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1 Introduction

The ability of an electron to tunnel across a potential barrier is one of the spectacular and fundamental quantum effects. It plays a particularly important role in nanodevices, where the transport is also dominated by the charging effects. An electron sitting on a small grain between the leads prevents other electrons from tunneling on it. In such a geometry one observes new quantum phenomena, like Coulomb blockade, quantization of the electric conductivity, appearance of the Kondo resonance, the spin Hall effect, etc.

The devices, called single electron transistors, which consist of a small island between two external electrodes allow the control of parameters and measurements of the transport characteristics precise enough to test the predictions of the many body theories for non-equilibrium charge [1] and heat [2] currents. The small central island, to be called quantum dot (QD), displays a rich physics very much similar to that of a magnetic impurity in a non magnetic host [3]. This situation enables exploration of the non-equilibrium regime which usually is not accessible in the condensed matter bulk systems.

Here we shall discuss the effect of strong Coulomb interaction (between electrons on an island) on the low temperature charge transport in the system with a bias voltage and temperature gradients applied between the electrodes.

2 Microscopic model

For a description of the tunneling through the quantum dot we use the single impurity Anderson model [3]

$$H = \sum_{k,\beta,\sigma} \xi_{k\beta\sigma} c^{+}_{k\beta\sigma} c_{k\beta\sigma} + \sum_{\sigma} \varepsilon_d d^{+}_{\sigma} d_{\sigma} + U d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow} + \sum_{k,\beta,\sigma} (V_{k\beta} c_{k\beta\sigma} d^{+}_{\sigma} + V^{*}_{k\beta} c^{+}_{k\beta\sigma} d_{\sigma}) , \qquad (1)$$

where $c_{k\beta\sigma}(c^{\dagger}_{k\beta\sigma})$ operators correspond to annihilation (creation) of electrons in the left $\beta = \mathrm{L}$ and right h.s. $\beta = \mathrm{R}$ leads. Energies of the electrons $\xi_{k\beta\sigma} = \varepsilon_{k\sigma} - \mu_{\beta}$ are measured from the chemical potentials

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which in a presence of the bias voltage V are shifted from each other by $\mu_L - \mu_R = eV$ and moreover, the electrodes can be characterized by different temperatures T_L and T_R. Operators d_σ, $d_\sigma^\dagger$ describe annihilation and creation of electron on a quantum dot whose spectrum consists of a single energy level ε_d. The on-dot Coulomb potential U describes repulsion between electrons of opposite spins. It leads effectively to another (high energy) level at $\varepsilon_d + U$.

The last term in the Hamiltonian (1) describes hybridization between localized electrons of the quantum dot and mobile electrons of the leads. It gives rise to a finite broadening of the energy levels centered around ε_d and $\varepsilon_d + U$. Moreover, when temperature is sufficiently low, the hybridization and Coulomb interactions give a combined effect observed as a narrow resonance at $\omega = \mu_\beta$. Under specific conditions (which are discussed below) the itinerant electrons from vicinity of the Fermi energy (chemical potential) can form a singlet state with the QD electron [3]. This low energy Kondo peak together with the high energy features have a qualitative influence on the transport properties which is the main object of our study here.

3 Conditions for the Kondo resonance

Formation of the many-body Kondo effect requires existence of the effective spin on the dot with charge fluctuations frozen out by the strong Coulomb repulsion U. To consider the mechanism responsible for the Kondo effect one can restrict to a perturbative treatment of the hybridization $H_{\text{hyb}} = \sum_{\boldsymbol{k},\beta,\sigma} [V_{\boldsymbol{k}\beta} c_{\boldsymbol{k}\beta\sigma} d_\sigma^+ + \text{h.c.}]$. It is convenient to construct a unitarily equivalent Hamiltonian $\tilde{H} = e^A H e^{-A}$ in which H_{hyb} is eliminated up to quadratic terms. Such canonical transformation has been designed for the model Hamiltonian (1) by Schrieffer and Wolff [5] using

$$A = \sum_{\boldsymbol{k},\beta,\sigma} \frac{V_{\boldsymbol{k}\beta}}{\varepsilon_d - \xi_{\boldsymbol{k}\beta}} \left[\frac{U}{\varepsilon_d + U - \xi_{\boldsymbol{k}\beta}} d_{-\sigma}^\dagger d_{-\sigma} - 1 \right] c_{\boldsymbol{k}\beta\sigma}^\dagger d_\sigma - \text{h.c.} \tag{2}$$

