Physics Letters A 380 (2016) 277–281

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Spin-dependent thermoelectric figure of merit in a quantum dot

Yonghong Yan [a,*], Feng Jiang [b], Hui Zhao [c]

[a] Department of Physics, Shaoxing University, Shaoxing 312000, China
[b] School of Mathematics and Physics, Shanghai University of Electric Power, Shanghai 200090, China
[c] Department of Physics, Tongji University, Shanghai 200092, China

ARTICLE INFO

Article history:
Received 19 May 2015
Received in revised form 7 September 2015
Accepted 4 October 2015
Available online 9 October 2015
Communicated by R. Wu

Keywords:
Spin-dependent Seebeck effect
Thermoelectric property
Quantum dot

ABSTRACT

We theoretically investigate the spin-dependent thermoelectric effects in a quantum dot that is connected with a normal metal lead and a ferromagnetic metal lead, by using the nonequilibrium Green's function method. The thermoelectric figure of merit ZT can be evaluated in several different ways, for example, by imposing a condition that the spin accumulation across the system is zero ($\Delta\mu_s = 0$) or that the spin current is zero ($I_s = 0$). We find that ZT in the case of $\Delta\mu_s = 0$ is always greater, especially when the spin polarization degree of the ferromagnetic lead is large. Meanwhile, in each case the ZT value drops when the spin polarization degree is increased. Effects of electron interaction on thermoelectric properties are also discussed briefly.

1. Introduction

Recently, there has been a renewed interest to develop high-efficiency thermoelectric materials for potential applications, e.g., power generation from waste heat and thermal management in electronics [1–4]. Generally, power generation from heat is realized via the Seebeck effect while the Peltier effect can be used to provide cooling at the cost of power. The efficiency of the energy conversion between heat and power is usually characterized by the dimensionless figure of merit ZT, which is defined as $ZT = S^2\sigma T/\kappa$. Here S is the Seebeck coefficient (or thermopower), σ is the electrical conductivity, T is the temperature, and κ is the total thermal conductivity including contributions from both phonons and electrons. As indicated by the definition, the possible ways to enhance ZT are thus to reduce the phonon conductivity through nanostructuring [5–7], or to optimize electronic properties by methods like band engineering [8,9].

Among various thermoelectric materials, low dimensional nanostructured systems are of particular interest as the reduced dimensionality provides great convenience for optimizing electronic properties [10–12]. Meanwhile, phonon thermal conductivity can be reduced largely due to phonon scattering by interfaces or boundaries [13]. In this respect, the zero-dimensional quantum dot typically exhibits a high ZT value when the dot is weakly coupled to electronic leads [14–18]. However, electrons carry not only charge but also spin, which adds new functionalities that may be used to improve the efficiency of thermoelectric devices. Indeed, the recent discovery of spin-Seebeck effect [19,20] in magnetic materials has stimulated intense research on thermoelectric properties of magnetic structures, leading to the appearance of a new field—spin caloritronics [21,22].

In the spin-dependent Seebeck effect involving a quantum dot [23–26], there may be heat, charge, and spin currents across the system with the driving forces being temperature gradient, charge electrochemical potential, and spin accumulation, respectively. In this case, we may follow several ways to define ZT. For example, we can evaluate ZT by imposing a condition that spin accumulation across the system is zero ($\Delta\mu_s = 0$) as usually done, or we impose a condition that the spin current is zero. The difference between these approaches and how ZT depends on magnetic properties of the system remain to be clarified.

In this paper, we consider the thermoelectric performance of a quantum dot that is connected to a normal metal lead and a ferromagnetic metal lead (NM-QD-FM). We show that the condition of $\Delta\mu_s = 0$ yields a larger value of ZT. Meanwhile, as the spin polarization degree of the ferromagnetic lead is increased, the ZT value reduces. We also discuss the effect of Coulomb interaction on thermoelectric properties. The results may be helpful for the design of thermoelectric devices based on magnetic materials.

2. Model and method

We consider a single-level quantum dot connected to two leads as shown in Fig. 1, and we assume that the left lead is a normal metal while the right lead is ferromagnetic. The total Hamiltonian reads

* Corresponding author. Tel.: +86 575 88342293.
E-mail address: yhyan@fudan.edu.cn (Y. Yan).

http://dx.doi.org/10.1016/j.physleta.2015.10.003
0375-9601/

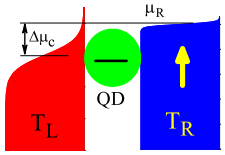

Fig. 1. (Color online.) A sketch of the thermoelectric setup: a single orbital quantum dot connected to a normal metal lead (left) and a ferromagnetic lead (right). The temperature of the left (right) lead is $T_{L,R}$ and we assume $T_L > T_R$. $\Delta\mu_c$ denotes charge electrochemical potential difference.

