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2002 J. Phys.: Condens. Matter 14 11747

(http://iopscience.iop.org/0953-8984/14/45/316)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 11747–11756 PII: S0953-8984(02)39512-2

Effect of the Kondo correlation on the thermopower in a quantum dot

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Received 16 July 2002
Published 1 November 2002
Online at stacks.iop.org/JPhysCM/14/11747

Abstract

In this paper we study the thermopower of a quantum dot (QD) connected to two leads in the presence of Kondo correlation by employing a modified second-order perturbation scheme at nonequilibrium. A simple scheme, Ng's ansatz (Ng T K 1996 *Phys. Rev. Lett.* **76** 487), is adopted to calculate the nonequilibrium distribution Green function and its validity is further checked with regard to the Onsager relation. Numerical results demonstrate that the sign of the thermopower can be changed by tuning the energy level of the QD, leading to a oscillatory behaviour with a suppressed magnitude due to the Kondo effect. We also calculate the thermal conductance of the system, and find that the Wiedemann–Franz law is obeyed at low temperature but violated with increasing temperature, corresponding to emerging and quenching of the Kondo effect.

1. Introduction

Observation of the Kondo effect in a semiconductor quantum dot (QD) [1, 2], which provided a testing ground of the quantum behaviour of electron wavefunctions and many-body effects, has stimulated a great deal of experimental [3, 4] and theoretical [5–9] investigation. So far, many interesting features in QDs, such as Kondo-assisted enhancement of conductance, specific temperature dependence, peak splitting in a magnetic field, zero-bias maximum of differential conductance in the Kondo regime and singlet–triplet Kondo effect have been successfully explored in early theoretical works, which described the electron transport through QDs using the well known impurity Anderson model [10].

A convenient way of describing transport through an Anderson impurity under out-of-equilibrium conditions is to employ the nonequilibrium Green function (GF) technique of Keldysh. In the framework of nonequilibrium GF, one needs consistent calculations of retarded (advanced) and distribution (lesser) GFs in order to study the out-of-equilibrium properties, while only the retarded GF is needed when studying equilibrium properties of the system. In the literature, the single-impurity Anderson model has been extensively studied for more than 30 years and many numerical and analytical methods have been developed to explore its equilibrium properties, such as the equation of motion (EOM) combined with the decoupling approximation [11], the second-order perturbation theory (SOPT) for on-site Coulomb interaction U [12] and the slave-boson non-crossing approximation (NCA) [13, 14]. However, it is still a great challenge to evaluate the distribution GF of the strongly correlated systems under out-of-equilibrium conditions, because one has to deal with both the on-site Coulomb interaction and the tunnellings between the dot and reservoirs simultaneously. To our knowledge, there have been three attempts to surmount this technical difficulty. The first one was carried out by Meir [6], who generalized the NCA to the nonequilibrium situation based on the Coleman slave-boson method in the limit of infinite Coulomb interaction $U \to \infty$ [13]. This scheme transforms the strong correlation Hamiltonian into a noninteracting equivalent one by introducing several auxiliary boson operators. Therefore, it evades the dilemma of how both the Coulomb interaction U and the mixing between QD and the two leads can be treated simultaneously in deriving the retarded and lesser (greater) self-energies of QD. It is well known that NCA provides a good description for the investigation of the excitation spectra of QD, but the necessary Fermi liquid behaviour was not reproduced at the low energy and low temperature limit. To extend the slave-boson method to study Kondo-type transport through double QDs at low temperature, especially at zero temperature, a slave-boson mean field approach has been presented by replacing the slave-boson operators with their expectation values [15]. Very recently, a finite-U slave-boson mean field scheme has been developed by us to explore Kondo-type transport through QDs [16] and double QDs [17]. Nevertheless, these slave-boson mean field approaches are at the same level of approximation in deriving the interacting retarded and lesser self-energies.

The third attempt was made by Ng [9], who has developed an approximative scheme, i.e., Ng's ansatz, to obtain the lesser GF from the EOM. It is impossible to obtain straightforwardly the distribution GF from the EOM without introducing additional assumptions. Ng assumed that the interacting greater or lesser self-energy of the QD is related to the noninteracting one, and the ratio parameter is determined by the interacting retarded self-energies derived by means of EOM. This simple and effective ansatz was later applied in more complicated structures involved QDs, such as normal metal–QD–superconductor [18] and superconductor–QD–superconductor [19] structures. Nevertheless, except for these three advantages pointed out by Ng in [9], up to now, no further inspection of the validity of the ansatz has been presented.