Focusing on the Hilbert space corresponding to the singly occupied QD states one obtains the following spin−spin interactions

$$\tilde{H} = \sum_{\boldsymbol{k},\beta,\sigma} \xi_{\boldsymbol{k}\beta} c_{\boldsymbol{k}\beta\sigma}^+ c_{\boldsymbol{k}\beta\sigma} - \sum_{\boldsymbol{k},\boldsymbol{q},\beta,\sigma,\sigma'} J_{\boldsymbol{k},\boldsymbol{q}}^{\beta,\beta'} \boldsymbol{S} (c_{\boldsymbol{k}\beta\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'} c_{\boldsymbol{q}\beta'\sigma'}) , \tag{3}$$

where $S^+ = d_\uparrow^\dagger d_\downarrow$, $S^- = d_\downarrow^\dagger d_\uparrow$, $S_z = 1/2(d_\uparrow^\dagger d_\uparrow - d_\downarrow^\dagger d_\downarrow)$ and vector $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ consists of the Pauli matrices. The effective exchange coupling between spins of the QD and itinerant electrons is given by

$$J_{\boldsymbol{k},\boldsymbol{q}}^{\beta,\beta'} = \frac{V_{\boldsymbol{k}\beta} V_{\boldsymbol{q}\beta'}}{2} \left[\frac{U}{(\varepsilon_d - \xi_{\boldsymbol{k}\beta})(\varepsilon_d + U - \xi_{\boldsymbol{k}\beta})} + \frac{U}{(\varepsilon_d - \xi_{\boldsymbol{q}\beta'})(\varepsilon_d + U - \xi_{\boldsymbol{q}\beta'})} \right]. \tag{4}$$

Near the Fermi surface ($\xi_{\boldsymbol{k}_F} = 0$) the coupling simplifies to $J_{\boldsymbol{k}_F,\boldsymbol{q}_F}^{\beta,\beta'} = V_{\boldsymbol{k}_F\beta} V_{\boldsymbol{q}_F\beta'} (U/\varepsilon_d(\varepsilon_d + U))$. It becomes negative (antiferromagnetic) for the chemical potential located between ε_d and $\varepsilon_d + U$. Absolute value of such antiferromagnetic coupling is large either for $\varepsilon_d \to \mu^-$ or for $\varepsilon_d + U \to \mu^+$.

One should however be cautious analyzing results of the Schrieffer-Wolff transformation because Eq. (4) may eventually diverge due to vanishing energy denominators. This ill-defined ultraviolet cutoff problem can be regularized using some other better controlled methods such as the Renormalization Group (RG) theory [6] or the Bethe ansatz [7]. Systematic improvement of the Schrieffer-Wolff transformation has been also proposed recently by Kehrein and Mielke [8]. These authors projected out the hybridization term H_{hyb} by means of the continuous canonical transformation $e^{A(l)} H e^{-A(l)}$. This idea has been introduced by Wegner [9] in analogy to a general scheme of the RG method.

