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Alternative equation of motion approach applied to transport through a quantum dot

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HIGHLIGHTS

- We study non-equilibrium electron transport through a quantum dot coupled to metallic leads.
- Equation of motion approach in which Green functions is differentiated over both time variables is used.
- We obtain the resonance Kondo state in the particle–hole symmetric case and in the asymmetric cases.
- We calculate the density of the states of quantum dot and the differential conductance as a function of bias voltage.

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ABSTRACT

We study non-equilibrium electron transport through a quantum dot coupled to metallic leads. We use an alternative equation of motion approach in which we calculate the retarded Green function of the impurity by differentiating Green functions over both time variables. Such an approach allows us to obtain the resonance Kondo state in the particle–hole symmetric case and in the asymmetric cases. We apply this technique for calculating the density of the states of quantum dot and the differential conductance as a function of bias voltage. The differential conductance dependence on temperature and on Coulomb interaction is also calculated.

1. Introduction

Electronic transport through quantum dots (QD) or single electron transistors (SET) has recently been widely investigated on both the experimental [1–5] and theoretical sides [6–12]. It has a large potential of applications in modern electronics (spintronic) based on nanoscopic structures. Quantum dot systems are excellent systems for studying the Kondo effect. They possess a resonance peak at the Fermi energy in the dot density of states and a zero-bias maximum in differential conductance.

In theoretical analysis the structure of a single quantum dot connected with two leads is well described by the single impurity Anderson model (SIAM) [13]. This model has an exact solution in the case of the noninteracting system ($U = 0$). At finite values of Coulomb interaction U there is no such solution and there are only approximate results. The SIAM model was solved approximately by different numerical techniques (e.g. quantum Monte Carlo [14], numerical renormalization group [14–16]) and analytical techniques (e.g. second-order perturbation theory, modified perturbation theory [9,12], noncrossing approximation). To solve the SIAM problem one can also use the equation of motion (EOM) technique [6,7,10,11,17]. This technique relies on finding the retarded Green function of the impurity, and requires the decoupling scheme breaking the infinite set of Green function equations.

One of the broadly used EOM techniques [6,7,10,11,17] is the decoupling scheme proposed by Lacroix [18]. This scheme was based on the Heisenberg equations of motion with differentiation over one time variable. There was a truncation in the chain of equations at the second order in hybridization term. In the original Lacroix work [18] there was an additional approximation of infinite Coulomb interaction ($U = \infty$). This approach allowed the narrow peak localized on the Fermi level to be obtained, but its width and height were too small resulting in an underestimation of the Kondo temperature [19]. The Lacroix scheme was used for quantum dots with infinite and finite Coulomb interaction. The weak point of this approach, when used at finite U, is the wrong result in the particle–hole symmetric case where Kondo peak vanishes. In effect, the unitary limit for the linear conductance is not reached [20]. Current flow in the symmetric case is small

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which disagrees with the experimental results showing a large conductance [2]. Away from the symmetric case, where the Kondo peak is small, the original EOM method does not fulfill the Fermi liquid relations and in the result linear conductance has very small values. In our report we develop an alternative EOM approach in which we calculate the retarded Green function of the impurity by differentiating Green functions over both time variables. This differs from the commonly used EOM solution by Lacroix [18] where the time derivative was taken only over primary time variable. Our approach allows us to obtain good results in the EOM method not only in the particle–hole symmetric case but also in the asymmetric cases.

The proposed method will be used for systems in the equilibrium state, as well as for systems with the finite bias voltage V applied between the leads coupled to the QD. At the finite bias voltage we calculate the electric current flowing through the dot and the differential conductance dI/dV dependence on temperature for different energy levels of the quantum dot and different Coulomb repulsions. This quantity is observed experimentally. In the particle–hole symmetric case due to the Kondo effect the differential conductance reaches unitary limit [20]. Initial experiments with quantum dots did not support this result. The unitary limit of Kondo effect was demonstrated after using semiconducting quantum dots [1].

The paper is organized as follows: in Section 2 we develop our approach to analyze the single impurity Anderson model. Using a modified EOM approach we obtain expressions for the self-energy and Green function in the presence of Coulomb repulsion. In Section 3 we present numerical results based on our approach. From the calculated dot Green function we obtain the density of states on the quantum dot and the differential conductance dI/dV as a function of the bias voltage. Dependence of the differential conductance dI/dV on temperature and on Coulomb interaction is also analyzed. It is shown that the increase of temperature reduces the value of the differential conductance dI/dV. At zero temperature and in the particle–hole symmetric case we obtain a unitary limit for conductance. Our results are compared with the experiment and previous calculations. Final conclusions are given in Section 4.