In this paper we will provide another validity check of Ng's ansatz by analysing the particle current and thermal flux through a QD connecting to two reservoirs on the basis of the Anderson single-impurity model by means of the nonequilibrium GF with the help of the Langreth continuation rules and Ng's ansatz. We find that the resulting particle current and heat flux driven by bias voltages and temperature gradients between two leads satisfy the Onsager relation in the near equilibrium regime [20], thus provide a natural check on the validity of derivation of the lesser GF.

To date, most theoretical calculations and experimental measurements on the thermopower of QDs have focused on the Coulomb blockade (CB) regime [21], and have revealed that when the gate voltage defining the QD is swept, the thermopower oscillates about zero (sawtooth behaviour) with a period equal to that of the CB oscillations in electric conductance. However, the thermopower across a QD in the Kondo regime is still much less studied [22, 23]. The second purpose of this paper is to investigate the Kondo effect on the linear thermopower of a QD based on Ng's ansatz.

We organize the rest of the paper as follows. In the second section we derive particle current and thermal flux formulae through an interacting QD within the framework of the nonequilibrium GF. The electric and thermoelectric transport coefficients are derived in the presence of both chemical potential and temperature gradients between two leads and automatically satisfy the Onsager relation in the linear transport regime. We note that within this approximation, the same current formula as that in [25] is derived without the presumption of proportional coupling $\Gamma_L(\omega) = \lambda\Gamma_R(\omega)$. In section 3, numerical calculations of linear Kondo-type thermopower S in QDs are reported as a function of gate voltage and temperature, which shows a gate-voltage-controlled change of sign and largely suppressed oscillatory magnitude due to the Kondo effect. We also discuss the thermal conduction coefficient κ and its violations of the well known Wiedemann–Franz law. Finally, a conclusion is given in section 4.

2. Thermal current formula and Onsager relation

Transport through a QD coupled to two reservoirs in the presence of external voltages and a temperature gradient between two reservoirs can be described by the Anderson single-impurity model:

$$H = \sum_{\eta,k,\sigma} \epsilon_{\eta k\sigma} c^\dagger_{\eta k\sigma} c_{\eta k\sigma} + \epsilon_d \sum_\sigma c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\eta,k,\sigma} (V_\eta c^\dagger_{\eta k\sigma} c_{d\sigma} + \text{H.c.}), \tag{1}$$

where $\epsilon_{\eta k\sigma}$ represents the conduction electron energy of the lead η, and ϵ_d is the discrete energy level in the QD. $c^\dagger_{\eta k\sigma}$ ($c_{\eta k\sigma}$) are the creation (annihilation) operators for electrons in lead η ($=L, R$), while $c^\dagger_{d\sigma}$ ($c_{d\sigma}$) for electrons in the QD. When a total external voltage V is applied between the two leads, their chemical potential difference is $\mu_L - \mu_R = eV$. The two leads are assumed to be in local equilibrium with respective temperature T_η and their distribution functions are given by $f_\eta(\omega) = [1 + \exp(\omega - \mu_\eta)/k_B T_\eta]^{-1}$ ($\eta = L$ or R). This assumption is practically correct because the two reservoirs respond to an external perturbation much faster than the centre region, i.e., the QD. The other parameters, U and V_η, stand for the Coulomb interaction, and the coupling between the QD and the reservoir η, respectively. For the transport problem considered in this paper, electrons in the QD are in a nonequilibrium state, to be determined by their coupling to two leads and by the applied voltage. In order to describe the nonequilibrium state of electrons, we define the retarded (advanced) and lesser (greater) GFs for the QD as follows: $G^{r(a)}_{d\sigma}(t,t') \equiv \pm \mathrm{i}\theta(\pm t \mp t')\langle\{c_{d\sigma}(t), c^\dagger_{d\sigma}(t')\}\rangle$, $G^<_{d\sigma}(t,t') \equiv \mathrm{i}\langle c^\dagger_{d\sigma}(t')c_{d\sigma}(t)\rangle$ and $G^>_{d\sigma}(t,t') \equiv -\mathrm{i}\langle c_{d\sigma}(t)c^\dagger_{d\sigma}(t')\rangle$.

The particle current J_η and energy flux $J_{E\eta}$ flowing from the lead η to the QD can be evaluated, respectively, from the rate of change of the electron number operator $N_\eta(t) = \sum_{k,\sigma} c^\dagger_{\eta k\sigma}(t)c_{\eta k\sigma}(t)$ and the rate of change of energy operator $H_\eta(t) = \sum_{k,\sigma} \epsilon_{\eta k\sigma} c^\dagger_{\eta k\sigma}(t)c_{\eta k\sigma}(t)$ of the lead η [24]:

$$\begin{aligned} J_\eta(t) &= -\frac{1}{\hbar}\left\langle \frac{\mathrm{d}N_\eta}{\mathrm{d}t}\right\rangle = -\mathrm{i}\frac{1}{\hbar}\left\langle\left[H, \sum_{k,\sigma} c^\dagger_{\eta k\sigma}(t)c_{\eta k\sigma}(t)\right]\right\rangle \\ &= \mathrm{i}\frac{1}{\hbar}\left\langle \sum_{k,\sigma}[V_\eta c^\dagger_{\eta k\sigma}(t)c_{d\sigma}(t) - V^*_\eta c^\dagger_{d\sigma}(t)c_{\eta k\sigma}(t)]\right\rangle, \end{aligned} \tag{2}$$

$$\begin{aligned} J_{E\eta}(t) &= -\frac{1}{\hbar}\left\langle \frac{\mathrm{d}H_\eta}{\mathrm{d}t}\right\rangle = -\mathrm{i}\frac{1}{\hbar}\left\langle\left[H, \sum_{k,\sigma} \epsilon_{\eta k\sigma} c^\dagger_{\eta k\sigma}(t)c_{\eta k\sigma}(t)\right]\right\rangle \\ &= \mathrm{i}\frac{1}{\hbar}\left\langle \sum_{k,\sigma}\epsilon_{\eta k\sigma}[V_\eta c^\dagger_{\eta k\sigma}(t)c_{d\sigma}(t) - V^*_\eta c^\dagger_{d\sigma}(t)c_{\eta k\sigma}(t)]\right\rangle, \end{aligned} \tag{3}$$

which involve the time-diagonal parts of the correlation functions: $G^<_{d\sigma,\eta k\sigma}(t,t') \equiv \mathrm{i}\langle c^\dagger_{\eta k\sigma}(t')c_{d\sigma}(t)\rangle$ and $G^<_{\eta k\sigma,d\sigma}(t,t') \equiv \mathrm{i}\langle c^\dagger_{d\sigma}(t')c_{\eta k\sigma}(t)\rangle$. According to [24], the thermal flux $J_{Q\eta}$ flowing from the lead η to the QD is determined as

$$J_{Q\eta} = J_{E\eta} - \mu_\eta J_\eta. \tag{4}$$

With the help of the Langreth analytic continuation rules [26], we obtain the following expressions:

$$J_\eta = \mathrm{i}\int \frac{\mathrm{d}\omega}{2\pi\hbar}\Gamma_\eta(\omega)\sum_\sigma\{G^<_{d\sigma}(\omega) + f_\eta(\omega)[G^r_{d\sigma}(\omega) - G^a_{d\sigma}(\omega)]\}, \tag{5}$$

$$J_{Q\eta} = \mathrm{i}\int \frac{\mathrm{d}\omega}{2\pi\hbar}\Gamma_\eta(\omega)\sum_\sigma(\omega-\mu_\eta)\{G^<_{d\sigma}(\omega) + f_\eta(\omega)[G^r_{d\sigma}(\omega) - G^a_{d\sigma}(\omega)]\}, \tag{6}$$

in terms of the QD GFs in Fourier space. Here $\Gamma_\eta(\omega) = 2\pi\sum_{k,\sigma}|V_\eta|^2\delta(\omega-\epsilon_{\eta k\sigma})$ denotes the strength of coupling between the QD level and lead η.

In the presence of both a strong Coulomb interaction in the QD and tunnellings between the QD and leads, it is difficult to evaluate the retarded GF $G^r_{d\sigma}$ of the QD accurately. Several approximation schemes have been proposed in the literature to derive $G^r_{d\sigma}$, such as EOM with the decoupling approximation, SOPT etc, where a retarded (advanced) self-energy for the interacting QD is written as $\Sigma^{r\,(a)} = \Sigma_0^{r\,(a)} + \Sigma_i^{r\,(a)}$, with $\Sigma_0^{r\,(a)} = \mp\mathrm{i}\sum_\eta\Gamma_\eta(\omega)/2$ being the noninteracting part coming from the tunnelling of electrons from the impurity state to outside leads, and $\Sigma_i^{r\,(a)}$ being the interacting part derived within these approximation approaches. The retarded (advanced) GF $G^{r\,(a)}_{d\sigma}$ thus has the form

$$G^{r\,(a)}_{d\sigma}(\omega) = \frac{1}{\omega-\epsilon_d-\Sigma^{r\,(a)}(\omega)}. \tag{7}$$