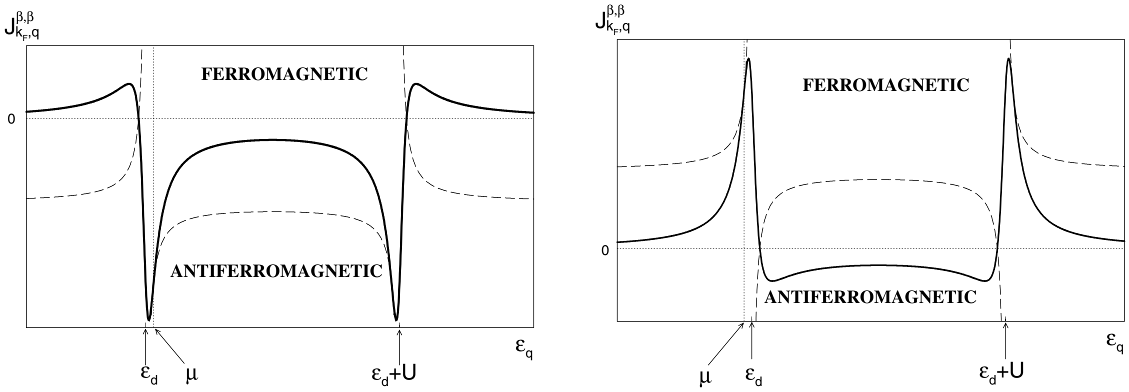


Fig. 1 Variation of the spin–spin coupling $J^{\beta,\beta}_{k_F,q}$ versus ε_q for $U = 1D$ in the equilibrium situation $V = 0$. The left h.s. panel corresponds to $\varepsilon_d = -0.03D$ (the Kondo regime) and the right h.s. one to $\varepsilon_d = 0.03D$ (the mixed valence regime). Thick solid lines show the results obtained by the continuous canonical transformation [8] which are compared with the standard Schrieffer–Wolff transformation [5] illustrated by the dashed lines.

Solution of the corresponding flow equations [8] improves the Eq. (4) and yields the following spin–spin coupling

$$J^{\beta,\beta'}_{k,q} = V_{k\beta} V_{q\beta'} U \, \frac{(\varepsilon_d - \xi_{k\beta})(\varepsilon_d + U - \tilde{\xi}_{k\beta}) + (\varepsilon_d - \tilde{\xi}_{q\beta'})(\varepsilon_d + U - \tilde{\xi}_{q\beta'})}{(\varepsilon_d - \tilde{\xi}_{k\beta})^2 (\varepsilon_d + U - \tilde{\xi}_{k\beta})^2 + (\varepsilon_d - \tilde{\xi}_{q\beta'})^2 (\varepsilon_d + U - \tilde{\xi}_{q\beta'})^2} \,. \tag{5}$$

Energies $\tilde{\xi}_{q\beta}$ of the mobile electrons are simultaneously renormalized hence the exchange coupling (5) is completely different from Eq. (4). In Fig. 1 we show variation of $J^{\beta,\beta}_{k_F,q}$ versus ε_q where, for simplicity, we neglected the renormalizations of energies $\tilde{\xi}_{q\beta} \simeq \xi_{q\beta}$. One notices that the extent of antiferromagnetic interactions (negative value of the exchange coupling J) spread over different regimes in both methods.

The spin–spin coupling $J^{\beta,\beta'}_{k,q}$ has a direct influence on the effective density of states of the QD. In particular, it determines the characteristic temperature T_K below which the resonance starts to be formed. In the literature there are various definitions of the Kondo temperature T_K. For instance, by using the Bethe ansatz it has been argued that T_K can be expressed as [7]

$$T_K \simeq \frac{2D}{\pi k_B} \exp\{-\Phi[2\rho_c(\mu)\, J^{\beta,\beta}_{k_F,q_F}]\} \,, \tag{6}$$

where $\Phi(x) = (1/|x|) - (\ln|x|)/2$ and $\rho_c(\mu)$ is the density of states for c electrons in a conduction band of the width D. The Eq. (6) is restricted to the equilibrium case $\mu_\beta = \mu$. Kondo temperature T_K is exponentially dependent on the effective spin–spin coupling J, however it is well defined only if the interactions are antiferromagnetic near the Fermi surface (see Fig. 1).

4 Role of the particle–hole symmetry

We can notice in Fig. (1) that $J^{\beta,\beta}_{k_F,q}$ is symmetric with respect to the point $\xi_q = \varepsilon_d + U/2$. For the equilibrium case this property is related to invariance of the Anderson model (1) with respect to the particle–hole transformation defined by

$$d_\sigma \equiv \tilde{d}^\dagger_\sigma, \qquad d^\dagger_\sigma \equiv \tilde{d}_\sigma, \qquad c_{k\beta\sigma} \equiv \tilde{c}^\dagger_{k\beta\sigma}, \qquad c^\dagger_{k\beta\sigma} \equiv \tilde{c}_{k\beta\sigma}. \tag{7}$$

