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Out of equilibrium Anderson model: Conductance and Kondo temperature

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ABSTRACT

We calculate the conductance through a quantum dot weakly coupled to metallic contacts by means of the Keldysh out of equilibrium formalism. We model the quantum dot with the SU(2) Anderson model and consider the limit of infinite Coulomb repulsion. The interacting system is solved with the numerical diagrammatic Non-Crossing Approximation (NCA) and the conductance is obtained as a function of temperature and gate voltage from differential conductance (dI/dV) curves. We discuss the results in comparison with those from the linear response approach which can be performed directly in equilibrium conditions. Comparison shows that out of equilibrium results are in good agreement with the ones from linear response supporting reliability of the method employed. The last discussion becomes relevant when dealing with general transport models through interacting regions. We also analyze the evolution of conductance vs gate voltage with temperature. While at high temperatures the conductance is peaked, when the Fermi energy coincides with the localized level it presents a plateau at low temperatures as a consequence of the Kondo effect. We discuss different ways to determine Kondo's temperature.

1. Introduction

Since the first observation of the Kondo effect in semiconducting quantum dots (QD) [1] the study of transport through nanoscopic devices has inspired a rich variety of experimental and theoretical works. Nowadays, measurements of transport properties in such systems, such as current versus bias voltage and conductance, are the main focus of the experiments due to the interesting and unusual features observed [2,3].

The behavior of the conductance at different temperatures and for different gate voltages has been studied for very general systems, including those showing strong correlations. While at equilibrium almost exact numerical methods have been developed for the theoretical treatment of these problems (numerical renormalization group (NRG) [4] or exact diagonalization (ED) [5]), the ones for non-equilibrium conditions are still in progress. Among them, the Scattering Bethe Ansatz (SBA) [6] and the Time dependent Density Matrix Renormalization Group (t-DMRG) [7] are promising ones.

In this work we study the transport properties of an interacting QD using the Non-Crossing Approximation (NCA) in its non-equilibrium [8] and equilibrium [9] versions. We consider mandatory the comparison between both schemes to support reliability for the more general procedure dealing with an out of equilibrium calculation. We discuss the results for conductance as a function of bias and gate voltage, and moreover, the dependence of transport properties on temperature.

2. Model

The transport properties through a quantum dot weakly coupled to metallic contacts is studied by describing the system with the Anderson model

$$H=\sum_{k\sigma v}\epsilon_{k\sigma v}c^{\dagger}_{k\sigma v}c_{k\sigma v}+\sum_{\sigma}E_d d^{\dagger}_{\sigma}d_{\sigma}+Ud^{\dagger}_{\uparrow}d_{\uparrow}d^{\dagger}_{\downarrow}d_{\downarrow}+\sum_{kv\sigma}V_{kv\sigma}c^{\dagger}_{kv\sigma}d_{\sigma}+H.c., \quad (1)$$

where $c_{k\sigma v}(c^{\dagger}_{k\sigma v})$ is the destruction (creation) operator of an electron with momentum k, spin σ and lead $v=L$ (left) or R (right), and d_{σ} ($d^{\dagger}_{\sigma}$) destroys (creates) an electron in the quantum dot.

The non-interacting conduction electrons in the leads are treated as being in thermal and chemical equilibrium with their reservoirs, thus $\epsilon_{k\sigma v}=\epsilon_{k\sigma}-\mu_v$, allowing for different chemical potentials μ_v in each of them. For the central region, we consider a spin degenerate localized level with energy E_d and Coulomb repulsion U. The leads and the dot are connected by means of the hybridizations $V_{k\sigma v}$.

The physical quantity accessible in transport measurements is the current. As shown by Meir and Wingreen [10], the current through a system described by the Hamiltonian equation (1) is

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given by

$$I = \frac{2\pi e}{h} Tr \int d\omega (\Gamma^L f_L(\omega) - \Gamma^R f_R(\omega)) \rho_d(\omega) + \frac{2\pi e}{h} Tr \int d\omega (\Gamma^L - \Gamma^R) i G_d^<(\omega)/2\pi, \quad (2)$$

where $\Gamma^\nu = 2\pi \sum_k |V_{k\sigma\nu}|^2 \delta(\omega - \epsilon_{k\sigma\nu})$ is the hybridization function and $f_L(f_R)$ is the Fermi function for the conduction electrons of the left (right) lead. The functions $\rho_d(\omega)$ and $G_d^<(\omega)$ represent the spectral density and the lesser Green function of the central region respectively. The calculation of such Green functions must be done in the presence of the leads and it is a non-equilibrium problem which might be handled within Keldysh formalism.

