Thermoelectric effects in strongly interacting quantum dot coupled to ferromagnetic leads

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We study thermoelectric effects in a Kondo correlated quantum dot coupled to ferromagnetic electrodes by calculating conductance, thermopower, and thermal conductance in the Kondo regime. We also study the effect of the asymmetry in the coupling to the leads, which has important consequences for antiparallel magnetization configuration. We discuss the thermoelectric figure of merit, tunnel magnetoresistance, and violation of the Wiedemann-Franz law in this system. The results agree with recently measured thermopower of the quantum dot defined in a two-dimensional electron gas.

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I. INTRODUCTION

Transport properties of the device consisting of the quantum dot attached to external leads are strongly affected by the appearance of the correlated many body Kondo state. The phenomenon discovered long ago has manifested itself as a low-temperature increase of the electrical resistance of diluted alloys. In quantum dots it shows up as an increase of conductance at low temperatures. The quantum dot devices allow the study of fundamental physics such as the Coulomb blockade phenomenon or Kondo effect in equilibrium and nonequilibrium conditions and in geometries not accessible in bulk systems. One or both of the external leads may be normal, superconducting, or magnetic. In this paper we shall study the systems in which the quantum dot is coupled with two ferromagnetic leads having the same or opposite magnetic polarization.

Spin-polarized transport, especially single electron tunneling, in magnetic nanostructures has attracted much interest due to its potential applications in, for example, spintronics and quantum computing. The Kondo effect in quantum dots attached to normal leads (N-QD-N structure) has been extensively studied both experimentally and theoretically. Many new effects have been predicted and observed in the transport characteristics, such as splitting of the zero bias resonance under magnetic field, absence of the even-odd parity effects, or out of equilibrium Kondo effect. The Kondo effect has also been observed in many other systems: single atom, single molecule, and carbon nanotubes. It has also been demonstrated in quantum dots attached to ferromagnetic leads, where transport properties can, in principle, be controlled with aid of the electron spin degree of freedom.

Recently we have observed growing interest in electronic transport properties of the Kondo correlated quantum dots coupled to ferromagnetic electrodes. In such geometry the Kondo resonance splits in parallel configuration (however, some of the works predict no splitting), while in the antiparallel configuration the Kondo effect remains virtually the same as for nonmagnetic electrodes. The shot noise studies reveal huge differences for spin up and spin down electrons in the parallel alignment and no differences in antiparallel configuration. It is well known that thermoelectric properties are the source of information complementary to that obtained from other transport characteristics. Thermal properties (thermopower and thermal conductance) of the quantum dot coupled to the normal leads in the Kondo regime have recently been investigated. Thermopower has been shown to be very sensitive and a powerful tool to study the Kondo effect. It manifests itself as an energy peak in the DOS slightly above Fermi energy and this leads to change of sign of the thermopower.

It is the purpose of the present work to study the thermoelectric properties of the quantum dot coupled to ferromagnetic leads. We shall concentrate on the conductance, thermal conductance, and related quantities such as tunnel magnetoresistance (TMR), thermoelectric figure of merit which directly informs on the usefulness of the system for applications and Wiedemann-Franz ratio which normalized value differing from 1 signals breakdown of the Fermi-liquid state.

We show that thermopower is very different for spin up and spin down electrons in parallel configuration and is similar to the nonmagnetic case for the antiparallel one. However, for parallel alignment the total (spin up plus spin down) thermopower is very small compared to the antiparallel alignment.

The organization of the rest of the paper is as follows. In Sec. II we present the model and discuss some aspects of our procedure. Results of calculations are presented and discussed in Sec. III. We end up with summary and conclusions.