$$H = \sum_{k\sigma,\alpha} \varepsilon_{k\sigma\alpha} c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} + \sum_\sigma \varepsilon_d d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow + \sum_{k\sigma,\alpha} [t_{k\sigma\alpha} c^\dagger_{k\sigma\alpha} d_\sigma + \text{H.c.}], \tag{1}$$

where $\varepsilon_{k\sigma\alpha}$ is the energy of a free electron with momentum k and spin $\sigma(=\uparrow$ or $\downarrow)$ in the lead $\alpha(=\text{L, R})$, and $c^\dagger_{k\sigma\alpha}$ $(c_{k\sigma\alpha})$ creates (destroys) such an electron. $n_\sigma = d^\dagger_\sigma d_\sigma$ is the number operator of electron occupying the dot with spin σ and energy ε_d, and U is the Coulomb interaction between electrons with opposite spins on the dot. The last term in Eq. (1) describes the coupling between the leads and the dot.

We assume the temperature of the right lead is $T_R = T$ whereas $T_L = T + \Delta T$ $(\Delta T > 0)$. The chemical potential of the right lead is $\mu_{R\sigma} = \mu$, while for the left lead we choose $\mu_{L\sigma} = \mu + \Delta\mu_c + \chi_\sigma \Delta\mu_s/2$ with $\chi_{\uparrow,\downarrow} = \pm 1$. Here $\Delta\mu_c$ is the charge chemical potential with respect to the right lead, and $\Delta\mu_s$ is the spin accumulation [21,25], which may be created by spin injection from other ferromagnets. According to the standard nonequilibrium Green's function formalism [27,28], the charge current I_c through the dot is

$$\begin{aligned} I_c &= \frac{ie}{\hbar}\sum_\sigma \int \frac{d\epsilon}{2\pi}[f_{L\sigma}(\epsilon) - f_{R\sigma}(\epsilon)]\frac{\Gamma^L_\sigma \Gamma^R_\sigma}{\Gamma^L_\sigma + \Gamma^R_\sigma} \\ &\quad \times [G^r_\sigma(\epsilon) - G^a_\sigma(\epsilon)] \\ &\equiv \frac{e}{h}\sum_\sigma \int d\epsilon\, \mathcal{T}_\sigma(\epsilon)[f_{L\sigma}(\epsilon) - f_{R\sigma}(\epsilon)], \end{aligned} \tag{2}$$

where $\mathcal{T}_\sigma$ may be viewed as an effective transmission, and $\Gamma^\alpha_\sigma(\epsilon) = 2\pi \sum_k |t_{k\sigma\alpha}|^2 \delta(\epsilon - \varepsilon_{k\sigma\alpha})$ is the tunnel coupling between the lead α and the dot. Here we assume that Γ^α_σ is energy-independent (the wide-band approximation) and that Γ^L_σ and Γ^R_σ are proportional to each other. $f_{L(R)\sigma}(\epsilon) = 1/(\exp[(\epsilon - \mu_{L(R)\sigma})/k_B T_{L(R)}] + 1)$ is the Fermi–Dirac distribution function in the left (right) lead. $G^{r(a)}_\sigma(\epsilon)$ is the retarded (advanced) Green's function for the dot.

Employing the equation-of-motion technique [27–29], we can obtain the following Dyson and Keldysh equations within the mean field approximation,

$$G^r_\sigma(\epsilon) = g^r_\sigma(\epsilon) + g^r_\sigma(\epsilon)\Sigma^r_\sigma(\epsilon)G^r_\sigma(\epsilon) \tag{3}$$

and

$$G^<_\sigma(\epsilon) = G^r_\sigma(\epsilon)\Sigma^<_\sigma(\epsilon)G^a_\sigma(\epsilon), \tag{4}$$

respectively. Here $g^r(\epsilon)$ is the exact retarded Green's function of the isolated quantum dot, and it is given by

$$g^r_\sigma(\epsilon) = \frac{1 - \langle n_{\bar\sigma}\rangle}{\epsilon - \varepsilon_d + i0^+} + \frac{\langle n_{\bar\sigma}\rangle}{\epsilon - \varepsilon_d - U + i0^+}. \tag{5}$$

The retarded and less self-energies are given by $\Sigma^r_\sigma(\epsilon) = -i(\Gamma^L_\sigma + \Gamma^R_\sigma)/2$ and $\Sigma^<_\sigma(\epsilon) = i\sum_\alpha f_{\alpha\sigma}(\epsilon)\Gamma^\alpha_\sigma$, respectively. From the less Green's function, we can obtain $\langle n_{\bar\sigma}\rangle$, i.e.,

$$\langle n_{\bar\sigma}\rangle = -i\int \frac{d\epsilon}{2\pi} G^<_{\bar\sigma}(\epsilon). \tag{6}$$

