Thermoelectric effects in transport through a quantum dot attached to ferromagnetic electrodes

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Abstract. We present a theoretical analysis of thermoelectric effects in a system consisting of a single-level quantum dot attached to two ferromagnetic leads. Calculations have been performed in terms of the Green function formalism based on the equation of motion method and Hartree-Fock approximation. The calculated thermopower shows an oscillatory-like behavior with increasing gate voltage and also depends on relative alignment of the magnetic moments of both electrodes and on the leads' spin polarization. External magnetic field applied to the system leads to an additional structure due to spin splitting of the dot level. Thermal conductance is also calculated and correlated with the electrical one.

1. Introduction

There is currently an increasing interest in thermoelectric and magneto-thermoelectric transport phenomena in nanoscopic systems [1,2]. Quantum confinement in such nanoscale systems as well as discrete charging with single electrons and the associated Coulomb blockade strongly affect not only charge transport properties, but also thermoelectric ones, leading to novel phenomena like for instance oscillations of the thermopower and thermal conductance with increasing gate voltage [3].

Spin-dependent thermoelectric phenomena in magnetic nanostructures also have been studied [2,4–6]. In fact, such phenomena are of particular interest as they offer a unique possibility of creating spin currents, which may be of some importance for future applications in spintronic devices [2]. Following the discovery of giant magnetoresistance in metallic magnetic multilayers, magneto-thermoelectric phenomena in such structures have been investigated, too. For instance, giant magneto-thermopower was found in some multilayer nanopillars [4], while Peltier and Seebeck effects in such structures were analyzed theoretically [5]. Some new results on thermoelectric phenomena in single-electron devices based on quantum dots have been reported as well [6]. Following the current interest, we consider in this paper thermoelectric phenomena in a system consisting of a quantum dot attached to two ferromagnetic leads. Our main interest is in variation of the thermoelectric effects with magnetic configuration of the system and with spin polarization of the leads.
2. Model

Thermopower is defined as the voltage drop $\Delta V$ created by a temperature gradient $\Delta T$, and is quantitatively described by the Seebeck coefficient, $S = \Delta V/\Delta T$, calculated on the condition of vanishing charge current, $I = 0$ [7]. In the linear response regime, the thermopower can be expressed as [7]

$$S = -L_1/(eTL_0),$$

where $e$ is the electron charge, while $L_n$ ($n = 0,1,2,...$) are defined as $L_n = (-1/h)\text{Tr} \int dE (\partial f/\partial E)\mathbf{T}(E) (E - E_F)^n$. Here $f(E)$ denotes the Fermi-Dirac distribution function in the leads, $h$ is the Planck constant, $E_F$ is the Fermi energy of the electrodes in equilibrium, while $\mathbf{T}(E)$ describes the transmission probabilities through the system and is a $2 \times 2$ matrix in the spin space. The thermal conductance $\kappa$ can be calculated in a similar way, and is given by

$$\kappa = (1/T)(L_2 - L_1^2/L_0),$$

with $L_n$ defined above. Thus, the key point is to calculate the matrix $\mathbf{T}(E)$ and indirectly the required parameters $L_n$.

Thus, we calculate now the matrix $\mathbf{T}(E)$ for a system consisting of a single-level quantum dot attached to ferromagnetic electrodes which are characterized by the spin polarization factor $p$. The system is described by the Hamiltonian

$$H = H_o + H_D + H_T,$$

where $H_o$ corresponds to the left (L) and right (R) leads, $H_D$ is the dot Hamiltonian, and $H_T$ describes tunneling processes between the dot and electrodes. Hamiltonian $H_D$ is taken in the following form:

$$H_D = \sum_\sigma \varepsilon_\sigma n_\sigma + Un_\uparrow n_\downarrow,$$

with $n_\sigma$ being the electron number operator, and $U$ describing the strength of electron correlations in the dot (Hubbard parameter). The energy level becomes spin split in an external magnetic field, $\varepsilon_\sigma = \varepsilon_0 - \sigma\Delta$ for spin-up ($\sigma = +$) and spin-down ($\sigma = -$) electrons, which gives rise to the splitting equal to $2\Delta$. The tunneling processes, in turn, are described by spin-dependent coupling parameters $\Gamma_{L(R)}^{\pm} = \Gamma (1 \pm p)$ for spin-majority (upper sign) and spin-minority (lower sign) electrons. The parameter $\Gamma$ characterizes the coupling strength and is treated as a constant.

