

# Correlation effects in the transport through quantum dots

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We study the charge and heat transport through the correlated quantum dot with a finite value of the charging energy  $U \neq \infty$ . The Kondo resonance appearing at temperatures below  $T_K$  is responsible for several qualitative changes of the electric and thermal transport. We show that under such conditions the semiclassical Mott relation between the thermopower and electric conductivity is violated. We also analyze the other transport properties where a finite charging energy  $U$  has a significant influence. They are considered here both, in the limit of small and for arbitrarily large values of the external voltage  $eV = \mu_L - \mu_R$  and/or temperature difference  $T_L - T_R$ . In particular, we check validity of the Wiedemann-Franz law and the semiclassical Mott relation.

Recent development in nanoelectronics has renewed the interests for studying the correlation effects in systems where the localized quantum states coexist and interact with a sea of itinerant electrons. Previously some related ideas have been explored in the solid state physics when investigating the screening of magnetic impurities hybridized with the conduction band electrons [1]. Correlations lead there to the Kondo effect [2] which shows up by a logarithmic increase of the electrical resistance at temperatures below  $T_K$ . Similar mechanism has been later found to be responsible for a superconductivity of the heavy fermion compounds [3].

In the nano- and mesoscopic systems (such as quantum dots or carbon nanotubes connected to external leads) there can also arise the Kondo effect [4]. This has been predicted theoretically [5, 6] and observed experimentally in measurements of the differential conductance  $G(V) = \frac{dI(V)}{dV}$  [7]. Recent experimental studies of the thermoelectric power  $S = -\frac{V}{\Delta T} |I(V)=0$  [8] provided an additional evidence in favor of the Kondo effect at low temperatures.

Various transport properties through the correlated quantum dots have been studied in quite a detail [5, 6, 7, 8, 9, 10, 11, 12, 13]. Authors investigated the quantum dots coupled to the normal, superconducting and ferromagnetic leads. In several cases there have been observed some qualitatively new effects, for instance a splitting of the zero bias resonance under magnetic field [7, 12], absence of the even-odd parity effects [10] or the out of equilibrium Kondo effect [9, 11, 14]. Kondo effect has been found in such nanosystems like the single atom [15], single molecule [16] and carbon nanotubes [17]. Moreover, it has been also observed in the quantum dots attached to ferromagnetic leads [18] where, in principle, transport is controlled by the spin degree of freedom.

Quantum dots are often thought to be promising objects for the nanotechnology e.g. in various spintronic applications [19], as the gates of quantum computers, in electron spin entanglers [20] or efficient energy conversion devices [21]. Therefore a detailed understanding of the charge and heat transport through mesoscopic systems seems to be of primary importance [22]. Besides the differential conductance it is important to analyze on

equal footing also the thermoelectric properties because they are very sensitive to dimensionality as well as the electronic spectrum near the Fermi level. In the Coulomb blockade regime the thermoelectric coefficient  $S$  has been shown [23] to oscillate as a function of the gate voltage (a characteristic saw-tooth shape). At temperatures of the order or smaller than  $T_K$  there forms a narrow resonance slightly above the Fermi energy. Its appearance is responsible for increasing the differential conductance (the zero bias anomaly) and simultaneously leads to a change of sign of the thermopower from positive (when  $T > T_K$ ) to negative values (for  $T$  smaller than  $T_K$ ). Both these effects are useful for detecting the Kondo effect in the quantum dots [13, 24].

In most of the experimental measurements it has been found that the charging energy (the on-dot Coulomb repulsion)  $U$  is large, yet being finite. Usually it varies between 2 and 5 in units of the effective coupling  $\Gamma$  whose meaning will be explained in the Section II.

It is a purpose of our work here to focus on studying the transport properties for the quantum dot with a finite Coulomb energy  $U$ . We analyze the linear response with respect to the bias  $V$  and temperature difference  $\Delta T$  applied across the junction and discuss some nonlinear effects in the case of arbitrary  $V$  and  $\Delta T$  values. Transport coefficients are determined with use of the non-equilibrium Keldysh Green's functions [25]. We treat the correlations using the equation of motion approach [26] whose justification has been recently thoroughly discussed in the Ref. [27].

Studying the equilibrium and the non-equilibrium aspects of the electric and thermal transport we shall check a validity of the Wiedemann-Franz law and the Mott relation. The paper is organized as follows. In Section II we briefly introduce the model and the approximation used for calculating the transport coefficients. Results obtained within the linear response theory are presented in Section III. In the next Section IV we discuss a non-equilibrium case corresponding to arbitrarily large values of  $V$  and  $\Delta T$ . We enclose this paper by a summary and some overview of the future prospects.

