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Spin Thermoelectric Effects in Transport through a Two-Level Quantum Dot Coupled to Ferromagnetic Leads

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We investigate spin thermoelectric effects in a two-level quantum dot attached to external ferromagnetic leads. The basic thermoelectric coefficients are calculated by means of the non-equilibrium Green functions approach in the mean field approximation for the Coulomb term. Specifically, we calculate spin-dependent thermopower (spin Seebeck coefficient) and the charge thermopower. These coefficients measure spin and charge voltage drops across the device, respectively. Moreover, the figure of merit and its spin analog (which measures the spin thermoelectric efficiency) are presented and discussed. We also show that the indirect (via the leads) coupling between the dot's levels can significantly enhance the thermoelectric effects.

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1. Introduction

The spin Seebeck effect has been recently observed in a metallic magnet subjected to a temperature gradient [1, 2]. This novel phenomenon is a spin version of the Seebeck effect, and enables conversion of heat current to a spin voltage. The latter may be used to drive non--equilibrium spin currents. Roughly speaking, the spin Seebeck effect occurs owing to different scattering rates and different densities of states for spin-up and spin-down conduction electrons. In other words, the two spin channels can be described by their own Seebeck coefficients which are different. It is worth nothing that generation of a pure spin current is of fundamental importance for spintronics applications.

It is well known that the thermoelectric effects become strongly enhanced in systems of reduced dimensionality [3]. They are also enhanced by the Coulomb blockade effects [4, 5]. All this leads to violation of the Wiedemann–Franz law and inholding of the Mott relation [6, 7]. Quantum dots possess the above properties and seem to be good candidates for heat to electrical energy conversion devices. Owing to these features and rather low thermal conductance, quantum dots can display high thermoelectric efficiency, which is measured by the dimensionless thermoelectric figure of merit $\mathrm{ZT}_{\mathrm{charge}}$, defined as $\mathrm{ZT}_{\mathrm{charge}} = GS^2T/\kappa$. Here, T stands for the temperature, G is the charge conductivity, S is the Seebeck coefficient, and κ is the total thermal conductivity. $\mathrm{ZT}_{\mathrm{charge}} > 1$ is required for good heat to charge voltage converters. When the spin accumulation exist in the external leads, one can introduce a spin analog of the figure of merit, given by $\mathrm{ZT}_{\mathrm{spin}} = G_{\mathrm{s}}S_{\mathrm{s}}^2T/\kappa$, where G_{s} and S_{s} denote the spin conductance (normalized to $\hbar/2e$) and the spin Seebeck coefficient, respectively. The system is a good heat to spin-voltage converter when $\mathrm{ZT}_{\mathrm{spin}} > 1$ [8].

A considerable spin thermoelectric efficiency has been reported in one- and two-level quantum dots attached to ferromagnetic leads in which spin accumulation is admitted [9, 10]. Moreover, further increase of the efficiency has been obtained when one of the dot's levels is partially decoupled from the leads [10, 11]. Additional increase of the thermoelectric efficiency can be achieved owing to quantum interference effects [12] in the presence of indirect (via the leads) tunneling [13] between different levels.

In this paper we consider a system consisting of a two-level quantum dot attached to ferromagnetic leads, whose magnetic moments are collinear. In general, both intralevel and interlevel Coulomb interactions are taken into account. Moreover, we assume an indirect coupling of the dot's levels via the electrodes, which leads to quantum interference effects. In the limit of no indirect coupling, the considered system is equivalent to that investigated in Refs. [10] and [11]. The basic thermoelectric characteristics are calculated using the nonequilibrium Green function approach with the relevant approximation for the Coulomb interactions. We show that the interference effects can significantly enhance the thermoelectric efficiency of the system.

2. Model and thermoelectric coefficients

The system consisting of a two-level quantum dot coupled to ferromagnetic reservoirs is described by the An-

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derson Hamiltonian of the following form, $H = H_{\rm c} + H_{\rm d} + H_{\rm T}$. The first term, $H_{\rm c} = \sum_{\boldsymbol{k}\beta\sigma} \varepsilon_{\boldsymbol{k}\beta\sigma} a^{\dagger}_{\boldsymbol{k}\beta\sigma} a_{\boldsymbol{k}\beta\sigma}$, describes the left ($\beta$ = L) and right (β = R) leads in the non-interacting quasi-particle approximation. The second term, $H_{\rm d}$, describes the two-level quantum dot isolated from the leads and acquires the following form:

$$H_{\rm d} = \sum_{i\sigma} \varepsilon_i d^{\dagger}_{i\sigma} d_{i\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} U_{ij} n_{i\sigma} n_{j\sigma'}, \tag{1}$$

