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Irreducible Green's functions method for a quantum dot coupled to metallic and superconducting leads

Grzegorz Górski*, Krzysztof Kucab

Faculty of Mathematics and Natural Sciences, University of Rzeszów, ul. Pigonia 1, 35-310 Rzeszów, Poland

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ABSTRACT

Using irreducible Green's functions (IGF) method we analyse the Coulomb interaction dependence of the spectral functions and the transport properties of a quantum dot coupled to isotropic superconductor and metallic leads (SC-QD-N). The irreducible Green's functions method is the modification of classical equation of motion technique. The IGF scheme is based on differentiation of double-time Green's functions, both over the primary and secondary times. The IGF method allows to obtain the spectral functions for equilibrium and non-equilibrium impurity Anderson model used for SC-QD-N system. By the numerical computations, we show the change of spectral and the anomalous densities under the influence of the Coulomb interactions. The observed sign change of the anomalous spectral density can be used as the criterion of the SC singlet-Kondo singlet transition.

1. Introduction

The Kondo effect in nanoscopic structures (quantum dots based on semiconductors, carbon nanotubes, nanowires) is actually widely studied both theoretically and experimentally. One of the interesting systems is a quantum dot coupled to one superconducting electrode and one metallic electrode (SC-QD-N). This system is intensively studied experimentally [1–5], and theoretically [6–15]. The connection of the superconducting electrode to a quantum dot through proximity effect induces electron pairing in quantum dot and it causes that the ground state of a quantum dot is the superconducting singlet state. The characteristic feature of the QD-SC connection is the appearance of subgap excitations in the quantum dot spectrum, so-called Andreev or Yu-Shiba-Rusinov bound states. These states play a crucial role in the transport properties of mesoscopic superconducting devices, especially in the subgap regime ($|\varepsilon| < \Delta$).

The strong Coulomb repulsion, between opposite spin electrons, opposes double occupancy of the quantum dot and prefers the doublet ground state. In SC-QD-N heterojunction the Kondo-type correlations have to compete with the proximity induced electron pairing. As a result of this competition, the system exhibits a quantum phase transition between the doublet and the singlet states [8,9,11,16]. The transition between the doublet and the singlet states is determined by different energy scales: the Coulomb interaction (U), the superconducting gap (Δ) and the coupling to the superconducting lead (Γ_S). In the large superconducting gap limit and strong coupling Γ_S, the singlet state is superconducting-like. For a weak coupling Γ_S and strong values of U, the dominant state is the Kondo singlet state [9]. The transition between these two states can be determined experimentally by means of transport spectroscopy. The measurements of the subgap differential conductance give the evidence for the Andreev bound states. Zero bias anomalies mark the quantum phase transition between the doublet and singlet state.

The properties of SC-QD-N systems have been studied using various theoretical approaches: Hartree-Fock theory (HF) [3,17], numerical renormalization group (NRG) [11,13,18], iterative perturbation technique (IPT) [8,9], equation of motion (EOM) [19,20] and noncrossing approximation (NCA) [21]. All of these methods have some restrictions. To describe the systems where Coulomb correlations are not very important one can use the Hartree-Fock theory; e.g. Lee and co-workers [3] used this approximation to describe the influence of external magnetic field on the value of the differential conductance dI/dV. The Coulomb correlations can be described by the use of the NRG, IPT and EOM approaches. The NRG method can be used only for equilibrium state, but IPT and EOM approaches can be used to study the local Coulomb interaction effect on the non-equilibrium transport properties.

In this work we use the irreducible Green's functions (IGF) technique [22] to describe the properties of SC-QD-N system. This technique involves the use of modified equation of motion scheme for the double-time temperature Green's functions. This scheme permits us to construct the relevant dynamic solutions in a self-consistent way,

* Corresponding author.
E-mail address: ggorski@ur.edu.pl (G. Górski).

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without decoupling the chain of equations of motion. This technique was used in many issues of solid-state physics, e.g. itinerant antiferromagnetism [23], itinerant [24] and Heisenberg [25] ferromagnetism, superconductivity in disordered transition metal alloys [26]. We also used this technique to describe the quantum dot coupled to two metallic leads (N-QD-N) [27]. The obtained results show that IGF-EOM method gives the results for density of states and the differential conductance comparable to the numerical methods results (NRG) both for the particle-hole symmetric case and also for the asymmetric cases. In this work, to describe a quantum dot coupled to one superconducting electrode and one metallic electrode (SC-QD-N) we will use the IGF-EOM method. In Section 2 we analyse the single impurity Anderson model using the IGF-EOM approach. In this approach, we can describe the SC-QD-N system. We also compute the expressions for the self-energy and the Green's function in the presence of the Coulomb repulsion. In Section 3 we present numerical results for the spectral density and the Andreev transmittance. We analyse the influence of the Coulomb interaction U on the spectral density and the Andreev transmittance. Additionally we study the influence of parameter Γ_N, which characterizes the coupling between the quantum dot and the normal lead, on the spectral density. The results of non-equilibrium transport are also shown in Section 3. Final conclusions are given in Section 4.

