Interpolative method for transport properties of quantum dots in the Kondo regime

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Abstract. We present an interpolative method for describing coherent transport through an interacting quantum dot. The idea of the method is to construct an approximate electron self-energy which becomes exact both in the limits of weak and strong coupling to the leads. The validity of the approximation is first checked for the case of a single (spin-degenerate) dot level. A generalization to the multilevel case is then discussed. We present results both for the density of states and the temperature dependent linear conductance showing the transition from the Kondo to the Coulomb blockade regime.

1 Introduction

The Kondo effect constitutes a prototypical correlation effect in condensed matter physics. Although originally studied in connection to magnetic impurities in metals, there is now a renewed interest in this many-body problem fostered by the recent observation of Kondo effect in semiconducting quantum dots [1,2]. Quantum dots provide an almost ideal laboratory where the relevant parameters can be controlled, which allow to test the predictions of theoretical models.

From the theoretical side, Kondo physics in quantum dots has been mainly analyzed in the light of the so called single level Anderson model. There were predictions for the Kondo effect in quantum dots based on this model since the early 90’s [3,4]. The theory predicts an enhancement of the linear conductance due to Kondo effect at very low temperatures, which is in qualitative agreement with recent experiments.

However, in most realistic situations, the single level Anderson model constitutes a crude approximation for a quantum dot. Actual semiconducting quantum dots contain a large number (∼ 100) of electrons and the single-particle level separation between dot levels may be not so large compared to the level broadening, which restricts the validity of the single-level approximation. The actual situation would be more appropriately described by a multilevel model, including several instead of a single dot level. Unfortunately, there are no simple theoretical approaches to extract the electronic and transport properties from such a microscopic model.

In this paper we present results on the Kondo effect in quantum dots based on the interpolative method. The basic idea of this method is to construct an interpolative electron self-energy which becomes exact both in the limits of weak and strong coupling to the leads. These ideas were first introduced in Ref. [5]
in connection to the single-level Anderson model and have, since then, been adapted by several authors to different problems involving strongly correlated electrons. In this way, the method has been used to study the Hubbard model [6], the non-equilibrium Anderson model [4], the metal-insulator transition in infinite dimensions [7], to incorporate correlation effects into band-structure calculations [8], the ac-Kondo effect in quantum dots [9] and finally extended by the present authors to analyze the multilevel Anderson model [10].

The paper will be organized as follows: In section 2 we present the interpolative method. We first discuss the single level case, showing the accuracy of the method with the help of a simple exactly solvable model. We then consider the multilevel situation. In section 3 we present results which illustrate the behavior of the conductance with temperature in a multilevel situation.

2 The interpolative method

For describing a multilevel quantum dot (QD) we consider a model Hamiltonian

\[ H = H_{\text{dot}} + H_{\text{leads}} + H_T \]

where

\[ H_{\text{dot}} = \sum_m \epsilon_m \hat{d}_m^{\dagger} \hat{d}_m + U \sum_{l>m} \hat{n}_m \hat{n}_l \]

corresponds to the uncoupled QD (\( \hat{n}_m = \hat{d}_m^{\dagger} \hat{d}_m \)); \( H_{\text{leads}} = \sum_{k \in L,R} \epsilon_k \hat{c}_k^{\dagger} \hat{c}_k \) to the uncoupled leads, and \( H_T = \sum_{m,k \in L,R} t_{m,k} \hat{d}_m^{\dagger} \hat{c}_k + \text{h.c.} \) describes the coupling between the dot and the leads. The labels \( m \) and \( l \) in \( H \) denote the different dot levels including spin quantum numbers. The number of dot levels will be denoted by \( M \) (i.e. \( 1 \leq m, l \leq M \)). We adopt the usual simplifying assumption of having the same electron-electron interaction \( U \) between any pair of dot states.

The main objective of our method is to determine the dot retarded Green functions

\[ G_m(\tau) = -i\theta(\tau) \langle [\hat{d}_m(\tau), \hat{d}_m^{\dagger}(0)] + \rangle \]

from which the different level charges and the dot linear conductance can be obtained. In the frequency representation we can write \( G_m \) as:

\[ G_m(\omega) = \frac{1}{\omega - \epsilon_m^{\text{HF}} - \Sigma_m(\omega) - \Gamma_{m,L}(\omega) - \Gamma_{m,R}(\omega)} \]

where \( \epsilon_m^{\text{HF}} = \epsilon_m + U \sum_{l \neq m} n_l \) is the Hartree-Fock level (we adopt the notation \( n_l \) for the mean charge on level \( l \)) and \( \Gamma_{m,L}, \Gamma_{m,R} \) are tunneling rates coupling the dot to the leads, given by

\[ \Gamma_{m,L(R)}(\omega) = \sum_{k \in L(R)} t_{m,k}^2 / (\omega - \epsilon_k + i0^+) \]

We shall neglect indirect coupling between dot levels through the leads (non-diagonal elements \( \Gamma_{m,m',L(R)} \)) and adopt the usual approximation of considering \( \Gamma_{m,L(R)} \) as a pure imaginary constant independent of the energy.