2. The model

Using the Anderson-type Hamiltonian we analyze the system that is build out of quantum dot connected to two metallic leads. The Hamiltonian of this model has the form

$$H = \sum_{\sigma} \varepsilon_d \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{\substack{k\sigma \\ \alpha=L,R}} (\varepsilon_{k\alpha} - \mu_\alpha)\hat{n}_{k\alpha\sigma} + \sum_{\substack{k\sigma \\ \alpha=L,R}} \left(V_{k\alpha} d_\sigma^+ c_{k\alpha\sigma} + h.c.\right) \tag{1}$$

where $d_\sigma^+ (d_\sigma)$ are the creation (annihilation) operators for the dot electron with spin σ, $c_{k\alpha\sigma}^+ (c_{k\alpha\sigma})$ are the creation (annihilation) operators for the conduction lead electron, $\alpha = L, R$ correspond to the left and right leads, $\varepsilon_{k\alpha}$ is the energy dispersion of α lead, μ_α is the chemical potential of α lead, ε_d is the dot energy, U is the on-site Coulomb interaction between electrons on the dot, and $V_{k\alpha}$ is the coupling between the α lead and the dot.

In our analysis we will use the Green functions method and the equation of motion technique. In the case of non-equilibrium situation the retarded, advanced, and the distribution Green functions have to be calculated. The EOM for Green functions was usually obtained by differentiation over primary time (t). For the retarded GF we have

$$i\frac{\partial}{\partial t}\langle\langle A(t); B(t')\rangle\rangle^r = \delta(t'-t)\langle[A(t), B(t')]_+\rangle + \langle\langle[A(t), H]_-; B(t')\rangle\rangle^r \tag{2}$$

and for the distribution Green function we have

$$i\frac{\partial}{\partial t}\langle\langle A(t); B(t')\rangle\rangle^< = \langle\langle[A(t), H]_-; B(t')\rangle\rangle^< \tag{3}$$

After Fourier transform these expressions become the following equations:

$$\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon^r = \langle[A, B]_+\rangle + \langle\langle[A, H]_-; B\rangle\rangle_\varepsilon^r \tag{4}$$

and

$$\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon^< = \langle\langle[A, H]_-; B\rangle\rangle_\varepsilon^< \tag{5}$$

which are the commonly used equations of motion form (see e.g. [6,7,10,11,17,18]). The deficiency of this approach is the lack of the Kondo resonance on the Fermi energy and unfulfilling the unitary limit for conductance [20] in the particle–hole symmetry case. Out of the particle–hole symmetric case we obtain a narrow Kondo resonance peak, whose height and width are small [19] resulting in an underestimation of Kondo temperature. To solve this problem the authors [19,21] used equations of motion at higher orders for hopping integral. Roermund and co-workers [21] applying the fourth order equation obtained the Kondo resonance no longer vanishing in the particle–hole symmetric case but the unitary limit was still not fulfilled.

In this paper we will use the alternative EOM approach based on the Heisenberg equation which includes differentiating over the second time (t'), resulting in EOM of the following form [22]:

$$-\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon^r = -\langle[A, B]_+\rangle + \langle\langle A; [B, H]_-\rangle\rangle_\varepsilon^r \tag{6}$$

and

$$-\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon^< = \langle\langle A; [B, H]_-\rangle\rangle_\varepsilon^< \tag{7}$$

Applying Eqs. (4) and (5) to the noninteracting case one can obtain the exact expression for self-energy. After including Coulomb interaction on the dot there is no exact solution for the self-energy and one has to construct an appropriate approximate solution. Frequently used Ng approximation [23] allows us to replace the distribution Green function by the retarded Green function.

Further on we will use the notation for the Green functions: $G_{d\sigma}(\varepsilon) = \langle\langle d_\sigma; d_\sigma^+\rangle\rangle_\varepsilon^r$. Using in Eq. (4) the Hamiltonian (1) and following the method of Kuzemsky [22], (Górski and Mizia [24]), we obtain:

$$[g_{d\sigma}(\varepsilon)]^{-1} G_{d\sigma}(\varepsilon) = 1 + U\langle\langle(\hat{n}_{d-\sigma} - n_{d-\sigma})d_\sigma; d_\sigma^+\rangle\rangle_\varepsilon^r \tag{8}$$

where

$$[g_{d\sigma}(\varepsilon)]^{-1} = \varepsilon - \varepsilon_d - Un_{d-\sigma} - i\Delta(\varepsilon) + i\eta \tag{9}$$

with η being a positive infinitesimal real number and $\Delta(\varepsilon)$ the hybridization coupling defined as

$$\Delta(\varepsilon) = \Delta_L(\varepsilon) + \Delta_R(\varepsilon) = \sum_{\substack{k \\ \alpha=L,R}} \frac{V_{k\alpha}^2}{\varepsilon - \varepsilon_{k\alpha}} \tag{10}$$

In further analysis we will assume that the hybridization coupling is the same for each electrode ($\Delta_L(\varepsilon) = \Delta_R(\varepsilon)$) and that it is energy independent. The asymmetric coupling with electrodes was analyzed by Krawiec and Wysokiński [11]. In addition we will assume that the hybridization coupling is the unit of energy, $\Delta(\varepsilon) = \text{const} \equiv 1$.

To solve Eq. (8) we have to write the EOM for a higher order Green function $\langle\langle(\hat{n}_{d-\sigma} - n_{d-\sigma})d_\sigma; d_\sigma^+\rangle\rangle_\varepsilon^r$. For this function we use