Electron correlation resonances in the transport through a single quantum level

A. Levy Yeyati, A. Martín-Rodero, and F. Flores
Departamento de Física de la Materia Condensada C-XII.
Facultad de Ciencias. Universidad Autónoma de Madrid.
E-28049 Madrid. Spain.

Correlation effects in the transport properties of a single quantum level coupled to electron reservoirs are discussed theoretically using a non-equilibrium Green functions approach. Our method is based on the introduction of a second-order self-energy associated with the Coulomb interaction that consistently eliminates the pathologies found in previous perturbative calculations. We present results for the current-voltage characteristic illustrating the different correlation effects that may be found in this system, including the Kondo anomaly and Coulomb blockade. We finally discuss the experimental conditions for the simultaneous observation of these effects in an ultrasmall quantum dot.

The transport properties of a quantum dot coupled to electron reservoirs have received considerable attention in recent years both from the experimental and theoretical sides. With the advent of nanotechnologies, the physically relevant regimes, showing how many-body resonances appear in the current-voltage characteristic. We pay particular attention to the situation where features related to the Kondo and charging effects may be simultaneously found. Based on these results, we shall also discuss in detail the experimental conditions necessary to observe those resonances in semiconductor nanostructures.

The transport properties of this model can be analyzed by using the Keldysh formalism, where the retarded, $G^r$, and the distribution, $G^{+-}$, Green functions are defined as follows

$$G^r_{i,j}(w) = -i \int dt \theta(t) \langle c_i(t) c_j(t) \rangle > e^{i w t} dt$$

$$G^{+-}_{i,j}(w) = i \int < c_i(t) c_j(0) > e^{i w t} dt.$$ (2)

These Green functions can be calculated by starting with the $L$ and $R$ reservoirs decoupled from the dot level. This case defines the unperturbed Green functions $G^{(0)}(w)$. Then $G(w)$ can be obtained by coupling the dot level to the reservoirs and by introducing the self-energies $\Sigma'$ and $\Sigma^{+-}$ which take into account the Coulomb correlations within the dot.

Once the different Green functions are obtained from the corresponding Dyson equations, the current intensity $I_\nu$ between reservoir $\nu$ and the dot level, is given by

$$I_\nu = \frac{2 e}{h} \sum_k \int dw \left[ G^r_{k,0}(w) - G^r_{0,k}(w) \right].$$ (3)

The crucial point in order to solve this problem is to find a reasonable approximation for the self-energies. For $U = 0$, $\Sigma = 0$ and the exact Green functions $G(w)$ can be easily obtained using conventional Green function techniques.

The effect of a finite $U$ can be included by using perturbation theory in $U$. This perturbative approach has been extensively analyzed by Yamada and Yoshida (hereafter referred to as YY and ZH) for the equilibrium Anderson Model (zero applied bias). Hershfield et al. have extended this approach to the nonequilibrium case by calculating $\Sigma^r_{\sigma \sigma}(w)$ and $\Sigma^{\sigma \sigma}_{\sigma \sigma}(w)$ up to second order in $U$.

In YY and ZH approach, $\Sigma^{(2)}_{\sigma \sigma}(w)$ is calculated from the second-order diagram shown in figure 1 (inset), where each Green function line is a Hartree Fock dressed propagator, whose retarded part is given by:

$$G^r_{k,0}(w) = -i \int dt \theta(t) \langle c_k(t) c_k(t) \rangle > e^{i w t} dt$$

$$G^{+-}_{k,0}(w) = i \int < c_k(t) c_k(0) > e^{i w t} dt.$$ (2)
\[ G_{0\sigma}^{HF}(w) = \frac{1}{w - \bar{\epsilon}_{0\sigma} + i\Gamma_L(w) + i\Gamma_R(w)}, \tag{4} \]

where \( \bar{\epsilon}_{0\sigma} = \epsilon_0 + U < n_{0\sigma} > \) and \( \Gamma_v = 2\pi \sum_k |T_k|^2 \delta(w - \epsilon_k) \).