The self-energy \( \Sigma_m(\omega) \) takes into account electron correlation effects beyond the Hartree approximation. The idea of the present approximation is to determine an interpolative self-energy which yields the correct exact results both in the \( \Gamma/U \to 0 \) limit (atomic limit) and in the opposite \( U/\Gamma \to 0 \) limit.

2.1 The single-level case

Let us first discuss how to proceed for the simple single-level case. In this case \( m = 1, 2 \), the two indexes corresponding to up and down spin orientations. These
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will be denoted by $\sigma$ and $\bar{\sigma}$. In the atomic limit $G_\sigma$ can be obtained using the equation of motion technique \[11\] as

$$G_\sigma^{(at)}(\omega) = \frac{1 - \tilde{n}_\sigma}{\omega - \epsilon + i0^+} + \frac{\tilde{n}_\sigma}{\omega - \epsilon - U + i0^+}$$  \(\text{(2)}\)

This expression can be formally written in the usual Fermi liquid form, i.e.

$$G_\sigma^{(at)}(\omega) = \frac{U^2 \tilde{n}_\sigma (1 - \tilde{n}_\sigma)}{\omega - \epsilon - U (1 - \tilde{n}_\sigma) + i0^+}$$

In the opposite limit, $U/\Gamma \to 0$, the electron self-energy can be calculated by second-order perturbation theory in $U$, which yields

$$\Sigma_\sigma^{(2)}(\omega) = U^2 \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \int_{-\infty}^{\infty} d\epsilon_3 \frac{\tilde{\rho}_\sigma (\epsilon_1) \tilde{\rho}_\sigma (\epsilon_2) \tilde{\rho}_\sigma (\epsilon_3)}{\omega + \epsilon_2 - \epsilon_1 - \epsilon_3 + i0^+} \times [f(\epsilon_1) f(\epsilon_3) (1 - f(\epsilon_2)) + (1 - f(\epsilon_1)) (1 - f(\epsilon_3)) f(\epsilon_2)],$$  \(\text{(3)}\)

where $f(\omega)$ is the Fermi distribution function and $\tilde{\rho}_\sigma (\omega) = \Gamma / \pi ((\omega - \bar{\epsilon}_\sigma)^2 + \Gamma^2)$ is the local density of states for an effective level $\bar{\epsilon}_\sigma$, which will be determined in order to fulfill exact Fermi liquid properties at zero temperature.

It is important to stress the following simple property of $\Sigma^{(2)}$:

$$\lim_{\Gamma \to 0} \Sigma_\sigma^{(2)}(\omega) = \frac{U^2 \tilde{n}_\sigma (1 - \tilde{n}_\sigma)}{\omega - \epsilon - U (1 - \tilde{n}_\sigma) + i0^+}$$

Thus, when extrapolated to the atomic limit $\Sigma^{(2)}$ has the same functional form as $\Sigma^{(at)}$. This property suggests that one can smoothly interpolate between the two limits. The ansatz proposed in Ref. \[5\] for the interpolative self-energy is:

$$\Sigma_\sigma (\omega) = \frac{\Sigma_\sigma^{(2)} (\omega)}{1 - \alpha \Sigma_\sigma^{(2)} (\omega)}$$  \(\text{(4)}\)

where $\alpha = (\epsilon - \bar{\epsilon}_\sigma - U (1 - \bar{n}_\sigma))/(U^2 n_\sigma (1 - n_\sigma))$. This ansatz has the desired property $\Sigma \to \Sigma^{(2)}$ when $U \to 0$ and $\Sigma \to \Sigma^{(at)}$ when $\Gamma \to 0$.

The final step is to impose the proper self-consistent condition for determining the effective level $\bar{\epsilon}$. At zero temperature, from the Luttinger-Ward relations \[13\] one can derive the Friedel sum rule for the Anderson model \[14\]

$$n_\sigma = -\frac{1}{\pi} \text{Im ln } G_\sigma^r(E_F)$$

which imposes an exact relation between the dot-level charge and the phase shift at the Fermi energy. The effective level can thus be determined in order to fulfill the Friedel sum rule. This condition is, however, not valid at finite temperature. In Ref. \[4\] we show that the condition $n_\sigma = \tilde{n}_\sigma$, i.e. imposing the same charge in the effective system as in the interacting system, is approximately
equivalent to the Friedel sum rule at zero temperature but can be also used at finite temperature.