where ε_i stands for the spin degenerate energy level of the dot, and $n_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$ is the corresponding level occupation operator — both for $i = 1, 2$ and $\sigma =\uparrow, \downarrow$. The second term of Eq. (1) takes into account both intra- and inter-level Coulomb repulsion. The last term, $H_{\rm T}$, describes tunneling processes between the quantum dot and electrodes, and takes the following form: $H_{\rm T} = \sum_{\boldsymbol{k}i\sigma\beta} V^{i\sigma}_{\boldsymbol{k}\beta} a^{+}_{\boldsymbol{k}\beta\sigma} d_{i\sigma} + \text{H.c.}$, where $V^{i\sigma}_{\boldsymbol{k}\beta}$ are the relevant matrix elements. The dot-lead coupling is parameterized by the linewidth function, $\Gamma^{\beta}_{ij\sigma} = 2\pi\rho^{\sigma}_{\beta} V^{\beta}_i V^{\beta *}_j$, where ρ^{σ}_{β} is the density of states in the lead β for spin σ, $\sigma = +\ (-)$ for the spin majority (minority) electrons. For the sake of simplicity we assume that the couplings are independent of energy. The nondiagonal elements, $\Gamma^{\beta}_{i\bar{i}\sigma} = q_{\beta}\sqrt{\Gamma^{\beta}_{ii\sigma}\Gamma^{\beta}_{\bar{i}\bar{i}\sigma}}$, are crucial for the interference effects under considerations. Moreover, one can change their impact on the thermoelectric phenomena by tuning the parameters $q_{\rm L}$ and $q_{\rm R}$. For simplicity, we assume $q_{\rm L} = q_{\rm R} \equiv q$ with $q \in \langle 0, 1\rangle$. The spin-dependent dot-lead couplings for symmetric barriers are expressed in the standard form: $\Gamma^{\beta}_{ii\sigma} = \Gamma(1 \pm p)$ with p denoting spin polarization of the lead $\beta = \text{L}, \text{R}$. As we are interested in the spin Seebeck phenomenon, we consider only parallel magnetic configuration.

The spin Seebeck effect relies on the compensation of spin-majority and spin-minority electron currents due to the temperature gradient by an appropriate spin bias applied to the system. This situation can be described by vanishing current in both spin channels. In the linear response regime this leads to the following formulae for the thermoelectric charge and spin Seebeck coefficients [9],

$$S = -\frac{1}{2eT}\left(\frac{L_{1\uparrow}}{L_{0\uparrow}} + \frac{L_{1\downarrow}}{L_{0\downarrow}}\right), \tag{2}$$

$$S_{\rm s} = -\frac{1}{2eT}\left(\frac{L_{1\uparrow}}{L_{0\uparrow}} - \frac{L_{1\downarrow}}{L_{0\downarrow}}\right), \tag{3}$$

respectively. In turn, the thermal conductance κ is given by

$$\kappa = \frac{1}{T}\sum_{\sigma}\left(L_{2\sigma} - \frac{L_{1\sigma}}{L_{0\sigma}}\right). \tag{4}$$

The charge and spin conductances are given by the following formulae: $G = e^2(L_{0\uparrow} + L_{0\downarrow})$ and $G_{\rm s} = e^2(L_{0\uparrow} - L_{0\downarrow})$, respectively. In the above formulae the integral $L_{i\sigma}$ is defined as $L_{i\sigma} = -(2/h)\int {\rm d}\varepsilon(\varepsilon-\mu)^i(\partial f/\partial\varepsilon)T_{\sigma}(\varepsilon)$, where f is the Fermi–Dirac distribution for equal chemical potentials and temperature T in both leads. Here, $T_{\sigma}(\varepsilon)$ is the transmission function for the σ channel, which can be expressed in terms of the retarded and advanced Green functions and the dot-lead coupling strengths [13]. These Green functions have been calculated from the relevant equation of motion with the appropriate mean field approximation [14]. The explicit form of the Green function and the used approximation can be found in Ref. [14]. The appropriate occupation numbers have been calculated self-consistently using the identity, $\langle n_{i\sigma}\rangle = -{\rm i}\int({\rm d}\varepsilon/2\pi)G^{<}_{i\sigma}$, where the lesser Green function has been calculated from the Keldysh equation.

3. Numerical results and discussion

In the numerical calculations we assume the following parameters: $\Gamma = 0.1$ meV, and $\varepsilon_2 = \varepsilon_1 + \Delta\varepsilon$ with $\Delta\varepsilon = 0.8$ meV. Let us consider first the case with no intra- and inter-level Coulomb interactions, $U_{ij} = 0$ in the derived formulae. Figure 1 shows the charge