Unfortunately, one cannot straightforwardly get the lesser GF for the strongly correlated systems under out-of-equilibrium circumstances, as for the retarded GF. Several years ago, Ng proposed a simple scheme to obtain the lesser GF $G^<_{d\sigma}$ from the retarded and advanced terms in order to study ac Kondo resonances in nonlinear transport based on the EOM approach. He assumed that $\Sigma^<(\omega) = A\Sigma_0^<(\omega)$ and $\Sigma^>(\omega) = A\Sigma_0^>(\omega)$ where A is an unknown function, while $\Sigma_0^< = \mathrm{i}\sum_\eta\Gamma_\eta(\omega)f_\eta(\omega)$ and $\Sigma_0^> = -\mathrm{i}\sum_\eta\Gamma_\eta(\omega)[1-f_\eta(\omega)]$ are noninteracting lesser and greater self-energies. These lesser and greater self-energies are requested to satisfy the Keldysh relation $\Sigma^< - \Sigma^> = \Sigma^r - \Sigma^a$, leading to

$$A = \frac{\Sigma^r-\Sigma^a}{\Sigma_0^r-\Sigma_0^a}, \tag{8}$$

or in explicit form,

$$\Sigma^<(\omega) = -2\mathrm{i}\frac{\sum_\eta\Gamma_\eta(\omega)f_\eta(\omega)}{\sum_\eta\Gamma_\eta(\omega)}\,\mathrm{Im}\,\Sigma^r. \tag{9}$$

The lesser GF $G^<_{d\sigma} = \Sigma^<|G^r_{d\sigma}|^2$ is thus obtained. This is the central result of Ng's scheme. It has three advantages, initially addressed by Ng, that

(i) it is exact in the equilibrium limit $\mu_L = \mu_R$,
(ii) it is exact in the noninteracting ($U = 0$) limit under general nonequilibrium situations and
(iii) the continuity equation $J_L(t) = -J_R(t)$ is automatically satisfied in the steady state limit [9].

With the help of this ansatz, as long as one obtains the retarded GF properly describing the strongly correlated system from a certain approximative method, the lesser GF can be derived, and thus the transport problem can be investigated. By means of equation (9), we easily obtain

$$J_\eta = -\frac{2}{h}\int \mathrm{d}\omega\, \Gamma(\omega)[f_\eta(\omega) - f_{\bar\eta}(\omega)]\mathrm{Im}\, G^r_{d\sigma}(\omega), \tag{10}$$

$$J_{Q\eta} = -\frac{2}{h}\int \mathrm{d}\omega\, \Gamma(\omega)(\omega-\mu_\eta)[f_\eta(\omega) - f_{\bar\eta}(\omega)]\mathrm{Im}\, G^r_{d\sigma}(\omega), \tag{11}$$

where $\Gamma(\omega) \equiv \Gamma_L(\omega)\Gamma_R(\omega)/[\Gamma_L(\omega) + \Gamma_R(\omega)]$ and $\bar\eta \neq \eta$. Note that here we arrive at exactly the same current formula (10) as that in [25] without introducing the assumption of a proportional coupling $\Gamma_L(\omega) = \lambda\Gamma_R(\omega)$ (λ is a constant). Since the pioneering work of Ng [9], several attempts have been made to generalize this ansatz to study Kondo-type transport in more complicated devices containing interacting QDs, such as normal metal–QD–superconductor [18] and superconductor–QD–superconductor structures [19]. Nevertheless, the validity of this ansatz is worth further examination. As mentioned in the introduction, verification of the Onsager relation is a natural choice for this purpose.

The Onsager relation is concerned with the linear response of the particle current J_η (equation (10)) and the heat flux $J_{Q\eta}$ (equation (11)) driven by small bias voltages $\mu_\eta - \mu_{\bar\eta} = \delta\mu$ and small temperature gradients $T_\eta - T_{\bar\eta} = \delta T$:

$$J_\eta = -\mathcal{L}_{11}\frac{\delta\mu}{T} - \mathcal{L}_{12}\frac{\delta T}{T^2} = -\frac{2}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)\left[\left(\frac{\partial f_\eta(\omega)}{\partial\mu}\right)_T \delta\mu + \left(\frac{\partial f_\eta(\omega)}{\partial T}\right)_\mu \delta T\right], \tag{12}$$

$$J_{Q\eta} = -\mathcal{L}_{21}\frac{\delta\mu}{T} - \mathcal{L}_{22}\frac{\delta T}{T^2} = -\frac{2}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)(\omega-\mu_\eta)\left[\left(\frac{\partial f_\eta(\omega)}{\partial\mu}\right)_T \delta\mu + \left(\frac{\partial f_\eta(\omega)}{\partial T}\right)_\mu \delta T\right], \tag{13}$$

with $\mathcal{T}(\omega) = \Gamma(\omega)\,\mathrm{Im}\, G^r_{d\sigma}(\omega)_{\delta\mu=0,\delta T=0}$ and