II. MODEL AND APPROACH

Schematic view of the quantum dot coupled to two leads $R$ and $L$, which may be magnetically polarized and/or at different temperatures and voltages is shown in Fig. 1. We assume that the interaction energy between two electrons on the quantum dot is the largest energy in the problem and thus model the system as the $U\infty$ single impurity Anderson Hamiltonian in the slave boson representation

$$H = \sum_{\lambda k} \epsilon_{\lambda k} n_{\lambda k}^c n_{\lambda k}^c + \sum_{\sigma} \epsilon_{\lambda k} f^c_{\lambda k \sigma} f_{\lambda k \sigma} + \sum_{\lambda k} \left( V_{\lambda k} c^c_{\lambda k \sigma} f^+_{\lambda k \sigma} + H.c. \right),$$

where $\lambda=L (R)$ denotes left (right) lead, $c^c_{\lambda k \sigma}$ ($c_{\lambda k \sigma}$) is the
creation (annihilation) operator for a conduction electron with the wave vector \( k \), spin \( \sigma \) in the lead \( \lambda \), and \( V_{\lambda k\sigma} \) is the hybridization matrix element between localized electron on the dot with the energy \( \epsilon_{\lambda k} \) and conduction electron of energy \( \epsilon_{\lambda k\sigma} \) in the lead \( \lambda \). Fermagnetism of the electrodes is modeled via modified conduction electron energy \( \epsilon_{\lambda k\sigma} = \epsilon_{\lambda k} \pm \alpha \hbar \omega_c \), where the magnetization points into \( z \) direction (the same or opposite in both leads). The constraint of no double occupancy is, in the present approach, \(^{36}\) exactly taken into account by the noncanonical commutation rules for fermion and boson operators.

The particle current \( J_\lambda \) and the energy flux \( J_{E\lambda} \) flowing from the lead \( \lambda \) to the central region can be calculated from the time derivative of charge and energy operator, respectively.\(^{39}\) We use the relation \( J_{\lambda 0} = J_{E\lambda} - \mu_\lambda J_\lambda \) for the thermal flux \( J_{\lambda 0} \) and express all currents in terms of Keldysh Green functions\(^ {40}\) in the standard form\(^ {23,32}\)

\[
J_\lambda = \frac{i e}{\hbar} \sum_\sigma \int_{-\infty}^{\infty} \frac{d \omega}{2 \pi} \Gamma_{\lambda \sigma}(\omega) \left[ G^>_{\sigma}(\omega) + 2i f_\sigma(\omega) \text{Im} G^<_{\sigma}(\omega) \right],
\]

\[
J_{Q\lambda} = \frac{i}{\hbar} \sum_\sigma \int_{-\infty}^{\infty} \frac{d \omega}{2 \pi} \Gamma_{\lambda \sigma}(\omega)(\omega - \mu_\lambda) \times [G^<_{\sigma}(\omega) + 2if_\sigma(\omega)\text{Im} G^>_{\sigma}(\omega)],
\]

where \( G^>_{\sigma}(\omega) \) is the Fourier transform of the retarded Green function (GF) \( G^>_\sigma(t, t') = i\theta(t)\langle f^\dagger_\sigma(t)f_\sigma(t') \rangle_\lambda \) and \( G^<_{\sigma}(\omega) = i\langle f^\dagger_\sigma(t)f_\sigma(t) \rangle \) is the Fourier transform of the lesser Keldysh GF.\(^ {40}\) \( \Gamma_{\lambda \sigma}(\omega) = 2\pi \sum_k |V_{\lambda k\sigma}|^2 \delta(\omega - \epsilon_{\lambda k\sigma}) \) denotes the strength of the coupling between dot and the lead \( \lambda \), \( f_\sigma(\omega) = \langle f^\dagger_\sigma(\omega)f_\sigma(\omega) \rangle \) is the Fermi distribution function in the lead \( \lambda \) with the chemical potential \( \mu_\lambda \) and temperature \( T_\lambda \).