Although this approximation gives a good description of the electron correlation effects in the symmetric case \( (\epsilon_0 = -U/2) \), it presents some drawbacks when one moves away from this condition. In the equilibrium case this is clearly illustrated by the failure of the Friedel-Langreth \[ \Sigma \] (hereafter referred as FL) sum rule, that relates the “impurity” charge \( < n_{0\sigma} > \) to the phase shift created by the impurity at the Fermi energy \( \eta(0) = Im [\ln G_{\sigma\sigma}(0)] \).

Figure 1a shows the degree of fulfillment of the FL sum rule, \( < n_{0\sigma} > = -\frac{1}{\pi} \eta(0) \), using the second order self-energy \( \Sigma^{(2)}_{0\sigma}(w) \) in the YY-ZH approach. In this figure we compare \( < n_{0\sigma} > \) with \( -\frac{1}{\pi} \eta(0) \) as a function of the dot level \( \epsilon_0 \), for \( U/\Gamma = 2.4\pi \), neglecting the frequency dependence in \( \Gamma_v \), and taking \( \Gamma_L = \Gamma_R = \Gamma/2 \).

Improvements over the above \( \Sigma^{(2)}_{0\sigma} \) are not easy to obtain. For instance, one could insert the full self-consistent dressed propagators instead of the Hartree-Fock ones for calculating the diagram in figure 1. This sort of self-consistent perturbation theory is charge conserving and would verify the FL sum rule. However, it has been shown that it leads to a poorer description of the quasiparticle spectral-density \[ \Sigma \].

Our proposal to improve the YY and ZH approach is the following: instead of using the Hartree-Fock solution for the calculation of \( \Sigma^{(2)}_{0\sigma} \), we use a different self-consistent field as a starting point. In this initial one-electron problem the Hartree-Fock solution does not yield the atomic limit when \( w \sim U \gg \Gamma \). To improve the solution given above in this region we introduce the following self-energy \[ \Sigma^{(2)}_{0\sigma}(w) = \frac{\Sigma^{(2)}_{0\sigma}(w)}{1 - \alpha \Sigma^{(2)}_{0\sigma}(w)}, \tag{5} \]

with

\[ \alpha = (1 - < n_{0\sigma} >)U + \epsilon_0 - \epsilon_{eff} \]

which has the virtue that it yields the appropriate atomic limit \( \Sigma^{(2)}_{0\sigma}(w) \), for \( w \sim U \) and \( \Gamma/U \to 0 \) and behaves like \( \Sigma^{(2)}_{0\sigma}(w) \) for \( U/\Gamma \to 0 \).

Let us now turn our attention to the non-equilibrium situation. For the sake of simplicity, we shall assume that in Eq. (1) \( \mu^L = -\mu^R = eV/2 \). Following our approach for the equilibrium Anderson model, we obtain the different nonequilibrium self-energies, \( \Sigma^L_{0\sigma} \) and \( \Sigma^R_{0\sigma} \), by introducing the effective levels \( \epsilon_{eff} \sigma \), \( \mu_{eff} \) and \( \mu_{eff} \) in the initial one-electron hamiltonian

\[ H_{eff}^{(transport)} = \sum_{\sigma} \epsilon_{eff}^{\sigma \sigma} n_{0\sigma} + \sum_{\nu, k, \sigma} (\epsilon_k^\nu + \mu_{eff}^\nu) n_{k\sigma}^\nu \]

\[ + \sum_{\nu, k, \sigma} T_k^\nu (\epsilon_{k\sigma}^\nu c_{0\sigma} + c_{0\sigma}^\dagger \epsilon_k^\nu). \tag{6} \]

As a natural extension of our procedure for the equilibrium case, \( \epsilon_{eff}^{\sigma \sigma}, \mu^L_{eff} \) and \( \mu^R_{eff} \) are determined by imposing self-consistency in the dot level charge and in the currents \( I_L \) and \( I_R \) defined by Eq. (3).

Eq. (6) allows us to calculate the one electron Green functions \( G^{\sigma \sigma} \) that will be used to obtain \( \Sigma^{(2)}_{0\sigma} \) and \( \Sigma^{(-2)}_{0\sigma} \) by means of a second order perturbative calculation, and finally \( \Sigma^{(2)}_{0\sigma}(w) \) and \( \Sigma^{(-2)}_{0\sigma}(w) \) by using the equivalent of Eq. (5) for the non-equilibrium case.