$$\mathcal{L}_{11} = \frac{2T}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)\left(\frac{\partial f_\eta(\omega)}{\partial\mu}\right)_T, \qquad \mathcal{L}_{12} = \frac{2T^2}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)\left(\frac{\partial f_\eta(\omega)}{\partial T}\right)_\mu, \tag{14}$$

$$\begin{aligned}\mathcal{L}_{21} &= \frac{2T}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)(\omega-\mu_\eta)\left(\frac{\partial f_\eta(\omega)}{\partial\mu}\right)_T,\\ \mathcal{L}_{22} &= \frac{2T^2}{h}\int \mathrm{d}\omega\, \mathcal{T}(\omega)(\omega-\mu_\eta)\left(\frac{\partial f_\eta(\omega)}{\partial T}\right)_\mu.\end{aligned} \tag{15}$$

We can easily see that Ng's ansatz equation (9) preserves the Onsager relation $\mathcal{L}_{12} = \mathcal{L}_{21}$ automatically. Furthermore, the result is independent of the approximation adopted in deriving the retarded GF.

3. Thermoelectric effects in the presence of Kondo correlation

As shown in equation (12), both the bias voltage and the temperature gradient between two reservoirs can give rise to particle current. The current induced purely by a small bias voltage reflects the electric conductance $G = -\frac{e^2}{T}\mathcal{L}_{11}$, while the thermopower S measures the voltage difference needed to eliminate the current due to the temperature gradient between the leads, given in the linear regime by

$$S = -\frac{1}{eT}\frac{\mathcal{L}_{12}}{\mathcal{L}_{11}}. \tag{16}$$

In this situation, we can simplify the thermal flux equation (13) as $J_{Q\eta} = -\kappa\delta T$, in which

$$\kappa = \frac{1}{T^2}\left(\mathcal{L}_{22} - \frac{\mathcal{L}_{12}^2}{\mathcal{L}_{11}}\right) \tag{17}$$

is the thermal conductance.

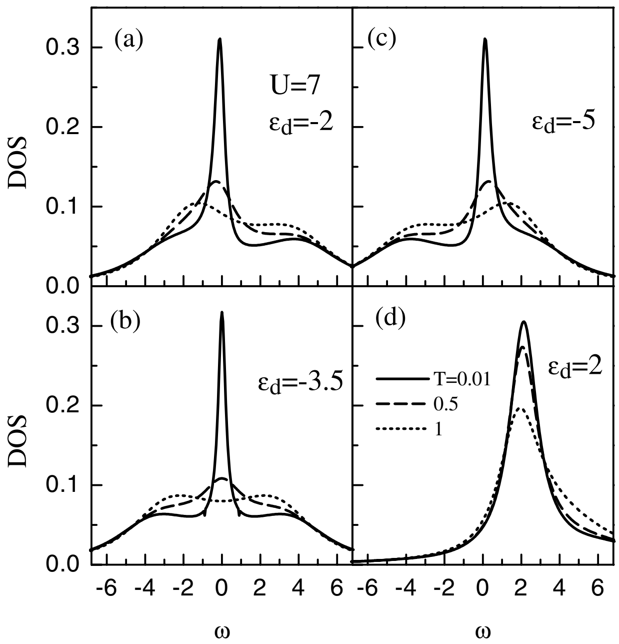

Figure 1. The DOS of the interacting QD $U = 7$ calculated from the modified SOPT with several energy levels $\epsilon_d = -2$ (a), -3.5 (b), -5 (c), 2 (d) and different temperatures $T = 0.01$, 0.5 and 1. In this and following figures, Γ is chosen as the energy unit.

Comparing the explicit expressions of $\mathcal{L}_{11}$ and $\mathcal{L}_{12}$ (equation (14)), we can roughly address that in low temperatures, the electric conductance G is determined by the transmission probability, or the density of states (DOS) of the QD, at the Fermi energy of the leads, while the linear thermopower S depends sensitively on the energy dependence of the DOS, implying that it contains information different from the electric conductance. So far, the thermopower of QDs in the Kondo regime is still much less studied in the literature. In this section, we attempt to numerically calculate the linear Kondo-type thermoelectric effects in QDs. The remaining task is to choose a suitable approximative scheme, which can provide the retarded self-energy (or DOS $\rho(\omega)$) capable of properly describing the Kondo physics in a wide range of parameters of interacting QDs. In the present paper, a modified SOPT developed in [8] is adopted, in which

$$\Sigma_i^r(\omega) = Un + \frac{a\Sigma^{(2)}(\omega)}{1 - b\Sigma^{(2)}(\omega)}, \tag{18}$$

with $a = n(1-n)/n_0(1-n_0)$ and $b = (1-2n)/n_0(1-n_0)U$. n is the occupation number of the QD level which should be determined self-consistently. $\Sigma^{(2)}$ and n_0 are, respectively, the second order self-energy in U and a fictitious particle number, both of which are obtained from the bare GF $G_0^r = 1/(\omega - \epsilon_d - Un - \Sigma_0^r)$.

