Zero bias anomalies in the Kondo regime of single and double quantum dots

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Abstract. The zero bias anomaly of the differential conductance of mesoscopic systems is a fingerprint of the electron-electron interaction. The common example is the peak of the differential conductance in Kondo mesoscopic systems.

We show that in complex mesoscopic systems, in particular in the side-coupled double dot, the dip of the differential conductance at zero bias is also possible due to simultaneous effects of interference and correlations. The external parameters that control this effect are the temperature and the gate potential on the lateral dot. We argue that even in single dots, in a multiple lead configuration, the shift from suppression to enhancement of $dI/dV$ with increasing bias is allowed if the bias applied on the leads is not symmetric. The differential conductance exhibits a peak-dip crossover, the effect being controlled by the strength of the asymmetry and the ratio of the dot-lead couplings.

The scaling of the differential conductance for the double-dot system is also discussed. The results are obtained using an extended Anderson model, the Keldysh transport formalism and the equation of motion technique extended to the non-equilibrium.

1. Introduction

The Coulomb repulsion leads to important electronic correlations, resulting in strong modifications of the density of states, the (perhaps) most significant such case being illustrated by the mesoscopic Kondo effect [1]. In the classical single-dot case, the Kondo effect manifests in the differential conductance $dI/dV$ as a pronounced peak at zero bias ($V = 0$), known as the zero bias anomaly (ZBA), meaning that the conductance is maximum close to equilibrium and decays rapidly when the bias is increased. The reason for the depletion of the differential conductance is that the applied bias kills the Kondo correlations.

A more subtle problem regards the bias dependence of the differential conductance in complex systems. The three lead-Kondo problem -for instance- was theoretically considered by, e.g., [2, 3, 4, 5] or experimentally realized by Leturcq et. al [6, 7]. It can be shown that the presence of the third lead allows for a conductance suppression around zero bias, instead of the usual enhancement, in conditions of asymmetrically applied bias [5]. The result is interesting due to its counter-intuitive aspect, but, more importantly, one can extract the ratio of dot-leads coupling from the threshold values of the asymmetry parameter corresponding to the peak-dip crossover.

Another complex Kondo problem arises when considering a second side-coupled dot, a set-up intensively addressed in literature [8, 9, 10, 11, 12, 13, 14]. The system is typical for exhibiting Fano resonances when a gate potential $V_g$ applied on the side dot is changed continuously. Our numerical results indicate that a dip-type ZBA can develop for values of $V_g$ around the Fano zero.
Next, we address the scaling of the differential conductance \( G = \frac{dI}{dV} \) for the double-dot system when the temperature and the bias are varied. The scaling properties resemble those for the single-dot case, provided that a suitable definition is used for the Kondo temperature of the double-dot system.

2. Three leads Kondo problem

A quantum dot connected to three leads is sketched in Fig.1. The electron current through one of the leads (say \( \alpha \)) is given by [2]:

\[
I_\alpha = -\frac{4e\Gamma_\alpha}{\pi\hbar\Gamma} \int_{-\infty}^{\infty} \text{Im} G_{dd}(\omega) \sum_{\beta \neq \alpha} \Gamma_\beta [f(\omega - \mu_\alpha) - f(\omega - \mu_\beta)] d\omega, \tag{1}
\]

where \( \Gamma_\alpha \) is the coupling of the lead \( \alpha \) to the dot, \( \Gamma = \sum \Gamma_\alpha \), and \( f(\omega - \mu_\alpha) \) is the Fermi distribution in the \( \alpha \)-lead. \( G_{dd} \) is the retarded Green function of the dot in the presence of the leads. Usually, one needs also the “lesser” Green function, however when the leads are all connected to the same site, the lesser function can be eliminated excepting for the case of magnetic leads [15]. The same simplification occurs for a geometrically symmetric many-site system [16].

![Figure 1](image_url)

**Figure 1.** (above) Sketch of a quantum dot connected to three leads. The bias is applied asymmetrically on the left and right leads (\( V_L = V \) and \( V_R = \lambda V \); the usual symmetric case corresponds to \( \lambda = -1 \)). (below) The differential conductance through the left lead for different values of the asymmetry parameter showing a change from peak to dip (around zero bias) : the crossover occurs at \( \lambda_0 = 1.58 \); the other parameters: \( \Gamma_R = \Gamma_L = 0.075, \Gamma_C/\Gamma_L = 3, T_K = 3.2 \cdot 10^{-4} \) (measured in the lead bandwidth), and \( T = T_K/10.\) [5]

If one applies the potential bias \( V_L - V_R = V(1 - \lambda) \) the differential conductance through the lead “L” can be calculated from eq.1:

\[
G_L(V) = \frac{dI_L}{dV} = \frac{4e^2\Gamma_L}{\pi\hbar\Gamma} \int_{-\infty}^{\infty} \left(\Gamma_R + \Gamma_C\right) \text{Im} G_{dd}(\omega) \frac{df(\omega - eV)}{d\omega} d\omega
\]
\[- \lambda \Gamma_R Im G_{dd}(\omega) \frac{df(\omega - \lambda eV)}{d\omega} \mathrm{d}\omega. \]  \hspace{1cm} (2)

