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Peak-dip crossover of the differential conductance in mesoscopic systems with quantum impurities.

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Abstract. We investigate the differential conductance dI/dV for the interacting T-shape model, using an approach based on the Keldysh formalism and the Lacroix solution for the equation of motion. A peak-dip crossover has been noticed by changing the hybridization between the two dots. For the same model, the combined interaction and interference processes give rise to the Fano-Kondo effect with an interesting crossing point of the isoterms below the Kondo temperature. A tentative explanation of these effects is given in terms of the many-body spectral properties of the system.

The differential conductance is a powerful instrument for the study of the electron transport in interacting meso-systems, as it can provide informations on the role of correlations at low temperatures, in particular on the Kondo correlations. Recently it was used also to probe the two-channel Kondo effect. The approach of the non-equilibrium situation arises theoretical difficulties since all quantities that enter the formalism depend on the applied bias, situation which is difficult to be tackled in practice. The theoretical modeling of the many-lead interacting quantum dots generally uses the tight-binding approach, and serious technical problems arises when the leads are attached to different sites. In this case, beside the retarded Green function at the impurity site, one has to calculate also the lesser Green function (in the Keldysh formalism) with supplementary approximations. More then this, not all the technical tools used for the calculation of the Green function are equally suitable for many-site mesoscopic systems. We shall follow the track of the equation of motion (EoM), which has been widely used in the Kondo problem. For the mesoscopic Kondo problem, the Lacroix’s approach has been developed by Entin-Wohlman et al for the Anderson impurity model embedded in a meso-system [1]. In the case of the N-fold degenerated model the same method has been used by Goldberg [2].

We shall evidentiate some properties of the differential conductance for the interacting T-shape model depicted in Fig.1 when both the inter-site hopping and gate potential may affect the nonlinear response. The expression of the electron current through the two leads (L,R) when the potentials \( V_L = -V_R = V \) are applied, deduced in the Keldysh formalism, reads [3]:

\[
I(V) = \frac{e}{\hbar} \sum_\sigma \int d\omega [f_L(\omega - eV) - f_R(\omega + eV)] \Gamma_\sigma(\omega) \left[ -\frac{1}{\pi} ImG_{00,\sigma}^{ret}(\omega) \right],
\]

(1)

where "0" is the index of the contact site. In principle, not only the Fermi function depends on the applied potentials, but also the coupling \( \Gamma \) and the Green function \( G_{00} \) itself. However, assuming that the system is not very far from equilibrium, commonly only the derivative
Figure 1. Sketch of the T-shape model: a) the quantum impurity is located at the contact site, b) the contact site is not interacting, c) the two one-particle levels $E_{1}^{\pm}$ in the well connected to reservoires.

df_{L,R}/dV \approx \pm \frac{e}{h} \delta(\omega \mp eV)$ is taken into account when deducing the expression of the differential conductance $G(V) = dI/dV$. So, for low temperatures, with $\Gamma_{\sigma}(\omega) = \Gamma_{\sigma}$ one gets:

$$G(V) = \frac{e^2}{2h} \sum_{\sigma} \Gamma_{\sigma}[\text{Im}G_{00,\sigma}^{\text{ret}}(-eV) + \text{Im}G_{00,\sigma}^{\text{ret}}(eV)]. \quad (2)$$

As long as $dI/dV$ is expressed in terms of the Green function at the contact site "0", any peak (dip) in the local density of states at $E = Ef (= 0)$ is automatically transferred into a peak (dip) of the differential conductance at zero bias $V = 0$. This suggests that, for such a case, the explanation of the effects may be given in terms of the many-body spectral properties of the system, as we shall discuss below.

One notes that for the T-shape model there is a distinct behavior when the quantum impurity is located at the contact site as in Fig.1a: in this case, the density of states at the contact is just the imaginary part of the impurity Green function (usually denoted as $-(1/\pi)\text{Im}G_{dd}$), which exhibits the Kondo peak. This means that the differential conductance shows definitely a peak behavior at $T < T_K$. Otherwise (situation described by Fig.1b) there is no a definite answer and the result depends on the interference effects controlled mainly by the hopping process between the two sites and a possible gate potential applied on one of the dots. The result is a Fano-Kondo effect [4].

At equilibrium, the conductance of the T-shape system shows a crossing point of the isoterms which separates regions with Kondo and non-Kondo temperature dependence (see Fig.2). We shall show below that, interestingly, also the differential conductance behaves quite different in the two regions, exhibiting a crossover from dip- to peak-behavior around the same crossing point. The usual model Hamiltonian describing the two non-interacting leads, the isolated meso-system and the coupling between them reads:

$$H = \sum_{k,\alpha \in L,R} (\epsilon_{k\alpha} - \mu_{\alpha})c_{k\alpha}^\dagger c_{k\alpha} + H_{\text{meso}}(\{d_{n\sigma}^\dagger, d_{n}\}) + \sum_{n,k,\sigma \in L,R} V_{k\sigma,n}c_{k\sigma}^\dagger d_{0\sigma} + H.c. \quad (3)$$

In our case (T-shape model) the meso-system consists of a two-site interacting molecule described by:

$$H_{\text{meso}} = \sum_{\sigma} [\epsilon_{0}d_{0\sigma}^\dagger d_{0\sigma} + \epsilon_{1}d_{1\sigma}^\dagger d_{1\sigma} + t_{01}(d_{1\sigma}^\dagger d_{0\sigma} + h.c.)] + U d_{0\uparrow}^\dagger d_{0\downarrow}^\dagger d_{0\uparrow} d_{0\downarrow}. \quad (4)$$

For infinite $U$ the system may accomodate up to three electrons, and the 1-, 2- (two singlets, one triplet) and 3- particle spectrum obtained by trivial diagonalization is shown in Fig.2a as function of the hybridization parameter $t_{01}$.