In actual calculation, an assumption that the tunnelling strength is independent of incident energy is taken in the wide-band limit and a symmetric system $\Gamma_L(\omega) = \Gamma_R(\omega) = \Gamma$ is focused. In the following we take the coupling strength Γ as the energy unit and the Fermi level of the lead to be zero.

In figures 1(a)–(d) we plot the equilibrium DOS $\rho(\omega)$ for the QD with $U = 7$ and several different energy levels $\epsilon_d = -2$, -3.5, -5 and 2 at different temperatures. We can observe

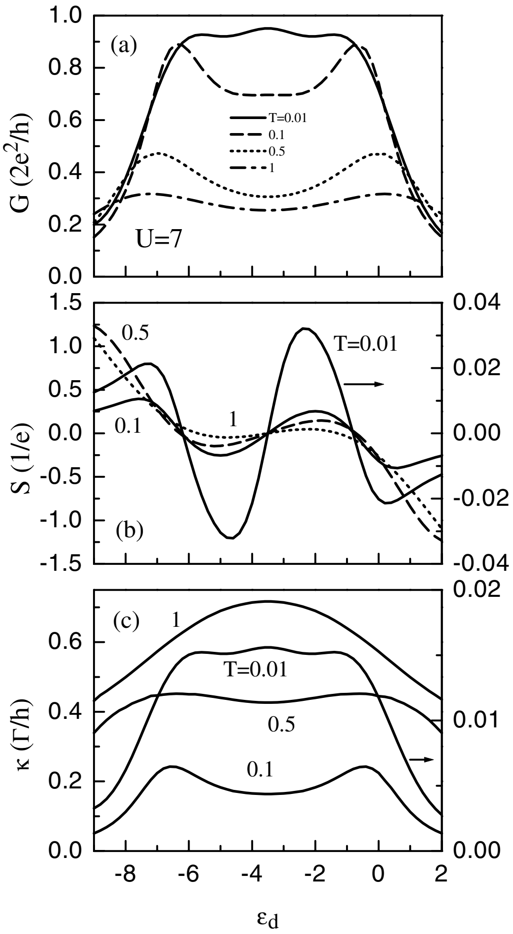

Figure 2. (a) The electric conductance G, (b) the thermopower S and (c) the thermal conductance κ, as functions of the energy level for several different temperatures $T = 0.01$, 0.5 and 1. The on-site Coulomb interaction in the QD is $U = 7$.

that the Kondo resonance peak in the DOS is clearly resolved for the Kondo systems $\epsilon_d = -2$, -3.5 and -5 at low temperature $T = 0.01$, but nearly disappears at high temperature $T = 1$. Of course there is no Kondo peak in the DOS for the non-Kondo system $\epsilon_d = 2$. In figure 2, the calculated electric conductance G (a), thermopower S (b) and thermal conductance κ (c) are displayed as functions of the gate voltage, i.e., the energy level in the QD. As expected, the conductance demonstrates a single-peak structure and nearly unitary limit near the symmetric point $\epsilon_d = -U/2$ at very low temperature, splitting peaks with increasing temperature and a minimum at $\epsilon_d = -U/2$ for very high temperature. It manifests the equilibrium DOS of the QD at the Fermi energy of the lead, $\rho(0)$, at low temperature, but not the concrete shape of the Kondo peak: symmetric or nonsymmetric (right or left of centre) around the Fermi energy of the lead. In order to detect the DOS in the whole range of energy, an attempt has been made to measure the differential conductance of a QD. However, the finite bias voltages between two leads result in a large change of DOS, giving rise to a splitting of the Kondo peak. As mentioned above, an alternative way of addressing this problem is to explore the thermopower, because it is relevant with the product of the incident electron energy ω and