Let us remark that our method eliminates, in a natural way, the pathologies that arise when the perturbation is performed upon the Hartree-Fock solution. In the non-equilibrium case these pathologies are reflected in the unphysical behavior of the dot level charge as a function of \( \epsilon_0 \) (around \( \epsilon_0 \sim -U/2 \)); the currents \( I_L \) and \( I_R \) exhibit also unphysical features \[ G^{\sigma \sigma} \] including violation of current conservation \( I_L \neq I_R \). A detailed comparison of the results given by the different approaches, together with a more comprehensive discussion of our method will be presented in a future publication.

In order to illustrate the kind of results obtained by our method we have considered two different situations, with the dot level below (Fig. 2) and above (Fig. 3) the Fermi energy respectively. In the second case the dot level is almost empty at zero bias.

Figure 2 shows the current intensity, \( I \), and the differential conductance \( g = \partial I/\partial V \), as a function of the applied bias, for \( \epsilon_0 = -\pi \) and \( U = 0, \pi/2, \pi, 2\pi, \) and
4π, where all the energies hereafter are measured in units of Τ. Our results for g show a single broad peak around $V = 2\pi$ for $U = 0$; this corresponds to the dot level $\epsilon_0 = -\pi$ crossing the right reservoir chemical potential $\mu_R = -V/2$. For small $U$ ($U < |\epsilon_0|$) this one-electron like resonance is shifted and adopts a somewhat asymmetric shape. On the other hand, for large $U$ (see case $U = 4\pi$ in Fig. 2) three different features are clearly present in the current-voltage characteristic. The conductance peak at $V = 0$ is related to the Kondo resonance appearing in the dot spectral density around the Fermi energy $\frac{\pi}{h}$, while the peaks at $V = 2\pi$ and $V = 4\pi$ correspond to the crossing of the dot “ionization” and “affinity” levels, $\epsilon_0$ and $\epsilon_0 + U$, with the reservoirs chemical potentials. We should comment that these two peaks reflect the charging effects associated with the dot level: the second level can only be filled when the applied bias overcomes the repulsion between the second and the first electron. For the particular case $U = 2\pi$ we have a symmetric problem with the two dot levels crossing the left and right chemical potentials at the same bias, $V = 2\pi$, leading to a single “charging effect” peak. Notice that in this case the conductance at $V = 0$ reaches its maximum value $2e^2/h$. Finally, the case $U = \pi$ illustrates the transition between small and large $U$, with a new correlation structure arising due to the overlap between both Kondo and charging effects, the resonances merging into a broad peak around $V = 0$. This transition is also apparent in the current intensity $I(V)$ shown in Fig. 2, where the case $U = \pi$ defines the border between the highly correlated limit (Kondo and charging effects completely separated) and the one-electron like behavior.

Figure 3 shows $I(V)$ and $g$ as a function of $V$ for $\epsilon_0 = 3\pi$ and $U = 0$, $2\pi$, $4\pi$ and $6\pi$. In these cases the dot level is above the Fermi energy, and for $V = 0$ no Kondo-like peak appears in the spectral density of states. As before, the two peaks appearing in the differential conductance for $U \geq 2\pi$ are related to the filling of the ionization, $\epsilon_0$, and affinity, $\epsilon_0 + U$, levels as a function of the applied voltage. As shown in figure 3b, the voltage difference between the two peaks for $U \geq 2\pi$ is approximately equal to $2U$. On the other hand, the conductance peak at $V = 2\epsilon_0$ is reduced to nearly half its $U = 0$ value when the interaction increases. It is also worth noting that the $I-V$ curve in this case exhibit a step-like behavior which is more pronounced for increasing values of $U$. The relative height of these steps is in agreement with calculations based on a simple atomic-like model for the dot Green functions [3].

Figure 2 and 3 show the different kind of current-voltage characteristics one gets for the single dot level described by hamiltonian (1). For $U$ sufficiently large, two resonances associated with the ionization and affinity levels can always be observed in the differential conductance. In this case correlation effects are very important giving rise to an additional resonance at $V = 0$ when the ionization level is initially filled.