## I. FORMULATION OF THE PROBLEM

### A. The model

To account for the correlation effects we focus on the simplest situation where QD is coupled to the normal leads as described by the non-degenerate single impurity Anderson Hamiltonian

$$H = \sum_{\mathbf{k},\beta,\sigma} \xi_{\mathbf{k}\beta} c_{\mathbf{k}\beta\sigma}^{\dagger} c_{\mathbf{k}\beta\sigma} + \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k},\beta,\sigma} \left( V_{\mathbf{k}\beta} c_{\mathbf{k}\beta\sigma} d_{\sigma}^{\dagger} + V_{\mathbf{k}\beta}^* c_{\mathbf{k}\beta\sigma}^{\dagger} d_{\sigma} \right). \quad (1)$$

Operators  $c_{\mathbf{k}\beta\sigma}$  ( $c_{\mathbf{k}\beta\sigma}^{\dagger}$ ) annihilate (create) electrons in the left ( $\beta=L$ ) or the right h.s. ( $\beta=R$ ) electrodes with the corresponding energies  $\xi_{\mathbf{k}\beta\sigma} = \epsilon_{\mathbf{k}\sigma} - \mu_{\beta}$  measured from the chemical potentials shifted by the external voltage  $\mu_L - \mu_R = eV$ . Operators  $d_{\sigma}$ ,  $d_{\sigma}^{\dagger}$  refer to the localized electrons of the dot which is characterized by a single energy level  $\epsilon_d$  as well as by the Coulomb potential  $U$ . The last term in (1) describes hybridization between the localized and itinerant electrons.

The retarded Green's function of the QD can be expressed in a general form

$$G_d^r(\omega) = \frac{1}{\omega - \epsilon_d - \Sigma_0(\omega) - \Sigma_I(\omega)}. \quad (2)$$

It consists of two contributions  $\Sigma_{\nu}(\omega)$  to the selfenergy, where the first part  $\Sigma_0(\omega) = \sum_{\mathbf{k},\beta} \frac{|V_{\mathbf{k}\beta}|^2}{\omega - \xi_{\mathbf{k}\beta}}$  corresponds to the noninteracting case  $U = 0$ . Twice of its imaginary part is often used as a convenient definition of the effective coupling  $\Gamma_{\beta}(\omega) = 2\pi \sum_{\mathbf{k}} |V_{\mathbf{k}\beta}|^2 \delta(\omega - \xi_{\mathbf{k}\beta})$ . We assume a flat function  $\Gamma_{\beta}(\omega) = \Gamma_{\beta}$  for  $|\omega| \leq D$  so, that the uncorrelated QD is characterized by the Lorentzian density of states centered around  $\epsilon_d$  with the halfwidth  $\Gamma_L + \Gamma_R$ .

The real many-body problem is encountered in (2) via additional part  $\Sigma_I(\omega)$  whenever  $U \neq 0$ . In the extreme limit  $U \rightarrow \infty$  one can use the slave boson approach which approximately yields the following Green's function [28]  $G_d^r(\omega) = [1 - \langle n_d \rangle] / \left[ \omega - \epsilon_d - \sum_{\mathbf{k},\beta} |V_{\mathbf{k}\beta}|^2 \frac{1+f_{\beta}(\omega)}{\omega - \xi_{\mathbf{k}\beta}} \right]$

where  $f_{\beta}(\omega) = 1 / [1 + \exp(\xi_{\mathbf{k}\beta} / k_B T)]$ . For sufficiently low temperatures the local density of states  $\rho_d(\omega) = -\frac{1}{\pi} \text{Im} G_d^r(\omega + i0^+)$  develops a narrow Kondo peak at the Fermi level as illustrated in figure 1.

One of the methods for studying the effects of Coulomb interactions  $U$  uses a truncation scheme for a set of the coupled Green's functions [29]. This, so called, equation of motion (EOM) technique is approximate. In particular, it is known that such procedure underestimates both the width and height of the Kondo resonance [28]. There are also other techniques like NCA or the large N expansion but all of them have only a limited range of applicability depending on the values of  $U$ ,  $V_{\mathbf{k}\beta}$  as well as temperature  $T$ . In this work we simply use the EOM to explore a qualitative behavior of the transport properties

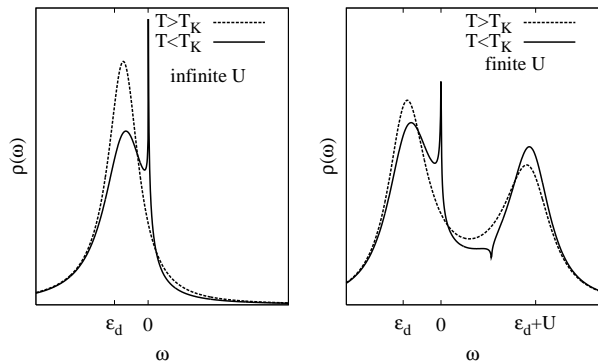


FIG. 1: Density of states  $\rho_d(\omega)$  of the QD in the equilibrium case. For a finite Coulomb energy  $U$  the spectrum consists of two Lorentzians centered around  $\epsilon_d$  and  $\epsilon_d + U$ . At sufficiently low temperatures  $T < T_K$  there appears a narrow Kondo resonance near the Fermi level (here it corresponds to  $\omega = 0$ ).

for the system (1). Our results can be eventually quantitatively improved by the more sophisticated methods.