In the absence of spin flip processes (eg. due to spin-orbit interaction), and when magnetic moments of the leads are collinear (parallel or antiparallel), the transmission matrix $\mathbf{T}(E)$ is diagonal and one can write $\text{Tr} \mathbf{T}(E) = \sum_\sigma T_\sigma(E) = \sum_\sigma A_\sigma(E)\Gamma_L^\sigma \Gamma_R^\sigma / (\Gamma_L^\sigma + \Gamma_R^\sigma)$, with $A_\sigma(E)$ being the spectral function calculated in terms of the Green function formalism based on the equation of motion method and Hartree-Fock approximation. Here, $T_\sigma(E)$ is the transmission coefficient in the spin channel $\sigma$.

3. Numerical results

Thermopower $S$ has been calculated numerically as a function of the dot’s energy level $\varepsilon_0$ (which can be tuned by an external gate voltage) for ferromagnetic electrodes with spin polarization $p$, and for both parallel (P) and antiparallel (AP) configurations of the leads’ magnetic moments. The influence of temperature and external magnetic field on the thermoelectric effects also has been taken into account. The results are presented in Fig. 1 for $\Gamma = 0.1$meV and $U = 2$meV.

All the calculations have been performed for the whole level position (gate voltage) range, i.e. when the dot is empty, singly occupied (Coulomb blockade regime), and doubly occupied. A typical oscillatory-like behavior of $S$ with increasing $\varepsilon_0$ has been found. Maximal absolute values...
Figure 1. Thermopower $S$ as a function of the dot’s level position, calculated for indicated values of the leads’ polarization $p$ (a), for two different configurations of the leads’ magnetic moments (b), and for different temperatures (c). The effects of level splitting $\Delta$ due to an external magnetic field are shown in (d). The energy parameters, like $kT$, $U$, $\Gamma$, $\Delta$, and dot’s energy level are measured in meV.

of $S$ occur for the dot level lying in the Coulomb gap. However, the thermopower vanishes in the symmetry point $\varepsilon_0 = -U/2$ (middle of the Coulomb gap), and also at resonances $\varepsilon_0 = E_F = 0$ and $\varepsilon_0 = -U$ [8,9]. As shown in figure 1a, the thermopower depends on the leads’ polarization and decreases with increasing $p$. It also decreases when the magnetic configuration is changed from the antiparallel to parallel one (figure 1b). These changes in $S$, though not very strong, are, however, quite remarkable, indicating that the optimal conditions for the generation of independent of spin voltage drop $\Delta V$ occur when transmissions are equal in both spin channels, which takes place in systems with non-magnetic electrodes or for ferromagnetic leads but in the antiparallel configuration of magnetic moments. In such a situation the charge current as well as spin current are simultaneously equal to zero.

Thermopower strongly varies with temperature (figure 1c). At relatively low temperatures, $kT \approx \Gamma$, well-defined maximum and minimum can be observed in the Coulomb blockade region. The blockade effects, however, become less significant with increasing $T$, and the curve representing $S$ as a function of the level position becomes flatter. External magnetic field applied to the system also leads to a suppression of the thermoelectric effect for gate voltages corresponding to the Coulomb gap (figure 1d). However, an additional structure appears then due to splitting of the dot level by an external field, $\varepsilon_0 \rightarrow \varepsilon_\sigma = \varepsilon_0 \pm \Delta$. When $\Delta$ increases, the spin splitting of the dot level strongly affects transport through the dot. This is especially visible in the electrical conductance, $G = e^2L_0$, presented in figure 2a, as well as in the thermal
Figure 2. Linear electrical conductance $G$ (a) and thermal conductance (b) in the parallel magnetic configuration, as a function of the dot’s level position for two different values of the splitting parameter $\Delta$. Spin resolved electrical conductance for nonzero magnetic field is also presented in (a). The energy parameters $kT$, $U$, $\Gamma$, $\Delta$, and energy of the dot’s level are measured in meV.