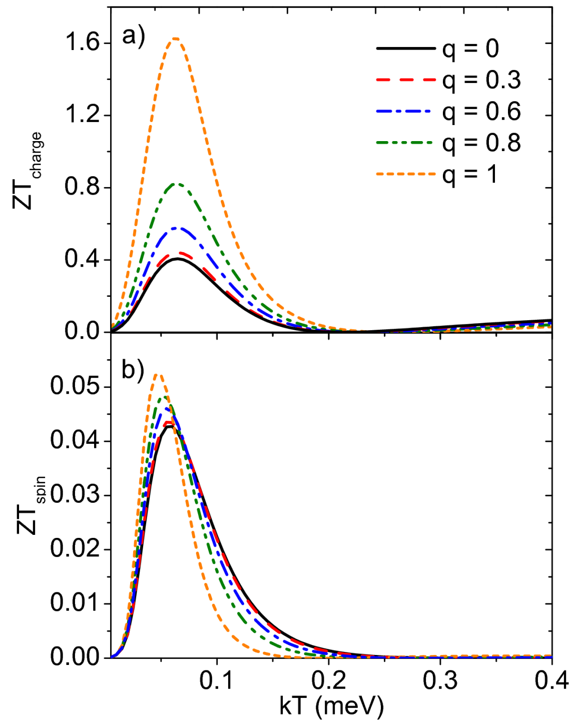

Fig. 1. Charge (a) and spin (b) figure of merit as a function of temperature, calculated for indicated values of the parameter q, $U_{ij} = 0$, $p = 0.3$, and $\varepsilon_1 = -0.2$ meV.

($\text{ZT}_{\text{charge}}$) and spin ($\text{ZT}_{\text{spin}}$) figures of merit as a function of temperature, calculated for different values of the parameter q. By tuning the parameter q, one can control the indirect coupling strength of the dot's levels through states of the electrodes. Both $\text{ZT}_{\text{charge}}$ and ZT_{spin} are nonmonotonic function of temperature, with the corresponding maxima at certain values of kT. In the case of

ZT_{charge}, position of the maximum is roughly independent of the parameter q. However, position of the relevant maximum in the temperature dependence of ZT_{spin} shifts slightly towards lower temperatures as q increases.

One can observe that the indirect coupling strength has a more significant influence on ZT_{charge} than on ZT_{spin}. The charge figure of merit first increases slightly with the increase in q and then grows rapidly for q approaching 1. One can note in Fig. 1a a significant increase in ZT_{charge} when q changes from $q = 0.8$ to $q = 1$. The charge figure of merit for $q = 1$ exceeds 1, which guarantees good thermoelectric efficiency of the system. On the other hand, the increase in q seems to have a weak impact on the maximum value of ZT_{spin} (see Fig. 1b).

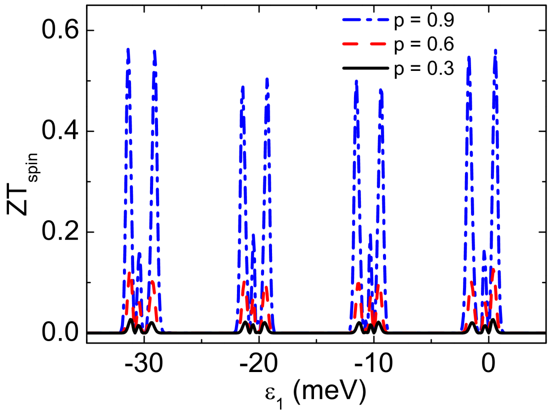

Fig. 2. Spin figure of merit as a function of ε_1 calculated for different values of the spin polarization factor p, and for $U_{ij} = U = 10$ meV, $kT = 0.1$ meV, and $q = 0$.

Now, let us consider the influence of intra- and inter-level Coulomb repulsion. For simplicity we assume equal Coulomb parameters, $U_{ij} = U$. In Fig. 2 we show the spin figure of merit, ZT_{spin}, as a function of dot energy level ε_1, calculated for different values of the spin polarization of the electrodes, and for $U = 10$ meV. From this figure follows that ZT_{spin} exhibits structure consisting of four groups of well resolved resonance-like peaks, separated by the Coulomb gaps. For the considered parallel magnetic configuration, ZT_{spin} strongly depends on the magnitude of spin polarization of the leads, and significantly grows with increasing value of p. As the ZT_{spin} is mainly determined by spin conductance and spin thermopower (i.e. the quantities which grow with increasing p) and less by the thermal conductance (which exhibits rather weak dependence on the leads polarization), this behavior is rather clear and understandable.

4. Summary

Charge and spin Seebeck effects in spin polarized transport through a system based on a two-level quantum dot coupled to ferromagnetic leads has been studied with the use of the non-equilibrium Green function approach. Conclusions regarding the best parameters for the most efficient conversion of heat to spin voltage in such a system can be summarized as follows. Firstly, the optimum value of charge and spin figures of merit can be found by adjusting the temperature. Secondly, coupling of the dot's energy levels via states in the reservoirs leads to constructive interference which results in a high charge thermoelectric efficiency. Thirdly, generation of a spin voltage in the system is greatly influenced by spin polarization of the electrodes. The largest spin thermoelectric efficiency can be noticed for near half-metallic ferromagnetic leads. Although the experimental realization of a spin battery based on quantum dot systems is still a matter of time, theoretical examinations provide insight into the nature of the effect, and also show how the effect can be tuned by a diversity of physical phenomena.

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