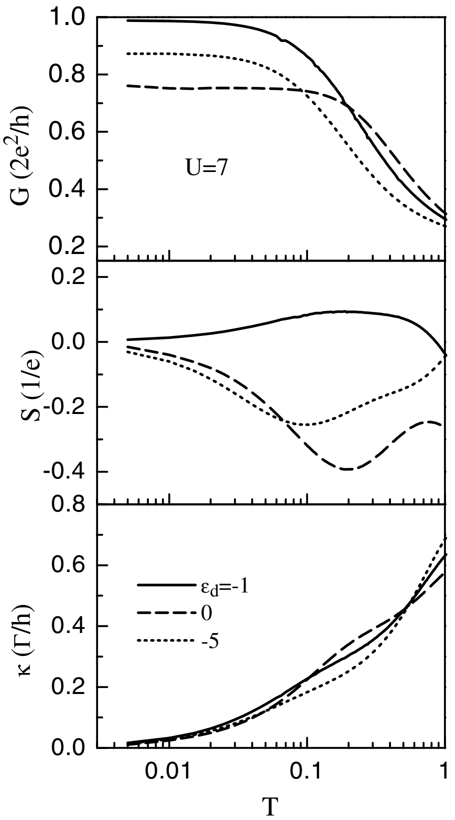

Figure 3. (a) The electric conductance, (b) the thermopower and (c) the thermal conductance versus temperature for the QD with $U = 7$ and $\epsilon_d = -1$, 0 and -5.

the DOS of QD $\rho(\omega)$. For example, the perfectly symmetric shape of DOS around $\omega = 0$ in the symmetric case $\epsilon_d = -3.5$, as shown in figure 1(b), results in exactly zero thermopower; while the positive (negative) thermopower is attributed to slight slanting of the DOS towards the left (right) for $\epsilon_d = -2$ (-5) (figures 1(a) and (c)), implying an oscillatory behaviour around zero which can be controlled by the gate voltage. We also observe from figure 2(b) that the magnitude of oscillations in thermopower is greatly decreased with lowering temperature due to the Kondo-suppressed deviation of DOS from the symmetric shape. Figure 2(c) reveals that the thermal conductance κ has similar behaviour to the electric conductance G at low temperature, but quite different at high temperature $T = 1$.

Figure 3 displays the temperature dependence of these three quantities. We observe from figure 3(b) that the thermopower shows a logarithmic rise with increasing temperature, leading to a broad maximum, and subsequently decreases in the high temperature regime. But temperature increase cannot cause a change of the sign of the thermopower, except for very high temperature where the Kondo effect is quenched. Figure 3(c) shows that the thermal conductance has similar temperature dependence for these different systems. As a result, the thermal conductance is not a suitable tool to explore the Kondo effect. The interesting physical quantity is the ratio between the thermal and electric conductances. The classical theory yields that thermal and electric transport in bulk metals satisfies the Wiedemann–Franz law $\kappa/TG = \pi^2/3e^2$. In a mesoscopic system transport occurs through a small confined region,

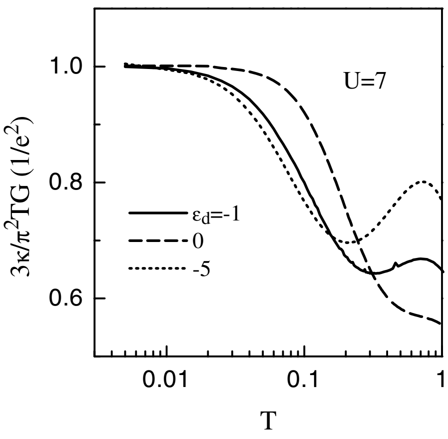

Figure 4. The ratio factor between the electric conductance and thermal conductance versus temperature for a QD with the same parameters as in figure 3.

and consequently does not satisfy the Wiedemann–Franz law in general. We depict this ratio in figure 4. Surprising recovery of the Wiedemann–Franz law is observed at very low temperature, where transport through the QD is dominated by Kondo correlation, implying that the Landau Fermi liquid state is rebuilt in this situation. But substantial deviation from the classical value emerges with increasing temperature due to disappearance of the Kondo effect. This temperature behaviour provides a good trademark for exploring the onset of Kondo correlation.

4. Conclusion

We have studied the particle current and thermal flux through an interacting QD on the basis of the nonequilibrium GF approach and Ng's ansatz. The advantage of the ansatz is its capability of evaluating the lesser (greater) GF from the retarded and advanced GFs derived in a certain rational approximation scheme. The validity of the ansatz and the resulting linear transport coefficients have been examined in terms of the Onsager relation. We have also emphasized that the same electric current formula as in [25] can be obtained without the assumption of proportional coupling $\Gamma_L(\omega) = \lambda\Gamma_R(\omega)$.

In the wide-band limit, a modified SOPT has been employed to calculate the retarded GF for an interacting QD and with this retarded GF the thermoelectric effect in the Kondo regime has been investigated. We have found that the thermopower exhibits a oscillatory behaviour around zero due to nonsymmetric shape of the Kondo peak in the DOS, giving rise to a change of sign of the thermopower which is controllable by tuning the gate voltage. These results demonstrate that measuring thermopower can provide useful information on the DOS in QDs. Furthermore, our calculation reveals that the magnitude of oscillation is greatly suppressed by the Kondo effect. Finally, we have explored the temperature characteristic of the thermoelectric effect and predicted that at low temperature regime thermal transport satisfies the classical Wiedemann–Franz law, which can be taken as a trace of the Kondo correlation.