We calculate the equilibrium conductance according to Eq.(1) in the limit of small $V$ as function of the hopping parameter $t_{01}$ at different temperatures; a crossing point of the isoterms
becomes evident in Fig.2a at $t_{01} = 2$ (see also the inset). On the left side, at small values of the inter-site hybridization, the conductance shows the Kondo-type temperature dependence, i.e. an increase with decreasing temperature. The dependence is most strongly at $t_{01} = 0$, which corresponds to the single impurity Anderson model (SIAM), but then diminishes with increasing hybridization. One notices that the crossing occurs at $t_{01} = 2$, where the one-particle eigen-energy $E_1^\pm$ of the Hamiltonian Eq.4 equals the Fermi energy $E_F = 0$ (see Fig.2b), indicating that the system is in the mixed valence (MV) regime. For $t_{01} > 2$ the temperature dependence becomes opposite, i.e. shows an increase with the temperature. It is obvious that the Kondo-type temperature dependence noticed at low hybridization is due to the presence of a Kondo peak in the density of states; it is however of interest to analyse more closely the density of states in the MV regime, in the attempt to understand the above mentioned change in the temperature behavior, and (as we shall see below) also the presence of a dip in the nonequilibrium case.

Three different situations are shown in Fig.3. The two main resonances correspond to the one-particle eigenvalues $E_1^\pm = (\epsilon_0 + \epsilon_1 \pm \sqrt{(\epsilon_0 - \epsilon_1)^2 + t_{01}^2})/2$ of the Hamiltonian Eq.4, broadened and shifted by the coupling to reservoirs. This correspondence can be easily checked at small coupling $\Gamma$. The left panel depicts the usual Kondo case. At $t_{10} = 2$ in the MV regime the DoS exhibits a significant drop at $E = E_F = 0$ (middle panel). This rapid variation with the energy is associated also with a tiny dip of the DoS at $E_F = 0$. These properties has been found also by Goldberg et al [2] using also the equation of motion approach, but with different approximations. By increasing the temperature or moving into the empty dot region by further increase of the hybridization this drop is swept out being replaced by a smooth energy dependence. This proves that the drop in DoS is a correlation effect that characterizes the mixed valence regime. An interesting picture can be obtained in the presence of a small bias, when both the drop and the Kondo peak may appear on the two sides of the resonance. This occurs in the non-equilibrium situation if the impurity resonance is located in between the two chemical potentials of the leads (right panel).

Since the crossover from the Kondo- to mixed valence regime gives rise to significant modifications of the DoS at the Fermi level, one expects also changes in the behavior of the differential conductance Eq.(2). In particular, the second derivative of $G(V)$ at $V=0$ is
Figure 3. DoS of the interacting T-shape model coupled to leads for three different situations: a) \( V = 0, t_{01} = 1 \); b) \( V = 0, t_{01} = 2 \); c) \( V = 0.4, t_{01} = 1.6 \); temperature \( T = 10^{-5} \).

Figure 4. Differential conductance versus the bias: a) Kondo regime \((t_{01} = 1)\), b) MV-regime \((t_{01} = 2.3)\), at three temperatures: \( T = 10^{-5} \) (red), \(10^{-3} \) (green), \(10^{-2} \) (blue).

\[ G''(0) = -\frac{e^4}{2\hbar} \Gamma \text{Im} G_{dd}''(0) \text{ (per spin)}, \] (5)

meaning that the second derivative of the density of states at \( V=0 \) determines the peak- or dip-type dependence of \( G(V) \) about \( V = 0 \). Obviously, in the Kondo regime, the differential conduction of the T-shape model shows the well known peak called 'zero bias anomaly', however this is not the case in the mixed valence regime, where the second derivative of the DoS may be positive at \( E=0 \). Indeed, the numerical calculation of the differential conductance \( G \) as function of the bias \( V \) shows in Fig.4 that both peak- and dip-type curves are obtained depending on the hybridization parameter \( t_{01} \). The two cases occur in the Kondo and mixed valence regime, respectively, and are separated by the critical value \( t_{01} = 2 \) at which \( E_{1}^{+} = 0 \). Such a dip of the differential conduction has been observed experimentally in the two-channel Kondo problem \([5]\). However, in this paper, the physics is different and the dip is obtained in the frame of one-channel problem of the T-shape interacting model.

In conclusion, the Tshape is the simplest model of meso-systems which exhibits both interaction and interference effects. By increasing the hybridization between the two dots the system moves from Kondo to mixed valence regime. Simultaneously, the zero bias density of states shows a crossover from the Kondo peak to a fast drop at the Fermi energy, while the differential conductance shows a peak-dip crossover.

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