From the results of different applied bias voltages, differential conductance dI/dV curves can be obtained by differentiation of Eq. (2). The value at zero bias $dI/dV|_0 = G(T)$ represents the usual equilibrium conductance at a given temperature. A simplified analytical expression for $G(T)$ can be obtained under the condition of proportional couplings, $\Gamma^L = \alpha \Gamma^R$ [8]

$$G(T) = 4\pi \frac{e^2}{h} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \Gamma(\omega) \rho_d(\omega), \quad (3)$$

where $\Gamma = \Gamma^L \Gamma^R / (\Gamma^L + \Gamma^R)$ is the effective hybridization and $\rho_d(\omega)$ is calculated in equilibrium. Thus, in contrast to Eq. (2) only equilibrium quantities enter Eq. (3).

3. Results

For the treatment of the model in and out of equilibrium, we use the diagrammatic NCA technique [8,11,12]. We consider the case of infinite repulsion, $U \to \infty$. It must be noted that different sets of self-consistent equations have to be solved in order to compute the equilibrium and non-equilibrium Green's functions. Therefore, computing the current from Eqs. (2) and (3) allows us to test the validity of the methods used.

For numerical evaluations, we consider a flat conduction band with band width $2D$ and also take $V_L = V_R = V$, $\Gamma^\nu = \pi V^2/D$. As it is clear from Eqs. (2) and (3), the main dependence of the conductance at low enough temperatures T is given by the spectral weight close to the Fermi level. It is then useful to understand the behavior of the spectral density of the QD for different conditions, specially in the Kondo regime, where an enhanced conductance is expected. In Fig. 1 we show the resulting ρ_d for different applied bias voltages. We take $\Gamma_L = 1$ as our unit and set $E_d = -4$, $D = 10$ and $T = 5 \times 10^{-5}$. We fix the Fermi level at $\epsilon_F = 0$. Note that $\epsilon_F - E_d \gg \Gamma_L$ so that the localized level is always occupied ($\langle n_\sigma \rangle \sim 1$). This corresponds to the Kondo regime, in which there is a localized spin interacting with the conduction electrons.

At zero bias there are two peaks in the spectral density. The one centered close to E_d, the charge transfer peak, is the result of a non-interacting orbital hybridizing with a conduction band. If the temperature were higher than the relevant low-energy scale of the problem, the Kondo temperature T_K, this would be the only peak in the spectral density. Since T is very low, the low-energy physics is dominated by the Kondo singlet between conduction electrons and the localized one. The localized spin leads electrons close to the Fermi level to suffer spin-flip processes giving rise to a screening effect. This is the reason for the increase of the spectral weight at ϵ_F shown in the figure, which corresponds to the Kondo peak. Its width is related with T_K. When the bias is turned on (dashed curves in Fig. 1) the Fermi level of each metallic contact is shifted. We set $\mu_L = -\mu_R = eV/2$. This energy shift produces a splitting of the Kondo resonance since conduction electrons coming from both leads contribute to the screening process. As a direct consequence, the spectral weight at the equilibrium Fermi level decreases and a lower conductance is expected. In Fig. 2, we show the differential conductance for several temperatures. Since the voltage is applied symmetrically, the current $I(V)$ is an odd function and thus the conductance $dI/dV(V)$ is an even one. dI/dV curves are Lorentzian-like with the maximum at zero bias. The value at the maximum and the width depend on temperature.

From the maximum of the curves of Fig. 2, we can build a point-by-point curve of G vs. temperature. The result is shown in Fig. 3. We show also a continuous line curve which corresponds to an equilibrium calculation of the conductance in the linear-response regime by means of Eq. (3). The dashed line curve is the empirical formula derived from the NRG calculations [13]. For high temperatures $T \gg T_K$, there is no Kondo resonance and thus the spectral weight at the Fermi level is low. There is an intermediate region where thermal fluctuations compete, and at low enough temperatures $T \ll T_K$, the Kondo effect is fully developed and conductance tends to a saturation value. However, at $T \ll T_K$, the NCA overestimates the Friedel's sum rule and therefore the conductance exceeds the unitary limit.