In order to check the accuracy of the interpolative method we have considered a simple two-sites problem that can be diagonalized exactly. One of the sites would describe the metallic leads and the other site corresponds to the dot. In order to analyze the more general situation we impose a finite splitting $\Delta = \epsilon_\sigma - \epsilon_{\bar{\sigma}}$ between the two spin orientations on the dot. Within this toy model the second order self-energy can be evaluated analytically.

In figure 1 we show the charge on the two dot levels as a function of gate voltage (the gate voltage is the distance between the lower dot level and the leads level). As can be observed, in the exact solution there is a blocking of the upper level charge until the gate voltage becomes larger than $\Delta + U$. The exact behavior is accurately reproduced by the interpolative method. It is instructive to consider another simple approximation widely used in the literature, which consist in just broadening the poles in the atomic Green function (2) by the non-interacting tunneling rates. This approximation corresponds to the so-called Hubbard I approximation [12]. As can be observed in the lower panel of Fig. 1, this approximation fails to give the blocking of the upper level found in the exact solution.

2.2 Multilevel case

The multilevel version of the interpolative method is somewhat more complex [10]. In the first place, the atomic limit Green functions do not contain just two poles but several poles corresponding to the various different charge states of the dot. The corresponding expression can be obtained using the equation of motion technique and is given by
\[
G_{m}^{(at)}(\omega) = \frac{\prod_{l \neq m}(1 - \hat{n}_l)}{\omega - \epsilon_m + i0^+} + \sum_{l \neq m} \frac{\hat{n}_l \prod_{(s \neq l)}(1 - \hat{n}_s)}{\omega - \epsilon_m - U + i0^+} + \ldots
\]
\[
+ \frac{\prod_{l \neq m} \hat{n}_l}{\omega - \epsilon_m - (M - 1)U + i0^+}.
\tag{5}
\]

The evaluation of this expression requires the knowledge of up to \(M - 1\)-body correlations functions \(<\hat{n}_1\hat{n}_2>, <\hat{n}_1\hat{n}_2\hat{n}_3>, \ldots\) etc. However, for sufficiently large \(U\) fluctuations in the dot charge by more of one electron with respect to the mean charge \(N\) are strongly inhibited. One can thus approximate Eq. (5) as follows

\[
G_{m}^{(at)}(\omega) \simeq \frac{A_N^{m-1}}{\omega - \epsilon_m - U(N - 1) + i0^+} + \frac{A_N^m}{\omega - \epsilon_m - UN + i0^+}
\]
\[
+ \frac{A_N^{m+1}}{\omega - \epsilon_m - U(N + 1) + i0^+},
\tag{6}
\]

where \(N = Int[N]\). In order to yield the exact first three momenta of the exact spectral density the weight factors \(A_N^m\) should satisfy the following sum rules

\[
A_N^{m-1} + A_N^m + A_N^{m+1} = 1
\]
\[
(N - 1)A_N^{m-1} + NA_N^m + (N + 1)A_N^{m+1} = \sum_{l \neq m} \hat{n}_l
\]
\[
(N - 1)^2A_N^{m-1} + N^2A_N^m + (N + 1)^2A_N^{m+1} = \sum_{l \neq m} \hat{n}_l + <\hat{n}>_m + \hat{n}^N >_m,
\tag{7}
\]

where \(<\hat{n}>_m = \sum_{l \neq k \neq m} <\hat{n}_l\hat{n}_k>\). For the special case \(N = 0\) \((N = M - 1)\) one has \(A_N^{m-1} = 0\) \((A_N^{m+1} = 0)\) and only the first two Eqs. in (7) have to be considered.

This approximated expression for \(G_{m}^{(at)}(\omega)\) is now fully determined by the average charges \(n_l\) and the two-body correlation functions \(<\hat{n}_l\hat{n}_k>\). As in the single-level case one can define an atomic self-energy, \(\Sigma_m^{(at)} = \omega - \epsilon_m^{HF} - [G_m^{(at)}(\omega)]^{-1}\), which can be written as the ratio of two polynomials in \(\omega\)

\[
\Sigma_m^{(at)} = \frac{a_m U^2(\omega - \epsilon_m + i0^+) + b_m U^3}{(\omega - \epsilon_m + i0^+)^2} + c_m U(\omega - \epsilon_m + i0^+) + d_m U^2,
\tag{8}
\]

where \(a_m = (N - n_m) [1 - (N - n_m)] + <\hat{n}>_m; c_m = N - n_m - 3N; d_m = <\hat{n}>_m + 3N^2 - 1 - (3N - 1)(N - n_m)\) and \(b_m = N^2(1 - N) - (N - n_m)d_m\).