According to the standard derivation based on the EOM and the Keldysh formalism [30] one obtains the following retarded Green's function (2) of the quantum dot [29]

$$G_d^r(\omega) = \frac{g_d^r(\omega)^{-1} - [\Sigma_0(\omega) + \Sigma_3(\omega) + U(1 - n_d)]}{[g_d^r(\omega)^{-1} - \Sigma_0(\omega)][g_d^r(\omega)^{-1} - (U + \Sigma_0(\omega) + \Sigma_3(\omega))] + U\Sigma_1(\omega)}, \quad (3)$$

where

$$g_d^r(\omega) = [\omega - \epsilon_d]^{-1}$$

$$\Sigma_1(\omega) = \sum_{\mathbf{k}\beta} |V_{\mathbf{k}\beta}|^2 \left( \frac{f_{\beta}(\omega)}{\omega - \xi_{\mathbf{k}\beta}} + \frac{f_{\beta}(\omega)}{\omega - U - 2\epsilon_d + \xi_{\mathbf{k}\beta}} \right),$$

$$\Sigma_3(\omega) = \sum_{\mathbf{k}\beta} |V_{\mathbf{k}\beta}|^2 \left( \frac{1}{\omega - \xi_{\mathbf{k}\beta}} + \frac{1}{\omega - U - 2\epsilon_d + \xi_{\mathbf{k}\beta}} \right).$$

In figure (1) we show the density of states  $\rho_d(\omega)$  computed for the equilibrium case ( $V=0$  and  $T_L = T_R$ ). The right h.s. panel illustrates the spectrum for the case of a

finite  $U$  which is characterized by two Lorentians, one at  $\varepsilon_d$  and another one around  $\varepsilon_d+U$ . The upper Coulomb satellite is missing (see the left h.s. panel) when  $U = \infty$ . At sufficiently low temperatures  $T < T_K$  there appears a narrow Kondo resonance due to the singlet state formed from the itinerant electrons and the localized electrons of the quantum dot.

## B. Definition of the transport coefficients

By applying some bias  $V$  or temperature imbalance  $T_L \neq T_R$  the system is driven out of its equilibrium [26]. Effectively there are induced the charge and heat currents through the QD. Using the nonequilibrium Keldysh Green's functions [25] one can derive the following Landauer-type expressions for the charge  $I(V, \Delta T)$  and heat currents  $I_Q(V, \Delta T)$  [12]

$$I = \frac{e}{h} \int_{-\infty}^{\infty} d\omega \Gamma(\omega) [f_L(\omega) - f_R(\omega)] \rho_d(\omega), \quad (4)$$

$$I_Q = \frac{1}{h} \int_{-\infty}^{\infty} d\omega \Gamma(\omega) (\omega - eV) [f_L(\omega) - f_R(\omega)] \rho_d(\omega). \quad (5)$$

We introduced here the symmetrized coupling  $\Gamma(\omega) = 2\Gamma_L(\omega)\Gamma_R(\omega)/[\Gamma_L(\omega) + \Gamma_R(\omega)]$  and factor 2 comes from the contributions of  $\uparrow$  and  $\downarrow$  electrons in the tunneling. We notice that both currents (4,5) are convoluted with the spectral function of the QD hence the behavior illustrated in figure 1 indirectly affects the transport properties.

In figure 2 we show the differential conductance  $G(V) = dI/dV$  obtained for temperatures higher and lower than  $T_K$ . We notice a clear increase of the zero voltage conductance (zero bias anomaly) when  $T < T_K$  while the other side-peaks in the conductance at  $|eV| \simeq U$  are not sensitive to temperature. In realistic systems there should be even more peaks because of the multi-level electronic structure containing a mesoscopic number of atoms at QD. We thus emphasize that from these features only the zero bias anomaly is driven by the many-body Kondo effect at temperatures  $T < T_K$ , usually being of the order of hundreds mK [7].

For a further analysis we introduce the following transport coefficients

$$S = - \left( \frac{V}{\Delta T} \right)_{I=0} \quad (6)$$

$$\kappa = - \left( \frac{I_Q}{\Delta T} \right)_{I=0} \quad (7)$$

which describe correspondingly the thermoelectric power (6) and the heat conductance (7). In the limit of small perturbations  $V$  and  $\Delta T$  the heat conductance is expected to obey the Wiedemann-Franz law  $\kappa/TG(0) = \pi^2/3e^2$ , however we will show that this relation is, in general, not obeyed for temperatures  $T \sim T_K$  (as has

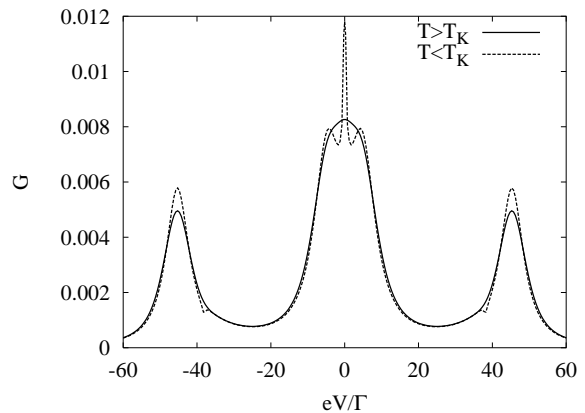


FIG. 2: The differential conductance  $G(V)$  versus the applied bias  $V$  for temperatures above and below  $T_K$  and a finite value of the Coulomb interaction  $U = 50\Gamma$ .

been independently pointed out by several authors, e.g. [24]).