Using the new operators introduced in Eq. (7) one finds that the Hamiltonian (1) preserves its initial structure upon simultaneously transforming the model parameters to

$$\tilde{\xi}_{k\beta} = -\xi_{k\beta}, \qquad \tilde{\varepsilon}_d = -\varepsilon_d - U, \qquad \tilde{U} = U, \qquad \tilde{V}_{k\beta} = -V^*_{k\beta} \,. \tag{8}$$

In particular, the single impurity Anderson model (1) has a particle−hole symmetry when $\varepsilon_d + U/2 = \mu_\beta$. For other values of ε_d, U and μ_β the particle excitation spectrum at ω is always identical with the hole excitation spectrum at $U-\omega$. Let us emphasize that this property has nothing to do with approximations employed either to the hybridization term (the preceding section) or to the on-site interaction (discussed in the next section). Such symmetry between the particle and hole excitations does clearly show up in the transport properties.

5 Transport properties

By applying a source-drain voltage V between the L and R electrodes (so that the chemical potentials get shifted $\mu_L - \mu_R = eV$) or by imposing some temperature difference $\Delta T = T_L - T_R$ one induces the charge and heat currents through the quantum dot. In this work we focus on the charge transport $I(V) = -e\,(\mathrm{d}/\mathrm{d}t)\,\langle N_L \rangle$. Within the non-equilibrium Keldysh formalism [4] one can determine a steady current using the generalized Landauer formula [10]

$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} \mathrm{d}\omega [f(\omega - \mu_L) - f(\omega - \mu_R)]\, T(\omega)\,, \tag{9}$$

where $f(\omega) = [1 + \exp(\omega)/k_B T]^{-1}$. It has been shown [4] that the transmission coefficient $T(\omega)$ is

$$T(\omega) = \sum_\sigma \frac{\Gamma_L(\omega)\, \Gamma_R(\omega)}{\Gamma_L(\omega) + \Gamma_R(\omega)}\, \rho_\sigma(\omega) \tag{10}$$

and, as usually, the weighted densities of states are defined by $\Gamma_\beta(\omega) = 2\pi \sum_{\boldsymbol{k}} |V_{\boldsymbol{k}\beta}|^2\, \delta(\omega - \varepsilon_{\boldsymbol{k}\beta})$. We further assume these functions $\Gamma_\beta(\omega)$ to be constant for energies $|\omega| \le D$. The density of states of the quantum dot $\rho_\sigma(\omega) = -(1/\pi)\,\mathrm{Im}\, G^r(\omega + i0^+)$ must be determined using the Fourier transform of the retarded Green's function $G^r_\sigma(t,t') = -i\theta(t-t')\,\langle d_\sigma(t)\, d^\dagger_\sigma(t') + d^\dagger_\sigma(t')\, d_\sigma(t) \rangle$.

In this work we focus on the semi-equilibrium situation (some more general case will be discussed separately [11]). For a qualitative study of the excitation spectrum we use the simplest procedure based on the equations of motion for the Green's function. Following the scheme described in Ref. [12] we determine the retarded Green's function

$$G^r_d(\omega) = \frac{g^r_d(\omega)^{-1} - [\Sigma_0(\omega) + \Sigma_3(\omega) + U(1-n_d)]}{[g^r_d(\omega)^{-1} - \Sigma_0(\omega)]\,[g^r_d(\omega)^{-1} - (U + \Sigma_0(\omega) + \Sigma_3(\omega))] + U\Sigma_1(\omega)}\,, \tag{11}$$

