^\dagger$ (d_σ) is the creation (annihilation) operator of an electron in the QD with spin index σ ($\sigma = \uparrow, \downarrow$), energy ε and electrostatic potential U. ε is the dot level at the equilibrium state. $H_\alpha = \sum_{k\alpha\sigma} \varepsilon_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma}$ describes the Hamiltonian of the αth electrode. Operator $c_{k\alpha\sigma}^\dagger$ ($c_{k\alpha\sigma}$) is the creation (annihilation) operator of an electron in the αth electrode with spin index σ ($\sigma = \uparrow, \downarrow$), energy $\varepsilon_{k\alpha\sigma}$ and momentum k. $H_T = \sum_{\alpha k \sigma} \left(V_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger d_\sigma + h.c. \right)$ describes the electron tunneling coupling Hamiltonian between the αth electrode and the QD. $V_{k\alpha\sigma}$ denotes the hopping matrix element between the αth electrode and the QD.

By nonequilibrium Green function [37,39], the charge current I can be expressed by:

$$I = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} [f_L(\omega) - f_R(\omega)] T(\omega, U) \tag{2}$$

Here $f_\alpha(\omega) = \{1 + \exp[(\omega - \mu_\alpha)/T_\alpha k_B]\}^{-1}$ is the Fermi–Dirac distribution function of the αth electrode with the chemical potential μ_α and the temperature T_α. $T(\omega, U)$ is the electron transmission function, $T(\omega, U) = Tr[\Gamma^L G^r(\omega, U) \Gamma^R G^a(\omega, U)]$. The Green function $G^x(\omega, U)$ ($x = r, a, <$) is 2×2 matrix in the Fourier space. $\Gamma^\alpha = 2\pi \sum_k \delta(\omega - \varepsilon_{k\alpha\sigma}) |V_{k\alpha\sigma}|^2$ denotes the level broadening. The electrostatic potential U becomes spin-dependent due to the presence of the ferromagnetic electrode, the voltage bias and the temperature shift. So the electrostatic potential $U = \sum_\sigma U_\sigma$ [9,22,36] is a function of the spin index σ ($\sigma = \uparrow, \downarrow$), the voltage bias V_α and the temperature shift θ_α, $U_\sigma = U(\{\theta_\alpha\}, \{V_\alpha\}, \sigma)$. In order to explicitly explain the spin-dependent screening effect, $T(\omega, U) = \sum_\sigma T_\sigma(\omega, U_\sigma)$. Without loss of generality, the spin-polarized electric current I_σ can be expressed as:

$$I_\sigma = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} [f_L(\omega) - f_R(\omega)] T_\sigma(\omega, U_\sigma) \tag{3}$$

The spin current I_s and the electric current I_c can be written as:

$$I_c = I_\uparrow + I_\downarrow \tag{4}$$

$$I_s = I_\uparrow - I_\downarrow \tag{5}$$

We use the equation of motion method and the Dyson equation [37–39] to derive the retarded Green function $G^r(\omega, U)$ in the Fourier space.

$$G_{\sigma\sigma}^r(\omega, U_\sigma) = \frac{1}{\omega - \varepsilon + U_\sigma + \frac{i}{2} \sum\limits_{\alpha = L, R} \Gamma_\sigma^\alpha} \tag{6}$$