In general, when both the strong on-dot Coulomb interaction and the tunneling between dot and leads occur, it is not possible to calculate \( G^<(r)(\omega) \) exactly. Several approximation schemes have been proposed to calculate \( G^<(r)(\omega) \). Here we use a recently proposed equation of motion technique for nonequilibrium GF.\(^ {41}\) This technique allows calculation of both \( G^>_\sigma(\omega) \) and \( G^<_{\sigma}(\omega) \) in a consistent way making similar approximations in the decoupling procedure of both \( G^>_\sigma(\omega) \)

and \( G^<_{\sigma}(\omega) \). The approach has been successfully applied to study systems containing quantum dot.\(^ {37,38}\) In the present case it yields

\[
J_\epsilon = -\frac{e}{\hbar} \sum_\sigma \int_{-\infty}^{\infty} d\omega \Gamma_{\sigma}(\omega) [f^\dagger_\sigma(\omega) - f_\sigma(\omega)] \text{Im} G^>_{\sigma}(\omega),
\]

\[
J_Q = -\frac{1}{\hbar} \sum_\sigma \int_{-\infty}^{\infty} d\omega \Gamma_{\sigma}(\omega)(\omega - eV) \times [f^\dagger_\sigma(\omega) - f_\sigma(\omega)] \text{Im} G^<_{\sigma}(\omega),
\]

where \( \Gamma_{\sigma} = \Gamma_{L\sigma} + \Gamma_{R\sigma}/[\Gamma_{L\sigma} + \Gamma_{R\sigma}] \) and \( eV = \mu_L - \mu_R \). The on-dot retarded GF reads

\[
G_{\sigma}(\omega) = \frac{1 - \langle n_{-\sigma} \rangle}{\omega - e_{\sigma} - \sum_\omega G_{\sigma}(\omega) - \sum_{\sigma} f_{\sigma}(\omega)},
\]

with noninteracting \( \Sigma_{0\sigma}(\omega) = \sum_k [\langle V_{k\sigma}^2 \rangle/2(\omega - \epsilon_{k\sigma})] \) and interacting self-energy \( \Sigma_{\sigma}(\omega) = \sum_k [\langle V_{k\sigma}^2 \rangle f_k(\epsilon_{k\sigma} - \epsilon_{k\sigma})/(\omega - \epsilon_{k\sigma} - e_{\sigma} - \epsilon_{k\sigma})] \). In order to get the splitting of the Kondo resonance in the presence of the ferromagnetic leads, which is consistent with the scaling analysis, we follow Ref. 17 and replace the bare dot energy level \( \epsilon_{d,\sigma} \) by \( \tilde{\epsilon}_{\sigma} \) found self-consistently from \( \tilde{\epsilon}_{\sigma} = e_{d,\sigma} + Re[\Sigma_{0\sigma}(\epsilon_{\sigma}) + \Sigma_{\sigma}(\epsilon_{\sigma})] \). In the numerical results presented below we have used constant bands of width \( D = 100t \), \( 1/2(\Gamma_{L\sigma} + \Gamma_{R\sigma}) = \Gamma \) and use \( \Gamma \) as our energy unit in the following. Let us mention that our treatment of correlations is equivalent to saddle point approximation in the standard slave boson technique.\(^ {42}\)

Within linear response theory (\( V \rightarrow 0 \)) for the particle current and the heat flux one defines the conductance \( G \) as equal to \( -(e^2/2T)L_{11} \), thermopower is given by \( S = -(1/eT)(L_{12}/L_{11}) \) and the thermal conductance by \( \kappa = (1/T)(L_{22} - L_{12}^2/L_{11}) \). The linear response coefficients read

\[
L_{11} = \frac{T}{\hbar} \sum_\sigma \int d\omega \Gamma_{\sigma}(\omega) \text{Im} G^<_{\sigma}(\omega) \left( -\frac{\partial f_\sigma(\omega)}{\partial \omega} \right) ,
\]

\[
L_{12} = \frac{T^2}{\hbar} \sum_\sigma \int d\omega \Gamma_{\sigma}(\omega) \text{Im} G^\sigma(\omega) \left( \frac{\partial f_\sigma(\omega)}{\partial T} \right) ,
\]

\[
L_{22} = \frac{T^2}{\hbar} \sum_\sigma \int d\omega \Gamma_{\sigma}(\omega)(\omega - eV) \text{Im} G^\sigma(\omega) \left( \frac{\partial f_\sigma(\omega)}{\partial T} \right) ,
\]

with the common distribution function \( f_\sigma(\omega) = f_{\sigma R}(\omega) \).