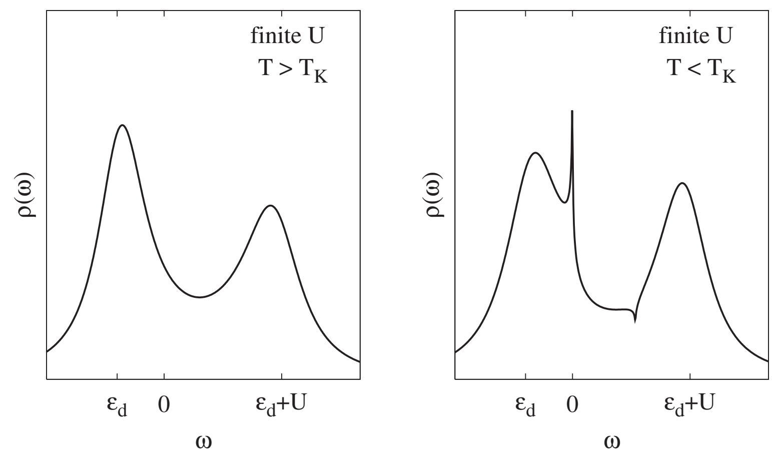
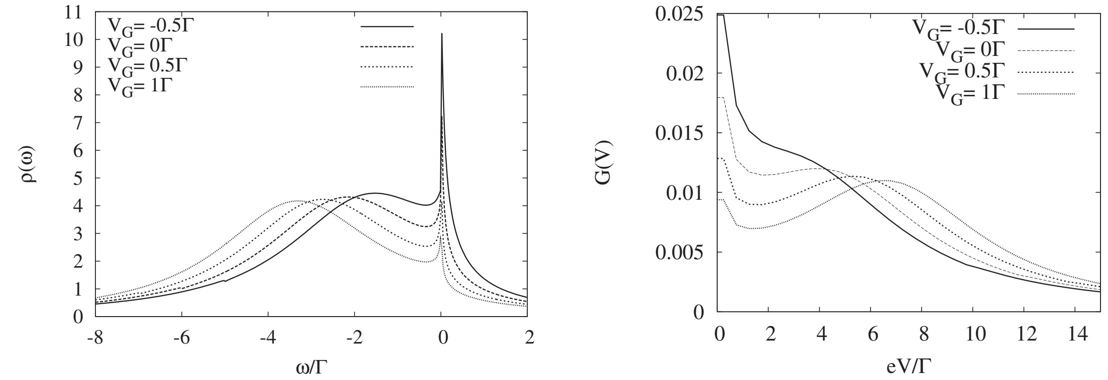


Fig. 2 Effective density of states $\rho(\omega)$ obtained when ε_d is located slightly below the Fermi energy μ.



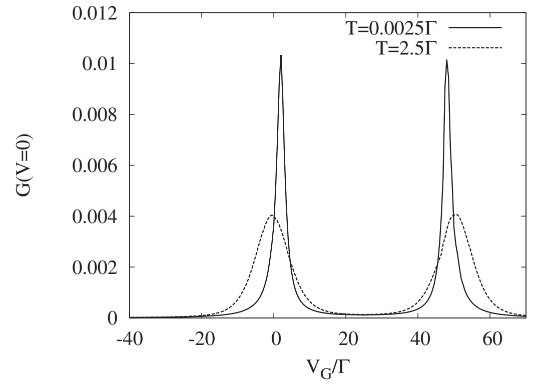


Fig. 3 Density of states $\rho(\omega)$ and the differential conductance $G(V) = \partial I(V)/\partial V$ for several values of the gate voltage V_{G} and $T < T_{\mathrm{K}}$. The bottom panel shows the zero bias conductance versus the gate voltage V_{G}.

where $n_d = \langle d_\sigma^\dagger d_\sigma \rangle$, $g_d^r(\omega) = [\omega - \varepsilon_d]^{-1}$ denotes the Green's function of non interacting system ($U = 0$) and $\Sigma_0(\omega) = \sum_{\boldsymbol{k}\beta} |V_{\boldsymbol{k}\beta}|^2 (\omega - \xi_{\boldsymbol{k}\beta})^{-1}$. The effect of finite Coulomb interaction U enters through the $\nu = 1, 2$ selfenergies given by $\Sigma_\nu(\omega) = \sum_{\boldsymbol{k}\beta} |V_{\boldsymbol{k}\beta}|^2 [(\omega - \xi_{\boldsymbol{k}\beta})^{-1} + (\omega - U - 2\varepsilon_d + \xi_{\boldsymbol{k}\beta})^{-1}] F_\nu(\omega)$ with $F_1(\omega) = f(\omega - \mu)$ and $F_3(\omega) = 1$. In Fig. 2 we illustrate the density of states $\rho_d(\omega)$ for high temperature $T > T_{\mathrm{K}}$ (panel on the left) and for $T < T_{\mathrm{K}}$ (panel on the right).