The thermoelectric power (6) is a quantity which is very sensitive to a particle-hole symmetry in the density of states of QD. For small perturbations  $V, \Delta T$  one can analytically prove that the thermopower is proportional to the energy weighted with respect to the Fermi level  $\mu$

$$S \simeq - \frac{\langle \omega - \mu \rangle}{eT} \quad (8)$$

in the range of thermal excitations  $k_B T$ . Appearance of the narrow Kondo peak should thus be accompanied by a change of sign in  $S(T)$  from the positive ( $T > T_K$ ) to negative ( $T < T_K$ ) values. Indeed, this behavior has been recently observed experimentally [8]. In the following sections we discuss in a more detail some properties of the thermopower for a representative set of  $U$  and for varying perturbations  $V, \Delta T$  ranging from the small to the arbitrarily large values.

## II. SMALL PERTURBATIONS $V$ AND $\Delta T$

For infinitesimally small perturbations  $V$  and  $\Delta T$  one can expand the currents (4, 5) up to linear terms

$$I = -\frac{1}{T} L_{11} \nabla \mu + L_{12} \nabla \left( \frac{1}{T} \right), \quad (9)$$

$$I_Q = -\frac{1}{T} L_{21} \nabla \mu + L_{22} \nabla \left( \frac{1}{T} \right). \quad (10)$$

These coefficients  $L_{ij}$  of the linear response theory can be determined from the corresponding correlation functions in the Kubo formalism [31]. The zero bias conductance is then given by  $G(0) = \frac{e^2}{T} L_{11}$ , the Seebeck coefficient by  $S = -\frac{1}{eT} \frac{L_{12}}{L_{11}}$  and the thermal conductivity by  $\kappa = \frac{1}{T^2} \left( L_{22} - \frac{L_{12}^2}{L_{11}} \right)$ . Coefficients  $L_{ij}$  can also be

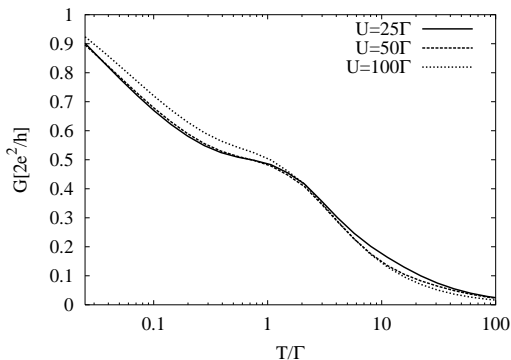


FIG. 3: Temperature dependence of the zero bias differential conductance  $G(V=0)$  obtained from the linear response calculations using the coefficient  $L_{11}$  (11).

derived directly from equations (4, 5) and they become functionals of the QD density of states via

$$L_{11} = \frac{T}{h} \int_{-\infty}^{\infty} d\omega \Gamma(\omega) \left[ -\frac{\partial f(\omega)}{\partial \omega} \right] \rho_d(\omega), \quad (11)$$

$$L_{12} = \frac{T^2}{h} \int_{-\infty}^{\infty} d\omega \Gamma(\omega) \left[ -\frac{\partial f(\omega)}{\partial T} \right] \rho_d(\omega), \quad (12)$$

$$L_{22} = \frac{T^2}{h} \int_{-\infty}^{\infty} d\omega \Gamma(\omega) \omega \left[ -\frac{\partial f(\omega)}{\partial T} \right] \rho_d(\omega) \quad (13)$$

where  $\rho_d(\omega)$  and derivatives of the Fermi function are to be computed for  $V=0$ . From the Onsager relation we have  $L_{21} = L_{12}$ .

From the equation (11) we conclude that at very low temperatures the zero bias conductance  $G(0)$  is proportional to the density of states  $\rho_d(\omega=0)$ . Appearance of the Kondo automatically enhances the zero bias conductance as has been indeed observed experimentally [7]. Moreover, for  $T \rightarrow 0$  it reaches the unitary limit value  $2e^2/h$ . With an increase of temperature there activated the scattering processes involving some higher energy sectors [32].

The linear response relations (11-13) are restricted to the external voltage  $V$  and/or temperature difference  $\Delta T$  being small (in terms of  $\Gamma$ ). In the remaining part of this section we give a brief summary of our numerical computations while the next section will be devoted to arbitrary large perturbations.

### A. Numerical results

Using the linear response relations (11-13) we explored numerically the transport properties for several values of  $T$ ,  $U$ ,  $\varepsilon_d$  keeping a fixed number of charge on the QD  $\langle n_d \rangle = 0.5$ . We assumed the flat coupling  $\Gamma_\beta(\omega) = \Gamma$  for energies  $|\omega| \leq D$  and  $\Gamma_\beta(\omega) = 0$  elsewhere.