The results found in this paper suggest that the Kondo-like resonance and the peaks associated with the charging effects of the quantum level could be found simultaneously in a quantum dot, provided that the temperature is sufficiently below the Kondo temperature. As an example, we consider a GaAs-dot of size $L \sim 100\text{Å}$ both in the vertical and lateral directions, sandwiched between two GaAs-wires and two AlGaAs-barriers, as those studied in reference [18]. A single bound level around $50meV$ is found by solving numerically a simple double barrier model with a barrier height $\sim 300\text{meV}$. The parameter $U$ can be evaluated as the Coulomb integral for the wave function corresponding to this bound level, which roughly yields $U \sim e^2/eL \simeq 15meV$, in agreement with the dot classical capacitance energy [3]. Then, varying the AsGa-wires doping around $10^{18}/\text{cm}^3$, one could get an experimental device close to some of the theoretical cases analyzed in figures 2 and 3. In particular, for $n = 10^{18}/\text{cm}^3$ and a barrier width of $30\text{Å}$, we find $\epsilon_0/\Gamma \simeq -3$ and $U/\Gamma \simeq 8$, not far from one of the cases presented in figure 2. We should recall that finite conduction band effects are not included in our present calculation; one should always keep in mind that for $V$ sufficiently large the effect of the bottom edge of the semiconducting wires would be present in the $I-V$ characteristic.

In conclusion, we have presented an accurate solution for the many-body problem of a single dot level between two biased reservoirs. Our results show the experimental conditions one should achieve to observe in the differential conductance a peak related to the Kondo-like structure in the density of states, and a complementary structure associated with the charging effects of the dot level. By adjusting appropriately the dimensions and the doping of a quantum semiconducting dot, we have shown how the different peaks could be determined by measuring the differential conductance.

Support by Spanish CICYT (contract no. PB89-0165) is acknowledged. We also thank Dr. J. Ferrer, Prof. J.P. Hernandez and Prof. S.Y. Wu for interesting discussions.

[1] M.A. Reed, J.H. Randall, R.J. Aggarwal, R.J. Matyi, T.M. Moore, and A.E. Wetsel, Phys.Rev.Lett.60, 535 (1988); U. Meirav, M.A. Kastner, and S.J. Wind, Phys. Rev.Lett. 65, 771 (1990); B. Su, V.J. Goldman, and J.E. Cunningham, Phys.Rev.B 46, 7644 (1992).
[2] C.W.J. Beenakker, Phys.Rev.B 44, 1646 (1991); Y. Meir,N.S. Wingreen, and P.A. Lee, Phys.Rev.Lett.66, 3048 (1991)
[3] T.K. Ng and P.A. Lee, Phys.Rev.Lett 61, 1768 (1988).
[4] S. Hershfield, J.H. Davies, and J.W. Wilkins, Phys.Rev. Lett. 67, 3720 (1991); and Phys.Rev.B 46, 7046 (1992).
[5] Y. Meir, N.S. Wingreen, and P.A. Lee, Phys.Rev.Lett.70, 2601 (1993).
FIG. 1. Fulfillment of the Friedel-Langreth sum rule as a function of the dot level position using the second order self-energy as calculated: (a) starting form the Hartree-Fock solution and (b) imposing self-consistency in the dot level charge. The full line corresponds to the dot level charge $\langle n_0 \sigma \rangle$ and the dotted line corresponds to $-\frac{1}{\pi} \eta(0)$. Inset: second order diagram used to calculate the self-energies.

FIG. 2. Current $I$ and differential conductance $g$ obtained using our method for $\epsilon_0 = -\pi$ and $U = 0$ (a), $\pi/2$ (b), $\pi$ (c), $2\pi$ (d), and $4\pi$ (e). All the energies are measured in units of the elastic decay rate at the dot $\Gamma$.

FIG. 3. Same as figure 2 for $\epsilon_0 = 3\pi$ and $U = 0$ (a), $2\pi$ (b), $4\pi$ (c), and $6\pi$ (d).