2. The model

Using the Anderson-type Hamiltonian we analyse the system which is built out of the quantum dot connected to one metallic lead and one superconducting lead. The Hamiltonian of this model has the following form

$$H = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma\alpha} (\varepsilon_{\mathbf{k}\alpha} - \mu_\alpha) n_{\mathbf{k}\alpha\sigma} + \sum_{k\sigma\alpha} (V_{\mathbf{k}\alpha} d_\sigma^+ c_{\mathbf{k}\alpha\sigma} + h.\,c.) - \Delta \sum_{\mathbf{k}} (c_{\mathbf{k}S\uparrow}^+ c_{-\mathbf{k}S\downarrow}^+ + c_{-\mathbf{k}S\downarrow} c_{\mathbf{k}S\uparrow}), \tag{1}$$

where $d_\sigma^+(d_\sigma)$ are creation (annihilation) operators for the dot electron with spin σ, $c_{\mathbf{k}\alpha\sigma}^+(c_{\mathbf{k}\alpha\sigma})$, $\alpha = N, S$ are creation (annihilation) operators for the electron in the normal (N) and superconducting (S) lead, $\varepsilon_{\mathbf{k}\alpha}$ 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 $V_{\mathbf{k}\alpha}$ is the coupling between the α lead and the dot.

We are looking for expressions for the matrix Green's function in the Nambu space defined as

$$\hat{\mathbf{G}}_d(t, t') = \begin{bmatrix} \langle\langle d_\uparrow(t); d_\uparrow^+(t')\rangle\rangle & \langle\langle d_\uparrow(t); d_\downarrow(t')\rangle\rangle \\ \langle\langle d_\downarrow^+(t); d_\uparrow^+(t')\rangle\rangle & \langle\langle d_\downarrow^+(t); d_\downarrow(t')\rangle\rangle \end{bmatrix}. \tag{2}$$

In our analysis, we will use the Green's function method and the equation of motion (EOM) technique. In general, the EOM for Green's functions is obtained by differentiation with respect to primary time (t). After taking the Fourier transform, we obtain the following equation

$$\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon = \langle [A, B]_+\rangle + \langle\langle [A, H]_-; B\rangle\rangle_\varepsilon. \tag{3}$$

Applying Eq. (3) to the Hamiltonian (1) we obtain the relation (see Appendix A)

$$\hat{\mathbf{g}}_d{}^{-1}\hat{\mathbf{G}}_d = \hat{\mathbf{I}} + U\hat{\boldsymbol{\tau}}_3\hat{\boldsymbol{\Gamma}}_d^{(1)}, \tag{4}$$

where

$$\hat{\mathbf{g}}_d{}^{-1} = \begin{bmatrix} \varepsilon - \varepsilon_d - \Sigma_{d11}^0 & -\Sigma_{d12}^0 \\ -\Sigma_{d21}^0 & \varepsilon + \varepsilon_d - \Sigma_{d22}^0 \end{bmatrix} \tag{5}$$

with self-energies $\hat{\boldsymbol{\Sigma}}_d^0$ given by Eq. (A.8). These self-energies come from the coupling between dot and the normal or superconducting lead. The two-particle, higher order Green's functions $\hat{\boldsymbol{\Gamma}}_d^{(1)}$ are given by

$$\hat{\boldsymbol{\Gamma}}_d^{(1)} = \begin{bmatrix} \langle\langle \hat{n}_{d\downarrow} d_\uparrow; d_\uparrow^+\rangle\rangle_\varepsilon & \langle\langle \hat{n}_{d\downarrow} d_\uparrow; d_\downarrow\rangle\rangle_\varepsilon \\ \langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; d_\uparrow^+\rangle\rangle_\varepsilon & \langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; d_\downarrow\rangle\rangle_\varepsilon \end{bmatrix}. \tag{6}$$

For the $\hat{\boldsymbol{\Gamma}}_d^{(1)}$ we will apply the technique of irreducible Green's functions [22,26]. These functions are defined as

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

where the z constant is given by $z = \langle [[A, H]_-; B]_\pm\rangle / \langle [A; B]_\pm\rangle$ and it represents the self-energy in the Hartree-Fock-Bogoliubov approximation. Using the irreducible Green's function technique we can express Eq. (6) as the sum of irreducible function and the mean-field solution. As a result the last part of Eq. (4) can be written as

$$U\hat{\boldsymbol{\tau}}_3\hat{\boldsymbol{\Gamma}}_d^{(1)} = U\hat{\boldsymbol{\tau}}_3{}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)} + \hat{\boldsymbol{\Sigma}}_U^{HF}\hat{\mathbf{G}}_d, \tag{8}$$

where the interaction part of self-energy, $\hat{\boldsymbol{\Sigma}}_U^{HF}$, is given by

$$\hat{\boldsymbol{\Sigma}}_U^{HF} = \begin{bmatrix} U\langle n_{d\downarrow}\rangle & U\langle d_\downarrow d_\uparrow\rangle \\ U\langle d_\uparrow^+ d_\downarrow^+\rangle & -U\langle n_{d\uparrow}\rangle \end{bmatrix}. \tag{9}$$