Figure 3 shows the temperature dependence of the zero bias conductance. We notice that  $G(0)$  decreases monotonously versus temperature. At low temperatures

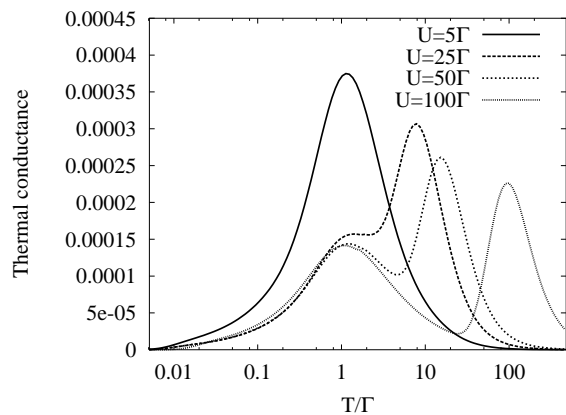


FIG. 4: Temperature dependence of the thermal conductance  $\kappa(T)$  obtained in the linear response theory.

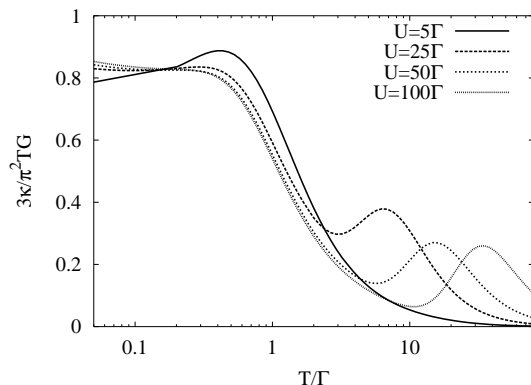


FIG. 5: The Wiedemann Franz relation obtained in the linear response theory for the same values of  $U$  as in figure 4.

$T \leq 0.1\Gamma$ , conductance decreases because of a gradual disappearance of the Kondo peak. For higher temperatures beyond the Kondo regime ( $T \sim \Gamma$ ) there is a bit of a plateau and then again there starts an exponential decrease with respect to  $T$ . This behavior seems to be universal and the Coulomb interaction  $U$  has merely a marginal effect on it.

On contrary, the effect of Coulomb interactions does show up in the temperature dependence of the thermal conductivity. In figure we can see 4 that at small temperatures  $\kappa(T)$  exponentially increases versus  $T$ . For  $T \sim \Gamma$  there appears one maximum (when the values of  $U$  is small so that the Lorentzians presented in figure 1 overlap with one another) and then the other maximum occurs at  $T \sim U$  (for sufficiently large  $U$ ). The heat current is thus enhanced either when transport occurs through the low energy sector (the Lorentzian around  $\varepsilon_d$ ) or it has an additional contribution by activating the high energy sectors (the Lorentzian around  $\varepsilon_d + U$ ). We checked that the Kondo state has no influence on  $\kappa(T)$ . The mutual relation between  $\kappa(T)$  and the  $G(0)$  is summarized in figure 4.

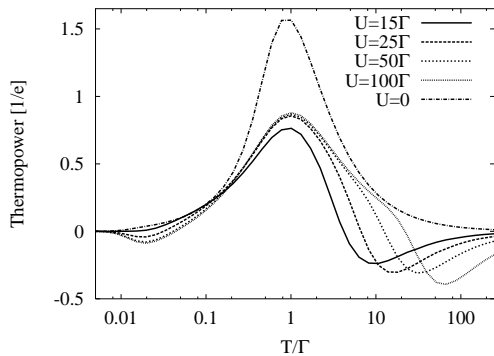


FIG. 6: Temperature dependence of the thermopower  $S(T)$  obtained in the linear response theory for several values of the Coulomb interaction:  $U = 50\Gamma$  (dotted line),  $U = 25\Gamma$  (dashed line) and  $U = 17.5\Gamma$  (solid curve).

Figure 6 illustrates the Seebeck coefficient  $S(T)$ . At low temperatures  $T < T_K$  the thermopower becomes negative due to the Kondo resonance slightly above the Fermi level (figure 1). A finite value of the Coulomb interaction  $U$  leads to a partial flattening of the minimum in the Kondo regime. At higher temperatures  $S(T)$  changes sign and considerably increases. For  $T \sim U$  there occurs an other change of sign (negative  $S(T)$ ) because of activating the high energy sector (the upper Lorentian in figure 1). Similar behavior has been independently reported for the periodic Anderson model [33]. At extremely large temperatures a magnitude of the thermopower asymptotically scales as  $|S(T)| \propto T^{-1}$ .

### B. The Mott relation

Within the linear response limit (i.e. for small perturbations  $V$  and  $\Delta T$ ) the following Mott formula [34]

$$S^M(T) = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \ln G(0)}{\partial \mu} \quad (14)$$

is often used in experimental studies of the thermopower  $S(T)$ . Dependence of the zero bias conductance  $G(V=0)$  on the chemical potential can be in practice measured by varying the gate voltage  $V_G$ . Since the gate voltage shifts the energy levels of the QD one can assume that  $-\partial \ln G(0)/\partial \mu \simeq \partial \ln G(0)/\partial V_G$ .