At low temperatures, approximating the derivatives of the Fermi functions by delta-functions, and under the assumption that the spectral function depends weakly on the applied bias, the above formula becomes:

\[ G_L(V) = - \frac{4e^2 \Gamma_L}{\pi \hbar} \left[ (\Gamma_R + \Gamma_C) Im G_{dd}(eV) - \lambda \Gamma_R Im G_{dd}(\lambda eV) \right]. \]  \hspace{1cm} (3)

In order to prove the peak- or dip-like behaviour of the differential conductance, one has to compute the second derivative:

\[ G_L''(0) = - \frac{4e^4 \Gamma_L \Gamma_R}{\pi \hbar \Gamma} Im G_{dd}''(0)[1 + \frac{\Gamma_C}{\Gamma_R} - \lambda^3] \]  \hspace{1cm} (4)

At this stage, one can make the following remarks:

i) in the above formulas \(- Im G_{dd}''(0)\) is the second derivative of the spectral function at equilibrium (i.e. at \(V = 0\)), and it is always negative for \(T < T_K\) indicating the presence of the Kondo peak in the density of states (also, one has \(Im G_{dd}'(0) = 0\)). This property will be used to determine the peak or dip behavior of the conductance.

ii) eq.(4) shows that the peak or dip aspect of the differential conductance is completely determined by the sign of the quantity \([1 + \Gamma_C/\Gamma_R - \lambda^3]\).

iii) the symmetric bias corresponds to \(\lambda = -1\), in which case the second derivative of the spectral function is positive. In other words, for the usual case of symmetric bias, the differential conductance is always enhanced at \(V = 0\) showing a peak-like behaviour.

iv) there is a crossover value of \(\lambda\) when the peak changes into dip; this value is \(\lambda_0 = \sqrt[3]{1 + \frac{\Gamma_C}{\Gamma_R}}\). This fact can be of interest for experimentalists: once the crossover value \(\lambda_0\) is identified from experiment, the ratio \(\Gamma_C/\Gamma_R\) of the two dot-lead couplings can be immediately extracted. Otherwise, the ratio of the two couplings is inaccessible to direct measurement.

The above general argumentation will be illustrated by calculating the spectral function of a single quantum dot connected to three leads; the system is described by the Anderson Hamiltonian:

\[ H_1 = \sum_{k,\sigma,\alpha} \epsilon_k c_{k\sigma,\alpha}^\dagger c_{k\sigma,\alpha} + \sum_{\sigma} E_d d_{\uparrow}^\dagger d_{\uparrow} + U_H n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma,\alpha} t_{kd} c_{k\sigma,\alpha}^\dagger d_{\sigma} + h.c. \]  \hspace{1cm} (5)

where the first term describes the three leads, \(E_d\) is the energy of the dot level, \(U_H\) is the Hubbard repulsion interaction inside the dot, and the last term describes the coupling to leads.

For the calculation of the spectral function we use the equation of motion method in the version of Ref.17 extended to the non-equilibrium situation. Details of this approach in the case of many-lead systems are given in Ref.5. By the use of eq.(3) the function \(G_L(V)\) can be obtained numerically. The differential conductance in Fig.1 is calculated for various \(\lambda\) and the crossover from the peak- to dip-like behaviour can be noticed with increasing asymmetry of the applied bias.

3. Non-equilibrium behaviour of the side-coupled double dot

The double-dot set-up can be realized by replacing the central lead in Fig.1 with a second dot. Only the the Kondo dot is directly coupled to leads, however the side dot influences the transport by allowing multiple electron paths resulting in non-trivial interference effects. We shall consider a multilevel non-interacting side-coupled dot, and focus on the Fano-Kondo regime of the system. In Kondo systems, due to the bias induced dephasing, the differential conductance is suppressed
around the zero bias, giving rise to a peak-like zero bias anomaly. However, the side-coupled double dot is characterized also by Fano interference which compete with the Kondo correlations, so that the behaviour of the differential conductance is no more obvious. The process is controlled by the gate potential applied on the lateral dot and temperature.

Qualitatively, the physical process can be described as follows. The charge current through the device is the result of the superposition of two transport channels: the resonant channel through the side dot and the continuous channel passing through the Kondo dot. The first channel is controlled by the gate potential $V_g$ applied on the lateral dot, while the Kondo channel is controlled mainly by temperature, but also by internal parameters describing the Kondo dot (e.g., $\Gamma, E_d$). The result of the interference depends on the transmittance amplitudes along the two channels, but also on the phase difference which can give rise to constructive or destructive interference depending on external parameters $T$ and $V_g$. This can be the origin of peak or dip-like aspect of the differential conductance in different ranges of the parameters space $\{T, V_g\}$. In [14] we show using the equation of motion method for the Green function that indeed the dip-like behavior of the ZBA is also possible in the vicinity of the Fano dips, where the interference effects are most pronounced. The numerical results are shown in Fig.2 which exhibits the peak-dip crossover when $V_g$ is varied at fixed temperature.