The leads considered here are magnetically polarized. In the following we shall characterize the degree of polarization by the parameter \( p = (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow) \), where \( n_\sigma \) is the concentration of spin \( \sigma \) electrons. The magnetization of both leads may point into the same direction (parallel configuration) or in opposite directions (antiparallel configuration).

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where \( T_K(p=0) \approx 2 \cdot 10^{-2} \Gamma \).

### III. THE RESULTS

In Fig. 2 linear conductance of the system in parallel configuration is calculated as a function of temperature for a number of lead polarizations \( p \). One observes the decrease of \( G \) for larger values of \( p \). This is due to the splitting of the Kondo resonance. Moreover, the decrease of \( G \) is not a universal function of \( p \). On the other hand, in antiparallel configuration, the conductance can be obtained from that for unpolarized leads, as it scales according to the relation \( G(p)/G(0) = 1 - p^2 \) for the whole temperature region.

Tunnel magnetoresistance is defined\(^{43}\) as the ratio

\[
\text{TMR} = \frac{G_P - G_{AP}}{G_{AP}},
\]

where \( G_{P(AP)} \) is the conductance calculated for parallel (antiparallel) configuration of the leads magnetization. It is shown in Fig. 3 as a function of polarization factor \( p \) for a number of temperatures for a system characterized by \( \epsilon_d = -1.75 \Gamma \). Note that the Kondo temperature itself is a function of \( p \). For unpolarized leads one finds \( T_K(p=0) \approx 2 \times 10^{-2} \Gamma \). The dependence is not symmetric with respect to \( p=0.5 \) and changes its character with temperature.

For small polarizations it is negative, as in this case \( G_{AP} \) is not much affected by the exchange field while \( G_P \) is strongly suppressed due to the splitting of the Kondo resonance. For large values of the polarization, TMR is positive, as in this case \( G_{AP} \) goes to zero with \( p \to 1 \) while \( G_P \) tends to finite value.

The thermal conductance \( \kappa \) vs temperature in the \( P \) configuration is displayed in Fig. 4. As one can see in Fig. 4 thermal conductance does not change much with the increasing of the leads polarization \( P \). This quantity is not a sensitive tool for the study of the Kondo effect. In the case of AP configuration for any temperature, \( \kappa \) scales with the polarization in the same way as \( G \) does, namely, \( \kappa(p)/\kappa(0) = 1 - p^2 \).

In Fig. 5 linear thermopower vs temperature is shown for a number of polarizations in the parallel configuration. The upper panel shows the total thermopower, the middle one the thermopower associated with spin up, while the lower one with spin down electrons. The \( p=0 \) curve corresponds to nonmagnetic leads. First of all one can see that for \( p=0 \) and around \( T = T_K \), where \( T_K \) is the Kondo scale, the thermopower reaches minimal value. It increases for elevated temperatures and eventually changes sign. This signals the disappearance of the Kondo peak. As it is well known, and in similar context has already been noted by Boese and Fazio,\(^{32}\) the thermopower is sensitive to the curvature of the energy dependence of the density of states. This curvature is negative at high temperatures and for \( \epsilon_d \) well below the chemical potential, while it becomes positive at low temperatures, when the Kondo resonance forms slightly above the chemical potential.