cannot be resolved for smaller values of $\Delta$. Similar features also appear in the thermal conductance. In the absence of magnetic field we find two peaks in the thermal conductance, whose position corresponds to the position of similar peaks in the electrical conductance. An additional peak develops between the two peaks (in the middle of the Coulomb gap). The peaks in thermal conductance are however broader, so the splitting in the external magnetic field assumed in figure 2 is not clearly resolved. The level splitting was also visible in the thermopower calculated as a function of the level position and discussed above (figure 1d).

Dimensionless figure of merit, defined as

$$ZT = \frac{GS^2}{\kappa}T,$$

quantitatively describes the thermoelectric efficiency of a device. Dependence of $ZT$ on the magnetic configuration, temperature, and external field applied to the system is presented in figure 3. Note, that the thermal efficiency diminishes considerably when configuration of the moments is changed from the antiparallel to parallel one. Such a behavior is a result of two effects, namely of a relatively strong decrease of the thermopower $S$ during the configuration change and also of an increase of thermal conductance $\kappa$ (not shown here). At low temperatures ($kT \approx \Gamma$) the Coulomb blockade effects are important and heat transport is suppressed in the Coulomb gap, so the figure of merit shows two high peaks in this region of gate voltages. In turn, $ZT$ is equal to zero in the symmetry point, $\epsilon_0 = -U/2$, and also at resonances, where the thermopower $S$ vanishes and changes sign. Moreover, for energies far from the resonant ones, small side maxima can be observed. The picture changes dramatically with increasing temperature (figure 3b). For higher temperatures ($kT > 3\Gamma$), the intensity of both central peaks
Figure 3. Figure of merit as a function of level position for a) two magnetic configurations, b) different temperatures and c) different level splitting.

rapidly drops, whereas the side maxima become enhanced and start dominating the whole dependence. Note, that for $kT > 5 \Gamma$ the thermal efficiency of the device is very small for the gate voltages corresponding to the Coulomb gap. At higher temperatures the blockade effects are strongly suppressed, which leads to increase of heat transmission. The strong increase fully determines the thermoelectric efficiency of the device. Though, at high temperatures $ZT$ shows well-developed side maxima, they are of no practical importance, as for these values of gate voltages the system is out of resonance and the electrical conductance is very low.

An external magnetic field has a strong influence on the figure of merit, as depicted in figure 3c for several values of the splitting parameter $\Delta$. As $\Delta$ increases, the central peaks in $ZT$ become narrower, so in strong fields the device can show the high thermoelectric efficiency only in a very narrow region of gate voltages close to the symmetry point $\epsilon_0 = -U/2$. It is due to the fact, that for large $\Delta$ the distance between split levels $\epsilon_0 + \Delta$ and $\epsilon_0 + U - \Delta$ is small and the width of the Coulomb gap is considerably reduced. One should note that the $ZT$ curve is strongly asymmetric and moreover, its shape is changed. As energy levels are split, $ZT$ shows additional small peaks and valleys corresponding to the situation when one of the split levels aligns with the Fermi level in the leads.

Finally, we have calculated the the voltage induced in the system due to a temperature gradient. To do this, the temperature of the right electrode is kept constant $kT_R = \Gamma$, while the temperature of the left one is changed. The induced voltage is determined under the condition that the charge current in the system vanishes. The calculated results are presented in figure 4 for two different values of gate voltages corresponding to positive and negative sign of the Seebeck
Figure 4. Voltage induced due to temperature gradient

coefficient $S$. The absolute values of the calculated voltage rapidly increases with increase in temperature of the left contact and then it starts to decrease slowly.

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