**Figure 2.** $\Delta G(V,T) = G(0,T) - G(V,T)$ as function of the bias (measured in units $T_k$) proves the peak-dip crossover when the gate potential $V_g$ is changed at the fixed temperature $T = T_K/100$ ($T_K$ = Kondo temperature).

The Hamiltonian of the double dot system can be written:

$$\begin{align*}
H &= \sum_{k,\sigma,\alpha} (\epsilon_k - \mu_\alpha)c_{k\sigma,\alpha}^\dagger c_{k\sigma,\alpha} + \sum_\sigma E_{dd}\sigma_d^\dagger \sigma_d + U_H n_d^\dagger n_d + \sum_\sigma E_{id}\sigma_i^\dagger \sigma_i + \frac{e^2}{2C} N^2 \\
&\quad + \sum_{k,\sigma,\alpha} t_{kd}(c_{k\sigma,\alpha}^\dagger \sigma_d + h.c.) + \sum_i \tau_{id}(c_{i\sigma}^\dagger \sigma_d + h.c.),
\end{align*}$$

where one may identify the Hamiltonian of the leads ($\alpha = L(left), R(right)$), the Hamiltonian of the small dot including the Hubbard term, and that one of the multilevel lateral dot which contains also the Coulomb repulsion in the orthodox (capacitance) model; the operator of the total occupation number reads $N = \sum_\sigma n_\sigma = \sum_\sigma \sigma_i^\dagger \sigma_i$. The last two terms stand for the coupling of the small dot to the leads and to the multilevel side dot.

Since only the Kondo dot is coupled to leads, the conductance takes the simple form (the symmetric bias will be considered in this case):

$$G(V) = \frac{dI}{dV} = \frac{e^2}{2h} \sum_\sigma \Gamma_\sigma \left[ ImG_{dd,\sigma}(-\frac{eV}{2}) + ImG_{dd,\sigma}(\frac{eV}{2}) \right]$$
Figure 3. (a) Two Fano-Kondo resonances as function on $V_g$. The scaling function $\Delta G$ will be plotted for different values of $V_g$ ($iV_g = -0.95, -0.7, -0.5, 0.1, 0.5, 0.95, 1.05, 1.1$) and considering three possible definitions for the Kondo temperature: (b) $T_{K0}$ - the SIAM Kondo temperature, which does not depend on $V_g$, (c) $T_{K1}$ - the half-width of the Kondo peak at $T = 0$, as estimated in [17], and (d) $T_{K2}$ - the half-width of the Kondo peak at a finite temperature as mentioned in [18]. In both cases (c) and (d) the Kondo temperature depends on $V_g$, and the scaling is satisfactory, resulting in the data collapse. For all curves, $V = T_K/100$. Other parameters are: $E_d = -0.25, \Gamma = 0.05, \tau = 0.006$ (measured in the lead bandwidth).

The equilibrium conductance described by the above formula in the limit $V = 0$ is plotted in Fig.3a as function of the gate potential $V_g$. Due to multilevel structure of the lateral dot the equilibrium conductance shows a sequence of resonances, their Fano character being obvious. The Fano zeros occur at integer values of $V_g$ which is measured in units of charging energy of the side dot.

At nonequilibrium, the conductance as function of the bias $V$ will present mainly the usual peak at $V = 0$, except for values of the $V_g$ in vicinity of the Fano zero, as mentioned. An important property of the conductance in the Kondo regime is the scaling. The usual function for which a scaling is searched is $\Delta G(V, T) = G(0, T) - G(V, T)$ [19, 20, 21]. In Fig.3 we check weather $\Delta G(V, T)$ can be expressed in terms of scaled variables $V/T_K$ and $T/T_K$; it turns out from Fig.3a that the scaling does not work if we choose as Kondo temperature that one of the isolated single dot (described by the single impurity Anderson model -SIAM, corresponding in our case to $\tau = 0$). Figs 3(c and d) shows however that the scaling works if a suitable definition of $T_K$ is considered for the double dot system.

In [14], we have shown that the scaling properties are preserved even in the Fano-Kondo regime, if $V_g$ is varied along a Fano line in the regions with peak-like behavior. Supplementary in this paper, we show that the good scaling properties maintain also when the gate is varied across multiple Fano resonances as seen in Fig.3.
4. Conclusions
In summary, we investigate the nonliner conductance in two different complex dot systems: i) many-lead single dot, and ii) side-coupled double dot (similar to a mesoscopic transistor set up). In both cases the bias dependence of the differential conductance can show a peak-dip crossover around the zero bias. The crossover is controlled by external parameters as the asymmetry of the applied bias in the case i) and the temperature or gate potential in the case ii). For the double dot, $\Delta G(V,T) = G(0,T) - G(V,T)$ shows scaling properties provided a proper definition of the Kondo temperature is chosen. The scaling cannot be universal because of different behaviour (peak/dip-like) of the differential conductance in different ranges of the parameters.

Acknowledgments
We acknowledge support from the Core Programme under the contract No 45N/2009 and from PNCDI2-Research Programme under the grant No.515/2008.

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