The low-temperature changes of \( S \) with polarization can also be understood. With increasing polarization in the leads thermopower decreases to zero, except at very high temperatures where the broad maximum (minimum) is observed. Small thermopower at low \( T \) for increasing leads polarization is due to the splitting of the Kondo resonance by the stray fields coming from the ferromagnetic leads. In this case DOS around the Fermi energy is almost symmetric. Moreover the thermopower is mostly positive in the whole range of the temperatures except for very small leads polarizations. It is worthwhile to note additional broad maximum (spin up) and minimum (spin down) of the thermopower at temperatures...
below $T=0.1$ for small polarizations. For such polarizations the distance between Kondo resonances $\delta$ is not so large ($\delta=1$) and thermal broadening significantly affects the DOS at the Fermi level, thus giving rise to the observed thermopower.

For AP configuration the thermopower does not depend on the polarization and is the same as for the QD with nonmagnetic leads. This can be easily understood as this quantity measures the curvature of the DOS around the Fermi energy, which does not change with the polarization in this case. Only the height of the Kondo resonance changes.

In Fig. 6 the total thermopower (upper panel), that in the spin up channel (middle panel), and in the spin down channel (lower panel), is plotted as a function of the lead polarization in $P$ configuration. Interestingly thermopower changes its behavior in a significant way only for small values of $p$ and at low temperatures it even changes sign. This is attributed to the splitting of the Kondo resonances. For small lead polarizations the splitting is small but significantly influences the DOS around the Fermi energy. For larger $p$ the Kondo peaks

FIG. 5. (Color online) The total thermopower of the quantum dot (upper panel), the thermopower associated with the spin up electrons (middle panel), and that one associated with spin down electrons (lower panel) as a function of the temperature for a number of lead polarizations.

FIG. 6. (Color online) Thermopower of the quantum dot as a function of the lead polarization for a number of temperatures. The upper panel shows the total thermopower, the middle one—that associated with spin up electrons, and the lower one—that for spin down electrons.
are far away from the Fermi energy and do not change low-energy DOS much.

So far the results for parallel configuration of the lead polarizations have been presented. However, as we have mentioned already, for antiparallel configuration the calculated quantities either do not depend on the value of the polarization and they are the same as for nonmagnetic leads (thermopower) or can be obtained from the solution for nonmagnetic leads due to the scaling relation $1 - p^2$ (electric and thermal conductance). This is easy to understand as for such polarizations the tunneling of spin up and spin down electrons on the dot are allowed to one of the electrodes. This is true for symmetric couplings. The situation is different when there is asymmetry in the coupling to the left and right lead. In this case the electric conductance behaves similarly as in parallel configuration (see Fig. 2). Thermal conductance also does not change much with increasing the leads polarization. It slightly decreases in the whole region of the temperatures.

On the other hand, behavior of the thermopower in asymmetrical AP configuration (which does not depend on $p$ for symmetric couplings) is similar to the case of the $P$ configuration (see Fig. 5). In Fig. 7 thermopower vs temperature for asymmetrical coupled quantum dot with $\Gamma_{Lp}/\Gamma_{Rd}=2$ is plotted. At high-$T$ thermopower goes to zero, eventually oscillating, with decreasing temperature.

Such behavior can be explained by the fact that for asymmetric couplings there is a splitting of the Kondo resonance. In symmetrically coupled quantum dot there is an equal number of electrons with spin up and down on the dot coming from different leads and one can show that this model can be mapped onto quantum dot with nonmagnetic leads. Here, when $\Gamma_{Lp}/\Gamma_{Rd} \neq 1$, due to different tunneling probabilities, quantum dot sees asymmetry in electron number with spins up and down and in this sense antiparallel configuration is very similar to a parallel one (see Fig. 5).

Thermoelectric figure of merit $Z = S^2 G / \kappa$ is a direct measure of the usefulness of the material or device for thermoelectric power generators or cooling systems. For simple systems it is inversely proportional to operation temperature and thus one conveniently plots $ZT$, which numerical value is an indicator of the systems performance. In Fig. 8 we show $ZT$ as a function of temperature in the $P$ configuration. Note that it is smaller than 1, which signals limited practical applicability of the studied device. The increase of polarization slightly increases $ZT$ but it never exceeds 1.