As it is shown in Fig. 3, there is an excellent agreement between the results from the non-equilibrium calculation and the equilibrium ones. Moreover, there is also a great correspondence with the results from NRG. We stress that the calculation of the linear response conductance implies only equilibrium quantities while the out of equilibrium solving procedure is more

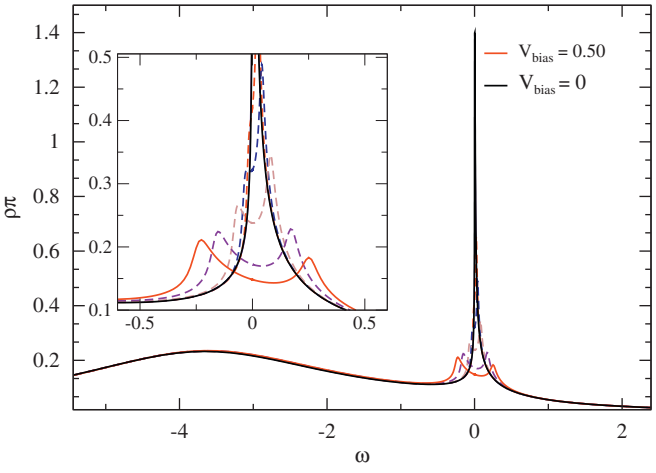

Fig. 1. QD spectral density for different applied bias voltages.

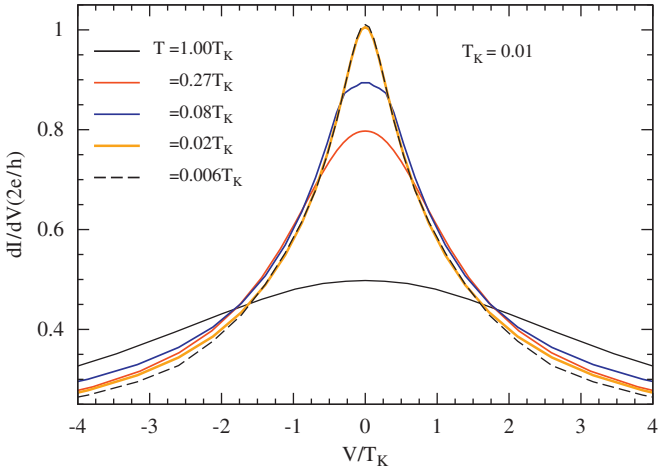

Fig. 2. dI/dV vs. V for different temperatures.

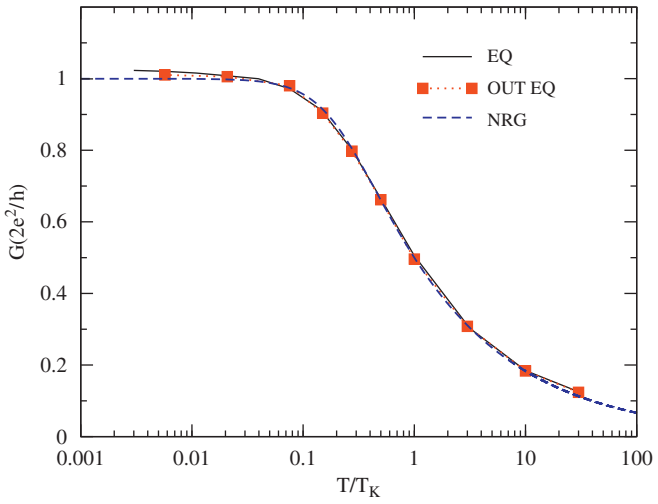

Fig. 3. Conductance as a function of temperature obtained from lineal response formalism (continuous curve) and differential conductance curves evaluated at zero bias (dots) and NRG predictions.

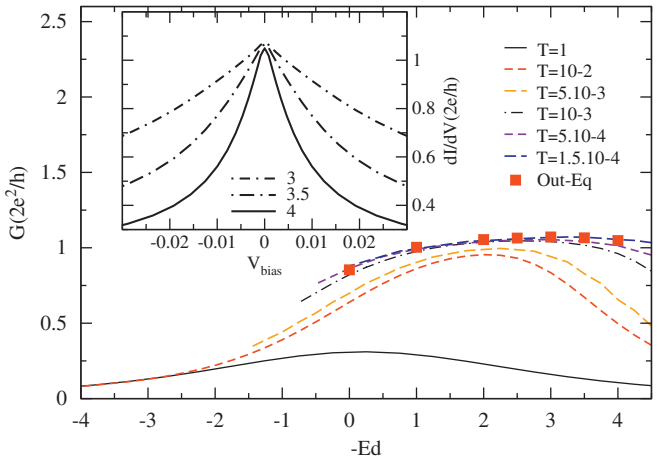

Fig. 4. Conductance as a function of gate voltage V_g for different temperatures obtained from lineal response formalism (continuous curve) and from differential conductance curves evaluated at zero bias (red dots). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