Acknowledgments

This work was supported by the National Natural Science Foundation of China, the Special Funds for Major State Basic Research Project (grant No 2000683), the Ministry of Science and Technology of China, the Shanghai Municipal Commission of Science and Technology and the Shanghai Foundation for Research and Development of Applied Materials.

References

[1] Goldhaber-Gordon D, Shtrikman H, Mahalu D, Abusch-Magder D, Meirav U and Kastner M A 1998 *Nature* **391** 156
[2] Cronenwett S M, Oosterkamp T H and Kouwenhoven L P 1998 *Science* **281** 540
[3] Goldhaber-Gordon D, Gores J, Kastner M A, Shtrikman H, Mahalu D and Meirav U 1998 *Phys. Rev. Lett.* **81** 5225
Schmid J, Weis J, Eberl K and Klitzing K v 1998 *Physica* B **256–258** 182
Schmid J, Weis J, Eberl K and Klitzing K v 2000 *Phys. Rev. Lett.* **84** 5824
van der Wiel W G, De Franceschi S, Fujisawa T, Elzerman J M, Tarucha S and Kouwenhoven L P 2000 *Science* **289** 2105
[4] Sasaki S, De Franceschi S, Elzerman J M, van der Wiel W G, Eto M, Tarucha S and Kouwenhoven L P 2000 *Nature* **405** 764
Nygård J, Cobden D H and Lindelof P E 2000 *Nature* **408** 342
[5] Meir Y, Wingreen N S and Lee P A 1991 *Phys. Rev. Lett.* **66** 3048
Hershfield S, Davies J H and Wilkins J W 1992 *Phys. Rev.* B **46** 7046
[6] Meir Y, Wingreen N S and Lee P A 1993 *Phys. Rev. Lett.* **70** 2601
Wingreen N S and Meir Y 1994 *Phys. Rev.* B **49** 11040
[7] Yeyati A L, Martín-Rodero A and Flores F 1993 *Phys. Rev. Lett.* **71** 2991
[8] Craco L and Kang K 1999 *Phys. Rev.* B **59** 12244
[9] Ng T K 1996 *Phys. Rev. Lett.* **76** 487
[10] Anderson P W 1961 *Phys. Rev.* **124** 41
[11] Lacroix C 1981 *J. Phys. F: Met. Phys.* **11** 2389
[12] Yosida K and Yamada K 1970 *Prog. Theor. Phys. Suppl.* **46** 244
Horvatić B and Zlatić V 1980 *Phys. Status Solidi* b **99** 251
[13] Coleman P 1984 *Phys. Rev.* B **29** 3035
[14] Bickers N E 1987 *Rev. Mod. Phys.* **59** 845
[15] Aono T *et al* 1998 *J. Phys. Soc. Japan* **67** 1860
Georges A and Meir Y 1999 *Phys. Rev. Lett.* **82** 3508
Aguado R and Langreth D C 2000 *Phys. Rev. Lett.* **85** 1946
[16] Dong B and Lei X L 2001 *Phys. Rev.* B **63** 235306
Dong B and Lei X L 2001 *J. Phys.: Condens. Matter* **13** 9245
[17] Dong B and Lei X L 2002 *Phys. Rev.* B **65** 241304(R)
[18] Fazio R and Raimondi R 1998 *Phys. Rev. Lett.* **80** 2913
Sun Q F, Guo H and Lin T H 2001 *Phys. Rev. Lett.* **87** 176601
[19] Cho S Y, Kang K and Ryu C M 1999 *Phys. Rev.* B **60** 16874
[20] Onsager L 1931 *Phys. Rev.* **37** 405
[21] Beenakker C W J and Staring A A M 1992 *Phys. Rev.* B **46** 9667
Dzurak A S, Smith C G, Barnes C H W, Pepper M, Martin-Moreno L, Liang C T, Ritchie D A and Jones G A C 1997 *Phys. Rev.* B **55** 10197
Andreev A V and Matveev K A 2001 *Phys. Rev. Lett.* **86** 280
[22] Kim T S and Hershfield S 2002 *Phys. Rev. Lett.* **88** 136601
[23] Boese D and Fazio R 2001 *Europhys. Lett.* **56** 567
[24] Mahan G D 1981 *Many-Particle Physics* (New York: Plenum)
[25] Meir Y and Wingreen N S 1992 *Phys. Rev. Lett.* **68** 2512
[26] Langreth D C 1976 *Linear and Nonlinear Electron Transport in Solids (NATO ASI, Series B, vol 17)* ed J T Devreese and V E Van Doren (New York: Plenum)