Inserting Eqs. (8), (A.5) and (A.8) into Eq. (4) we obtain the following relations

$$\hat{\mathbf{g}}_d^{HF-1}\hat{\mathbf{G}}_d = \hat{\mathbf{I}} + U\hat{\boldsymbol{\tau}}_3{}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}, \tag{10}$$

where $\hat{\mathbf{g}}_d^{HF-1} = \hat{\mathbf{g}}_d^{-1} - \hat{\boldsymbol{\Sigma}}_U^{HF}$. Neglecting the irreducible function ${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}$ in Eq. (10) we obtain the well-known Hartree-Fock-Bogoliubov approximation which is widely applied to the systems with quantum dot, for which the Coulomb correlations are less important (e.g. for metallic dots, see [15,28]). Because we are interested in the influence of the Coulomb correlations on the transport properties, we have to calculate the irreducible function ${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}$.

In the previous papers where the classic EOM approach in the SIAM model was used (e.g. [29–31]), the higher order Green's functions $\hat{\boldsymbol{\Gamma}}_d^{(1)}$ was calculated by reusing of Eq. (3). Such approach allows to obtain Abrikosov-Suhl resonance outside the particle-hole symmetric system. For $n_d = 1$ the Abrikosov-Suhl peak disappears. The classic EOM approach does not fulfil the unitary limit for conductance in the particle–hole symmetry case. Out of the particle–hole symmetric case one obtain a narrow Abrikosov-Suhl resonance peak, whose height and width are small, resulting in an underestimation of Kondo temperature.

In order to correct this defect of the classic EOM approach, by calculating the ${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}$ function we will use the extended equation of motion approach based on differentiating Green's function over the second time variable (t'). In the energy representation this leads to the equation [22]

$$-\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon = -\langle [A, B]_+\rangle + \langle\langle A; [B, H]_-\rangle\rangle_\varepsilon. \tag{11}$$

Using this equation we obtain the following relation for the irreducible Green's function

$$-\varepsilon\,{}^{ir}\langle\langle A; B\rangle\rangle_\varepsilon = {}^{ir}\langle\langle A; [B, H]_-\rangle\rangle_\varepsilon, \tag{12}$$

which gives the following expression for the ${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}$ function

$${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(1)}\hat{\mathbf{g}}_d^{0-1} = \sum_{\mathbf{k}\sigma\alpha} {}^{ir}\hat{\boldsymbol{\Gamma}}_{d\mathbf{k}\alpha}^{(1)}\hat{\mathbf{V}}_{\mathbf{k}\alpha}^*\hat{\boldsymbol{\tau}}_3 + U\,{}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(2)}\hat{\boldsymbol{\tau}}_3, \tag{13}$$

where

$${}^{ir}\hat{\boldsymbol{\Gamma}}_{d\mathbf{k}\alpha}^{(1)} = \begin{bmatrix} {}^{ir}\langle\langle \hat{n}_{d\downarrow} d_\uparrow; c_{\mathbf{k}\alpha\uparrow}^+\rangle\rangle_\varepsilon & {}^{ir}\langle\langle \hat{n}_{d\downarrow} d_\uparrow; c_{\mathbf{k}\alpha\downarrow}\rangle\rangle_\varepsilon \\ {}^{ir}\langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; c_{\mathbf{k}\alpha\uparrow}^+\rangle\rangle_\varepsilon & {}^{ir}\langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; c_{\mathbf{k}\alpha\downarrow}\rangle\rangle_\varepsilon \end{bmatrix} \tag{14}$$

and

$${}^{ir}\hat{\boldsymbol{\Gamma}}_d^{(2)} = \begin{bmatrix} {}^{ir}\langle\langle \hat{n}_{d\downarrow} d_\uparrow; n_{d\downarrow} d_\uparrow^+\rangle\rangle_\varepsilon & {}^{ir}\langle\langle \hat{n}_{d\downarrow} d_\uparrow; \hat{n}_{d\uparrow} d_\downarrow\rangle\rangle_\varepsilon \\ {}^{ir}\langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; n_{d\downarrow} d_\uparrow^+\rangle\rangle_\varepsilon & {}^{ir}\langle\langle \hat{n}_{d\uparrow} d_\downarrow^+; \hat{n}_{d\uparrow} d_\downarrow\rangle\rangle_\varepsilon \end{bmatrix}. \tag{15}$$