complex and deals with lesser and greater Green functions. Since the first of these approaches is valid just under the condition of proportional couplings, the agreement we find is a useful check that supports reliability to the most general procedure based on the calculation of the current by means of Eq. (2).

We turn now the discussion to the conductance as a function of gate voltage V_g. The energy of the localized level of the QD is proportional to this voltage $eV_g = -E_d$ and it is thus possible to perform a transistor-type experiment by the control of this parameter. In Fig. 4, we present the NCA results for different temperatures. The understanding of this outcome is directly connected to our previous analysis of the spectral density. For high temperatures (black continuous line in the figure) the conductance shows just a symmetric peak centered at $V_g=0$. This corresponds to the localized level placed at the Fermi energy, the optimum condition for the conduction electrons to pass from the left to the right metallic contact. For temperatures lower than T_K (dashed curves in the figure) the behavior is completely different. As soon as the energy of the localized level is below the Fermi energy, the Kondo effect develops and the spectral density shows not only the charge transfer peak but also the Kondo resonance. This is the reason for the plateau in the conductance as a function of gate voltage. Our results qualitatively agree with those obtained previously with NRG [14]. As it is shown in Fig. 4, at finite temperature the conductance starts to decay at some V_g. This feature has to do with the fact that $T_K \sim \exp\{E_d\}$. Since the temperature is finite, T turns larger than $T_K(E_d)$ at some point, destroying the Kondo effect and the plateau. It must be noticed that for $T < T_K$, the NCA results are not reliable within the empty orbital regime, $E_d \geq 0$, due to the appearance of a spike with non-physical spectral weight at the Fermi energy.

For $T = 1.5 \times 10^{-4}$ we show (with dots) in Fig. 4 the conductance values obtained by the procedure stated previously from the out of equilibrium calculations. In the inset of the figure we show differential conductance curves for several values of V_g's. We observe that the maximum of the conductance remains the same while the curves get narrower for greater values of the gate voltage. This is a direct indication of the variation of T_K with V_g.

There are three different ways to define the characteristic energy scale, T_K, from the physical magnitudes addressed in this work: at equilibrium it can be obtained from the half-width at half of the maximum (HWHM) of the spectral density for $T \to 0$ (T_K^{ρ}). Out of equilibrium it follows from the HWHM of the differential conductance curves, $T_K^{dI/dV}$. Using the equilibrium conductance, T_K^G can be defined as the temperature for which that $G(T) = G(0)/2$. From our results, $T_K^G = 8.2 \times 10^{-3}$, $T_K^{\rho} = 9.1 \times 10^{-3} = 1.11 T_K^G$ and $T_K^{dI/dV} = 12.1 \times 10^{-3} = 1.48 T_K^G$. As expected, the three values are of the same order of magnitude.

4. Conclusions

We study the transport through an interacting quantum dot described with the Anderson model. We use the NCA to calculate the conductance as a function of bias, gate voltage, and temperature. We find a good agreement between the results coming from non-equilibrium calculations and those from the linear response regime, which implies only equilibrium quantities. The results for conductance versus temperature also agree with those from the NRG calculations. The conductance as a function of gate voltage shows the formation of a plateau for low enough temperatures within the Kondo regime in agreement with previous results. At finite temperature, the conductance decays for a given gate voltage destroying the plateau. We finally discuss several procedures, in and out of equilibrium, which allow the determination of the Kondo temperature scale. We find that the values obtained are of the same order of magnitude and provide numerical relations among them. While the conductance at equilibrium of the used model is known from NRG calculations, we show that NCA is able to provide reliable results at a lower computational cost in and out of equilibrium, for which few alternative techniques exist. Moreover, the NRG can miss features in the spectral density which are not near to the Fermi energy [15,16], this turned out recently to be important to explain a plateau observed in the $G(T)$ of C_{60} QDs [2] on the triplet side of a quantum phase transition, using the NCA [16].

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