In the limit $V \to 0$ the differential conductance $G(V) = \mathrm{d}I/\mathrm{d}V$ simplifies to

$$G(V \to 0) = \frac{2e^2}{h} \int_{-\infty}^{\infty} \mathrm{d}\omega \left[-\frac{\mathrm{d}f(\omega - \mu)}{\mathrm{d}\omega} \right] T(\omega) \tag{12}$$

and at very low temperatures (12) implies that $G(0) = (2e^2/h)\, \Gamma_{\mathrm{L}} \Gamma_{\mathrm{R}}/(\Gamma_{\mathrm{L}} + \Gamma_{\mathrm{R}}) \sum_\sigma \rho_\sigma(\mu)$. Therefore the zero bias conductance $G(0)$ is proportional to the density of states of the quantum dot on the Fermi level $\omega = \mu$. In Fig. 3 we show the low temperature density of states $\rho(\omega)$ and the corresponding differential conductance $G(V)$ computed for identical leads $\Gamma_{\mathrm{L}} = \Gamma_{\mathrm{R}} \equiv \Gamma$ with the Coulomb interaction $U = 50\Gamma$ and the single particle energy level assumed to depend on the gate voltage through $\varepsilon_d = -3\Gamma - V_G$. Although the zero bias conductance shows a strong enhancement we can notice that the equation of motion technique does not reproduce a well defined value of the unitary limit $(2e^2/h)$. For this reason in the right h.s. panel of Fig. 3 we do not obtain a plateau typical for the Kondo regime. Such fine behaviour could be obtained within better controlled treatments as the NCA or the numerical renormalization group method.

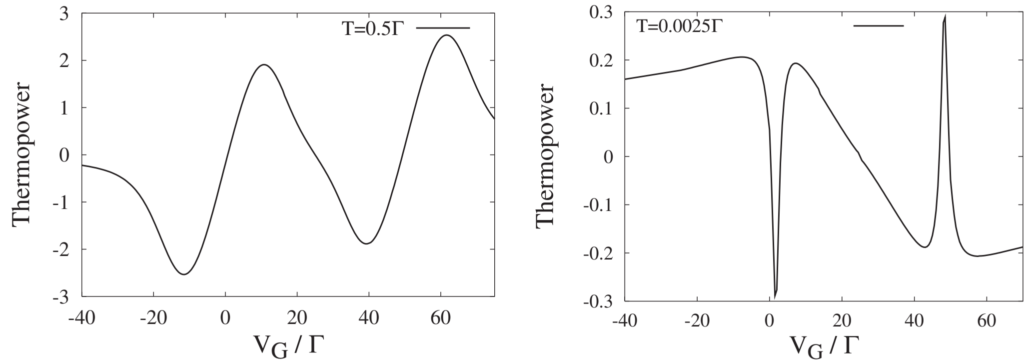


Fig. 4 Variation of the thermopower S versus the gate voltage V_G for two representative temperatures $T > T_K$ (left h.s. panel) and $T < T_K$ (right h.s. panel).

Figure 4 presents the thermopower $S = (-V/\Delta T)|_{I(V)=0}$ calculated in the linear response limit $V \to 0$. At high temperatures S has a characteristic saw-tooth shape which, roughly speaking, follows the semi-classical Mott relation $S = (\pi^2 k_B^2 T/3e)\, \partial \ln G/\partial\mu$. For low temperatures, on top of this shape there arise two additional anomalous features: one of them comes from the typical Kondo effect (which occurs ε_d approaches the Fermi energy μ from below) and the other one corresponds to a similar Kondo effect for holes (when $\varepsilon_d + U$ approaches μ from above). Existence of these two features is strictly related to the particle-hole symmetry of the Anderson model (1).

6 Summary

We studied the charge transport through a correlated quantum dot. In agreement with the experimental data [1] we found that the differential conductance G oscillates as a function of the gate voltage V_G and temperature shows merely a quantitative effect on it. The thermoelectric power S is characterized by a saw-tooth shape versus V_G. For low temperatures we observe an emergence of the anomalous features related with the Kondo resonance either for particles or for holes. The lower feature has been already observed experimentally [2] and we hope that the other one could be checked in the future measurements.

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