For the realistic multilevel QDs the Mott relation (14) implies for the thermopower to have a sawtooth shape as a function of  $V_G$  [23]. Similar property can be observed even in the single level QD as a consequence of the Coulomb blockade [35]. The dashed lines in figure 7 show the variation of the thermopower obtained from the Mott relation (14) for temperatures higher (the upper panel) and lower than the Kondo temperature  $T_K$  (the bottom panel). In the Kondo regime we notice a clear discrepancy between the Mott formula and the results computed directly from (4) and (6).

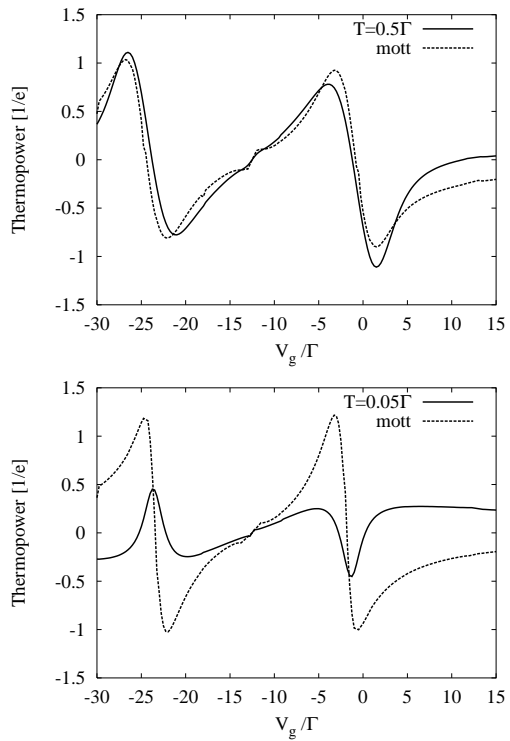


FIG. 7: The thermopower  $S(T)$  obtained directly from the linear response theory (solid lines) and using the Mott relation (14) (dashed lines).

In order to clarify a limited range of applicability for the semi-classical Mott relation we briefly recollect some basic constraints used for derivation of (14) as has been also independently stressed by other authors [35]. The Landauer-type expression (4) can be expanded with respect to the small perturbations  $V$  and  $\Delta T$ . If one neglects the temperature dependence of  $\rho_d(\omega)$  (which obviously is not valid for  $T \sim T_K$ ) then such expansion is carried out only in the Fermi distribution functions  $f_\beta(\omega)$

$$f_\beta(\omega) = f(\omega) - \frac{\partial f(\omega)}{\partial \omega} \left[ (\mu_\beta - \mu) - \frac{\omega - \mu}{T} (T_\beta - T) \right]. \quad (15)$$

Substituting  $\mu_L = \mu + \frac{1}{2}eV$  and  $\mu_R = \mu - \frac{1}{2}eV$  together with (15) into the equation (4) we search for such a bias  $V$  which compensates the current induced by the temperature imbalance  $\Delta T = T_L - T_R$ . Using the definition (6) we finally obtain [35]

$$S(T) = \frac{\int_{-\infty}^{\infty} d\omega (\omega - \mu) \Gamma(\omega) \rho_d(\omega) \left[ -\frac{\partial f(\omega)}{\partial \omega} \right]}{eT \int_{-\infty}^{\infty} d\omega \Gamma(\omega) \rho_d(\omega) \left[ -\frac{\partial f(\omega)}{\partial \omega} \right]}. \quad (16)$$

For a quantitative determination of (16) one can apply the Sommerfeld expansion  $\int_{-\infty}^{\infty} d\omega f(\omega) Y(\omega) \simeq \int_{-\infty}^{\mu} d\omega Y(\omega) + \frac{\pi^2}{6} (k_B T)^2 Y'(\mu)$  which is valid only at low temperatures. Within the lowest order estimation one

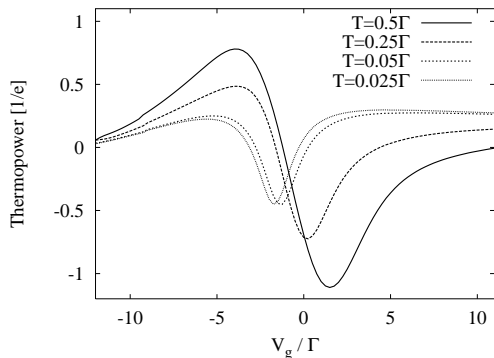


FIG. 8: The thermopower  $S(T)$  computed within the linear response theory in a range of the gate voltage  $V_G$  where the Kondo effect has the most strong influence.

finally gets

$$S(T) = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \ln \rho_d(\omega=0)|_{T=0}}{\partial \mu} \quad (17)$$

because  $\lim_{T \rightarrow 0} \frac{\partial f(\omega)}{\partial \omega} \simeq -\delta(\omega - \mu)$ . According to (11) the zero bias conductance  $\lim_{T \rightarrow 0} G(V=0) = \text{const} \times \rho_d(\omega=0)|_{T=0}$  hence we finally arrive at the relation (14)

$$S(T) = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \ln G(V=0)|_{T=0}}{\partial \mu} \quad (18)$$

It is now clear that deviation from the Mott relation shown in figure 7 are due to the temperature dependence of the QD spectrum  $\rho_d(\omega)$  when the Kondo peak gradually builds in.