Again, in the AP configuration the thermoelectric figure of merit does not depend on $p$, which can be easily deduced from the definition of this quantity. On the other hand, in the asymmetrical AP configuration it changes little but unlike for $P$ configuration, it slightly decreases with increasing the polarization.

Finally we discuss Wiedemann-Franz (WF) law which relates thermal and electrical transport via relation $\kappa = (\pi^2/3 e^2) T G$. This law describes transport in Fermi liquid bulk metals and in general is not obeyed in QD systems where the transport occurs through a small confined region. However, at very low temperatures, where the Kondo effect develops and the ground state of the system has Fermi-liquid nature, the WF law is recovered. At high temperatures transport is dominated by sequential tunneling processes leading to the larger suppression of the thermal transport than the electrical one. This behavior is illustrated in Fig. 9 in $P$ configuration (upper panel) and in asymmetrical AP configuration (lower panel) for a number of the polarizations. In the AP configuration with symmetric couplings to the leads WF ratio does not depend on $p$ due to its definition and behavior of the quantities entering into it.

IV. COMPARISON WITH EXPERIMENT

It is worth noting that the thermopower of the quantum dot in the Kondo regime has recently been measured experimentally albeit for nonmagnetic electrodes. The dot itself and the electrodes were defined in the two-dimensional electron gas. In the experimental situation the charging energies (i.e., $U$) were finite and varied between 2 and 5 in units of effective coupling $\Gamma$. This precludes the detailed comparison with our calculations (for $p=0$) as we have taken $U=\infty$ limit. Experimentally one applies the bias $V_{SD}$ between source and drain and measures thermopower as a function of gate voltage $V_g$. Theoretically this dependence can be modeled by plotting $S$ as a function of on-dot energy level $e_\sigma$. 

FIG. 7. (Color online) Thermopower vs temperature for asymmetrical ($\Gamma_{Lp}/\Gamma_{Rd}=2$) coupled quantum dot in the anti-parallel configuration.

FIG. 8. (Color online) Temperature dependence of the thermoelectric figure of merit $Z = S^2 G / \kappa$. 

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Experimental data, shown in Fig. 4 of Ref. 44 qualitatively agree with our calculations for $p=0$ presented in Fig. 10.

To understand the results, as the first approximation one can use so-called Mott formula, which states that thermopower is proportional to the logarithmic derivative of the conductance with respect to the energy evaluated at the actual Fermi energy. The Kondo effect shows up as additional maximum appearing in conductance via quantum dot when the temperature decreases. It is essentially due to Abrikosov-Suhl resonance in the density of states, which appears at low temperatures and is located slightly above the Fermi level of the leads. The slope of conductance thus changes and the thermopower changes sign. The similarity between theoretical and experimental results is very encouraging. However, for qualitative comparison one has to take few energy levels on the dot, assume finite $U$ values and selfconsistently calculate the shift of $\varepsilon_d$ with changing gate voltage. Also the nonlinear conductance and thermopower for actual value of $V_g$ and $V_{SD}$ have to be obtained. This is outside the scope of the present paper. The detailed comparison between experimental data and calculations will be the subject of future work.

V. SUMMARY AND CONCLUSIONS

In summary, we have studied thermal properties of the strongly correlated quantum dot coupled to the ferromagnetic leads in the Kondo regime. We have found that thermopower is strongly suppressed at low temperatures due to the splitting of the Kondo resonance in parallel configuration of the lead polarization. In antiparallel configuration Kondo effect behaves in a way similar to the system with nonmagnetic electrodes so the results do not depend on the value of the polarization in the leads. Moreover we have shown that asymmetry in the coupling to the leads in antiparallel configuration has important consequences as it lifts spin degeneracy on the dot thus leading to the suppression of the thermopower at low temperature, similarly as in the parallel polarization configuration. Finally we have checked the Wiedemann-Franz relation which does not hold in general, but similarly as for QD with nonmagnetic leads it is recovered at low temperatures where the Kondo effect develops. The results qualitatively agree with experimental data.

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