Thus we see that $\langle n_{\bar\sigma}\rangle$ depends on the retarded Green's function of the quantum dot $G^r_{\bar\sigma}$, which in turn depends on $\langle n_\sigma\rangle$. Using numerical techniques, a self-consistent solution can be obtained. Here it should be mentioned that the mean field approximation is valid when $T_{L,R} \gg T_K$, where T_K is the Kondo temperature, and in this paper we restrict our attention to cases where $T_{L,R} \gg T_K$. In a similar way, the spin current and heat current flowing out from the left lead are given respectively by

$$I_s = \frac{\hbar}{2h}\sum_\sigma \chi_\sigma \int d\epsilon\, \mathcal{T}_\sigma [f_{L\sigma}(\epsilon) - f_{R\sigma}(\epsilon)] \tag{7}$$

and

$$J_L = \frac{1}{h}\sum_\sigma \int d\epsilon\, (\epsilon - \mu_{L\sigma})\mathcal{T}_\sigma [f_{L\sigma}(\epsilon) - f_{R\sigma}(\epsilon)]. \tag{8}$$

From Eq. (8), it follows that

$$\begin{aligned} J_L &= J_R - I_c\frac{\Delta\mu_c}{e} - I_s\frac{\Delta\mu_s}{\hbar} \\ &\equiv J_R + P_c + P_s, \end{aligned} \tag{9}$$

where J_R is the heat current flowing *into* the right lead. Eq. (9) indicates that the heat current flowing out from the left lead partly flows into the right lead, and is partly converted to power corresponding to charge current and spin current respectively. Throughout this paper, we consider the case where the setup acts as a power generator $(P_c > 0)$. The thermoelectric efficiency is then specified by $\eta = P_c/J_L$.

In the linear response regime, the three currents can be expanded respectively as

$$\begin{aligned} I_c &= \frac{e^2}{h}\int d\epsilon\, \mathcal{T}_+ F(\epsilon)\frac{\Delta\mu_c}{eT} + \frac{\hbar e}{2h}\int d\epsilon\, \mathcal{T}_- F(\epsilon)\frac{\Delta\mu_s}{\hbar T} \\ &\quad + \frac{e}{h}\int d\epsilon\, \mathcal{T}_+(\epsilon - \mu)F(\epsilon)\frac{\Delta T}{T^2}, \end{aligned} \tag{10}$$

$$\begin{aligned} I_s &= \frac{\hbar e}{2h}\int d\epsilon\, \mathcal{T}_- F(\epsilon)\frac{\Delta\mu_c}{eT} + \frac{\hbar^2}{4h}\int d\epsilon\, \mathcal{T}_+ F(\epsilon)\frac{\Delta\mu_s}{\hbar T} \\ &\quad + \frac{\hbar}{2h}\int d\epsilon\, \mathcal{T}_-(\epsilon - \mu)F(\epsilon)\frac{\Delta T}{T^2}, \end{aligned} \tag{11}$$

and

$$\begin{aligned} J_L &= \frac{e}{h}\int d\epsilon\, \mathcal{T}_+(\epsilon - \mu)F(\epsilon)\frac{\Delta\mu_c}{eT} \\ &\quad + \frac{\hbar}{2h}\int d\epsilon\, \mathcal{T}_-(\epsilon - \mu)F(\epsilon)\frac{\Delta\mu_s}{\hbar T} \\ &\quad + \frac{1}{h}\int d\epsilon\, \mathcal{T}_+(\epsilon - \mu)^2 F(\epsilon)\frac{\Delta T}{T^2}. \end{aligned} \tag{12}$$

Here $F(\epsilon) = \{4k_B \cosh^2[(\epsilon - \mu)/2k_B T]\}^{-1}$, $\mathcal{T}_+ = \sum_\sigma \mathcal{T}_\sigma$, and $\mathcal{T}_- = \mathcal{T}_\uparrow - \mathcal{T}_\downarrow$. Equivalently, we can rewrite these equations in a matrix form,

$$\begin{pmatrix} I_c \\ I_s \\ J_L \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} & \mathcal{L}_{13} \\ \mathcal{L}_{21} & \mathcal{L}_{22} & \mathcal{L}_{23} \\ \mathcal{L}_{31} & \mathcal{L}_{32} & \mathcal{L}_{33} \end{pmatrix} \begin{pmatrix} \Delta\mu_c/eT \\ \Delta\mu_s/\hbar T \\ \Delta T/T^2 \end{pmatrix}, \tag{13}$$

where the kinetic coefficients $\mathcal{L}_{ij}$ are defined by Eqs. (10), (11), and (12), and remain unchanged under the exchange of the spin indices [30]. The kinetic coefficients here are analogous to those in the absence of a magnetic field, and satisfy the Onsager relation, $\mathcal{L}_{ij} = \mathcal{L}_{ji}$ [31]. In the presence of a magnetic field B, the Onsager relation becomes $\mathcal{L}_{ij}(B) = \mathcal{L}_{ji}(-B)$; for its implication in thermoelectric properties, see Refs. [32,33]. One can also notice that each