On the other hand, in the \(U/\Gamma \rightarrow 0\) limit the self-energy is accurately given by second order perturbation theory as in the single level case. The second order
self-energy $\Sigma_m^{(2)}$ now takes into account the interaction of an electron on the dot level $m$ with electron-hole pairs on each one of the other channels.

For the interpolation one notices that both $\Sigma_m^{(2)}$ and $\Sigma_m^{(\text{op})}$ have the same functional form when extrapolated to the corresponding opposite limit. The natural generalization of the ansatz in the single level case now has the form of a continued fraction

$$\Sigma_m(\omega) = \frac{\alpha_m \Sigma_m^{(2)}(\omega)}{1 - \beta_m \Sigma_m^{(2)}(\omega) - R_m(\omega)}, \quad R_m(\omega) = \frac{\gamma_m (\Sigma_m^{(2)}(\omega))^2}{1 - \delta_m \Sigma_m^{(2)}(\omega)},$$

with coefficients $\alpha_m = U^2 a_m/\Delta_m$, $\beta_m = (\epsilon_m - \tilde{\epsilon}_m + (b_m/a_m - c_m)U)/\Delta_m$, $\gamma_m = ((\epsilon_m - b_m/a_m)b_m/a_m - d_m)U^2/\Delta_m^2$ and $\delta_m = (\epsilon_m - \tilde{\epsilon}_m + U b_m/a_m)/\Delta_m$.

As in the single-level case the final step is to determine the effective levels self-consistently. In the multilevel case one has, in addition to self-consistently determine the two-body correlations $<\hat{n}_l \hat{n}_m>$ that appear in the atomic self-energy. This can be done by means of the relation

$$\sum_{l \neq m} <\hat{n}_l \hat{n}_m> = -\frac{1}{\pi U} \int_{-\infty}^{\infty} f(\omega) \text{Im} [(\omega - \epsilon_m - \Gamma_m) G_m(\omega)] d\omega,$$

connecting the two-body correlations and the Green functions that can be derived from the equation of motion for $G_m(\omega)$. This step turns out to be essential in order to obtain the correct values of the charges in the large $U$ limit.

Finally, the temperature dependent dot linear conductance can be obtained using the expression [15]

$$G = \frac{e^2}{h} \sum_m \frac{|\Gamma_{m,L} \Gamma_{m,R}|}{(|\Gamma_{m,L}| + |\Gamma_{m,R}|)} \int_{-\infty}^{\infty} \left( \frac{\partial f}{\partial \omega} \right) \text{Im} G_m^*(\omega) d\omega.$$

### 3 Results

The multilevel formalism allows to study the importance of the multilevel structure in the QD transport properties. For this purpose we have analyzed the $M = 4$ case which corresponds to two consecutive dot levels plus spin degeneracy. We have studied this case as a function of the level separation $\Delta$.

Figure 2 shows the dot conductance as a function of Fermi energy and temperature for the cases $\Delta = 0, 0.1$ and 0.5 (in units of $U$).

This figure illustrates the transition from a two-fold degenerate situation ($\Delta = 0$), where the conductance reaches a maximum value $4e^2/h$ for the half-filled case at zero temperature, to the case of well separated dot levels, where the maximum conductance $2e^2/h$ is reached for the quarter and three quarter filling case. The increase of conductance with decreasing temperature is due to the Kondo effect. While in the case of well separated levels one observes only the Kondo effect due to the spin-degeneracy of the individual levels, when $\Delta$ is
small compared to $\Gamma$ one can observe Kondo features involving the two nearby dot levels. When the temperature is raised above the Kondo temperature (which is around 0.005 for the parameters used in this figure) one recovers the sequence of dot resonances at the charge degeneracy points characteristic of the Coulomb blockade regime.

The Kondo effect should manifest also as a zero-bias anomaly in the dot non-linear conductance. This anomaly is directly related to the appearance of a narrow peak around the Fermi energy in the dot spectral density. In cases where the splitting between dot levels is of the order of $\Gamma$ we expect to have a zero-bias anomaly not only between dot resonances corresponding to the same dot level but also in between resonances corresponding to different levels. This feature is illustrated in Fig. 3 where we plot the density of states around $E_F$ for the same three cases of Fig. 2 with $E_F = 1.5$. The appearance of a zero-bias anomaly in between resonances corresponding to different levels is a clear manifestation of the multilevel structure of the QD which has already been observed in recent experiments on semiconducting quantum dots [16].

This work has been funded by the Spanish CICyT under contracts PB97-0028 and PB97-0044.

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Fig. 3. Density of states around the Fermi energy for increasing temperatures values (0.01, 0.02 and 0.03) for the same three cases in Fig. 2 and $E_F = 1.5$.

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