In figure 8 we present the qualitative changes of the thermopower caused by the Kondo effect. For high temperatures  $T > T_K$  we see a piece of the saw-tooth behavior [23]. Upon lowering the temperatures to  $T < T_K$  the Kondo resonance is formed in the density of states (see figure 1) and through the relation (16) this affects a sign of the thermopower. Such physical effects have been recently observed experimentally [8].

It is interesting to notice that the qualitative changes of the thermopower occur on both teeth of the *saw*. We explain in the appendix that this is related to the particle or hole type of the Kondo resonance.

### III. BEYOND THE LINEAR RESPONSE

We also studied the charge (4) and heat currents (5) going beyond the limit of small bias  $V$  and temperature difference  $\Delta T$ . Figure 2 shows the differential conductance computed numerically for  $T_L = T_R$ . When temperatures  $T_\beta$  differ from one another the differential conductance has still qualitatively the similar behaviour with only the zero bias anomaly being gradually smeared for increasing  $\Delta T$ .

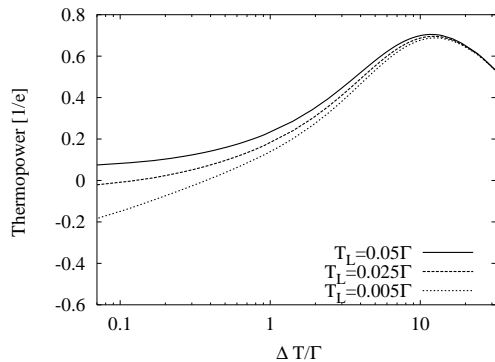


FIG. 9: The thermopower  $S(T) \equiv \frac{V}{\Delta T}|_{I=0}$  determined beyond the linear response theory in the Kondo regime for  $\varepsilon_d = -3\Gamma$  and  $U = 50\Gamma$ .

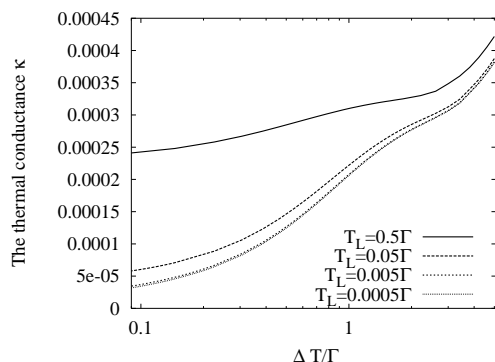


FIG. 10: Variation of the thermal conductance  $\kappa(T)$  as a function of the applied temperature difference  $\Delta T$  at low temperature region (upper panel) and at higher temperatures (the bottom panel).

To account for nonlinear effects of the other transport quantities we determined the thermopower and thermal conductivity directly from the definitions (6-7). Following [24], we solved numerically the integral equation

$$I(V, \Delta T) = 0 \quad (19)$$

for the fixed temperature difference  $\Delta T$  determining the bias  $V(\Delta T)$ . The thermopower is then given by the ratio (6). To compute the thermal conductance we determined the heat current  $I_Q(V, \Delta T)$  and substituted it to (7) using  $V(\Delta T)$ .

In figure 9 we show influence of the finite temperature difference  $\Delta T$  on the thermopower  $S(T)$  as function of the average temperature  $T = (T_L + T_R)/2$ . Our results prove that the nonlinear effects play a considerable role. In general, by increasing the temperature difference  $\Delta T$  we notice that the system acquires such properties which are characteristic for the high temperature behaviour shown previously in figure 6.

Thermal conductance  $\kappa$  is a physical quantity which is rather weakly sensitive to any particular structure of the low energy excitations. In the linear response limit

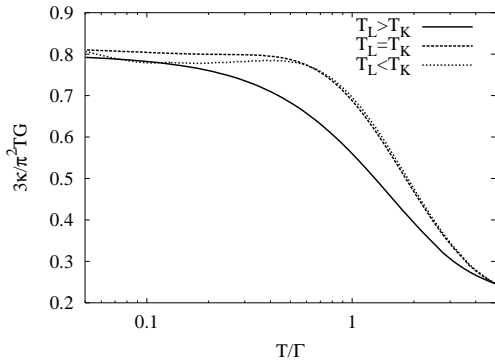


FIG. 11: The Wiedemann-Franz relation beyond the linear response limit determined for several values of  $T_L$  with the Coulomb energy  $U = 25\Gamma$ . On abscissa we put the average temperature defined as  $T = T_L + \frac{\Delta T}{2}$ .

it is known to vanish for  $T \rightarrow 0$  as well as for the opposite limit  $T \rightarrow \infty$  [14, 24]. The maximum value of  $\kappa$  occurs usually at temperatures  $T \sim \Gamma/k_B$  (see figure 4). This situation changes radically if the applied temperature difference  $\Delta T$  is large. Obviously,  $\kappa(T)$  gradually increases as a function of  $\Delta T$  (see the figure 10) but this dependence is irregular. We further illustrate it in figure 11 where we plot the Wiedemann-Franz ratio versus the average temperature  $T$  for several fixed values of  $T_L$ .

#### IV. SUMMARY

We studied the influence of correlations on various properties of the charge and heat transport through the quantum dot connected to the normal leads. In the regime of linear response theory (for the small applied bias  $V$  or temperature difference  $\Delta T$ ) we find the qualitative changes caused strictly by appearance of the Kondo resonance at low energies. In particular, it leads to the zero bias anomaly and to the change of sign of the thermopower. Moreover, the Coulomb interactions have additional effects by activation of the high energy channels in the QD spectrum for the transport of charge and heat. Presence of such high energy states manifests by the non-monotonous variation of the thermopower (figure 6) and thermal conductance (figure 4).

Appearance of the Kondo effect has a further strong influence on deviation from the semiclassical Mott-relation. The Mott formula (14) fails for  $T \sim T_K$  because of the temperature dependence of the spectral function.

The Wiedemann-Franz law seems to be rather well preserved unless temperatures are small, for increasing temperatures we observe a systematic departure from the well known Wiedemann-Franz ratio. The nonlinear effects studied within the Landauer formalism show an additional effect on the transport properties for practically all transport quantities. This issue has been previously pointed also by some other authors [24].

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#### APPENDIX

In this appendix we briefly explain under what conditions there can arise the Kondo effect in the system described by Hamiltonian (1). For this purpose let us first explore the particle hole transformation

$$\begin{aligned} d_\sigma &\rightarrow \tilde{d}_\sigma^+ & c_{\mathbf{k}\beta\sigma} &\rightarrow \tilde{c}_{\mathbf{k}\beta\sigma}^+ \\ d_\sigma^+ &\rightarrow \tilde{d}_\sigma & c_{\mathbf{k}\beta\sigma}^+ &\rightarrow \tilde{c}_{\mathbf{k}\beta\sigma} \end{aligned}$$

Substituting these operators into the Hamiltonian (1) we obtain

$$\begin{aligned} H &= \sum_{\mathbf{k},\beta,\sigma} \tilde{\xi}_{\mathbf{k}\beta} \tilde{c}_{\mathbf{k}\beta\sigma}^+ \tilde{c}_{\mathbf{k}\beta\sigma} + \sum_{\sigma} \tilde{\epsilon}_d \tilde{d}_\sigma^+ \tilde{d}_\sigma + \tilde{U} \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \\ &+ \sum_{\mathbf{k},\beta,\sigma} \left( \tilde{V}_{\mathbf{k}\beta} \tilde{c}_{\mathbf{k}\beta\sigma} \tilde{d}_\sigma^+ + \tilde{V}_{\mathbf{k}\beta}^* \tilde{c}_{\mathbf{k}\beta\sigma}^+ \tilde{d}_\sigma \right) + const \end{aligned}$$

where

$$\tilde{\xi}_{\mathbf{k}\beta} = -\xi_{\mathbf{k}\beta} \quad (\text{A.1})$$

$$\tilde{\epsilon}_d = -\epsilon_d - U \quad (\text{A.2})$$

$$\tilde{U} = U \quad (\text{A.3})$$

$$\tilde{V}_{\mathbf{k}\beta} = -V_{\mathbf{k}\beta}^* \quad (\text{A.4})$$

and  $const = U + 2\epsilon_d + \sum_{\mathbf{k},\beta,\sigma} \xi_{\mathbf{k}\beta\sigma}$ . We thus notice that the Hamiltonian (1) preserves its structure under the particle-hole transformation and simultaneously the model parameters are scaled as given in (A.1-A.4). This property will be useful for us when determining conditions necessary for the Kondo effect to appear.

The standard way to specify when electron of the QD is perfectly screened by the mobile electrons is obtained using the Schrieffer-Wolf transformation. This perturbative method eliminates the hybridization terms  $V_{\mathbf{k}\beta}$  to linear terms. In the present case one derives the following effective superexchange coupling [36]

$$J = \frac{U |V_{k_F,\beta}|^2}{(\epsilon_d + U)(-\epsilon_d)}. \quad (\text{A.5})$$

In the equilibrium case (i.e. for  $V=0$ ) this formula (A.5) means that antiferromagnetic interactions arise when the energy level  $\epsilon_d$  of the QD is located slightly below the chemical potential (we assumed here  $\mu=0$ ). This situation is schematically illustrated in figure 1.

The other possibility for the Kondo state to appear corresponds to holes rather than particles. In a simple

way one can verify that under the particle hole transformation the superexchange coupling transforms to

$$J = \frac{\tilde{U} |\tilde{V}_{k_F, \beta}|^2}{(-\tilde{\varepsilon}_d)(\tilde{\varepsilon}_d + \tilde{U})}. \quad (\text{A.6})$$

This result could be expected on more general grounds

due to the fact that the XY model is invariant on the particle hole transformation. We hence conclude that the Kondo effect should be present for the small negative value of  $\tilde{\varepsilon}_d$ , in other words for  $\varepsilon_d$  located slightly above  $U$ . We would like to emphasize that this is not an artifact depending on the approximations used in this work.

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