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Electronic Transport through Quantum Dot Above and Below Kondo Temperature using Equation of Motion Method

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Abstract We study theoretically the Kondo effect in the quantum dot within the whole range of temperature including the Kondo temperature T_K by using the equation of motion method based on the non-equilibrium Green function techniques. We have taken account of the finite Coulomb correlation and the non-equilibrium effect by calculating the correlation terms emerged from the decoupling approximation using the equation of motion method for the lesser Green function. Our results are the generalization into the pseudo-equilibrium state of the results of reference [5] and can be used to describe a non-equilibrium state under the bias voltage that is not so large.

Key words non-equilibrium Green function, equation of motion method, Kondo temperature

Introduction

The Kondo effect [1] in electronic transport through quantum dot (QD) strongly coupled to metallic leads was predicted theoretically and also observed experimentally.

The Kondo effect is a typical instance to demonstrate an importance of the many-body effect in QD.

One of the techniques used in the non-equilibrium situations is the non-equilibrium Green function (NGF) techniques [2]. To calculate density of state (DOS) and electric current one needs both retarded and lesser Green functions. The former one is usually calculated by the equation of motion (EOM) method in the framework of some decoupling approximation schemes.

The most commonly used approximation [2] describes the situation rather well for temperatures close to the Kondo temperature T_K as well as above T_K. However, it is not correct for much smaller temperatures $T << T_K$. In this regime, the approximation developed by ref. [3] is more appropriate.

The decoupling approximation [2] was applied to most of literatures [4－7] used EOM, and therefore very low temperature region $T << T_K$ could not be considered.

On the other hand, the Kondo effect in the whole range of temperature including T_K was studied [5] by using the approach developed [3], however, they [5] considered only the equilibrium state and calculated the correlation functions using fluctuation-dissipation theorem that is valid for the equilibrium state.

In this paper, we investigate theoretically the Kondo effect in QD with finite Coulomb correlation in the whole range of temperature including the Kondo temperature T_K by using EOM method based on NGF techniques.

1. Theoretical Formalism

1.1. Model

We consider a single-level QD coupled to metallic leads by tunneling barriers. In this case, the Hamiltonian of whole system can be described as follows:

$$H = \sum_{k\beta\sigma} \varepsilon_{k\beta\sigma} c^{+}_{k\beta\sigma} c_{k\beta\sigma} + \sum_{\sigma} \varepsilon_{\sigma} d^{+}_{\sigma} d_{\sigma} + U d^{+}_{\uparrow} d_{\uparrow} d^{+}_{\downarrow} d_{\downarrow} + \sum_{k\beta\sigma} T_{k\beta\sigma} c^{+}_{k\beta\sigma} d_{\sigma} + \text{H.C.} \tag{1}$$

where $\varepsilon_{k\beta\sigma}$ is the single-electron energy in the β^{th} $(\beta = L/R)$ lead for the wave vector k and electron spin σ, $c^{+}_{k\beta\sigma}$ and $c_{k\beta\sigma}$ denote the corresponding creation and annihilation operators. ε_{σ} denotes the energy of the discrete dot level, d^{+}_{σ} and d_{σ} are the corresponding creation and annihilation operators, U denotes Coulomb correlation parameter. $T_{k\beta\sigma}$ are the components of the tunneling matrix and describe coupling between QD and β^{th} leads.

The electric current I flowing from the left to right electrodes can be written in form

$$I = \frac{ie}{2\hbar}\int \frac{dE}{2\pi} Tr\left\{[\boldsymbol{\Gamma}^{L}(E) - \boldsymbol{\Gamma}^{R}(E)]\boldsymbol{G}^{<}(E) + [f_L(E)\boldsymbol{\Gamma}^{L}(E) - f_R(E)\boldsymbol{\Gamma}^{R}(E)][\boldsymbol{G}^{r}(E) - \boldsymbol{G}^{a}(E)]\right\} \tag{2}$$

where $\boldsymbol{G}^{\eta}(E)$ $(\eta = r,\ a,\ <)$ are the Fourier transforms $G^{\eta}_{\sigma\sigma}(E) \equiv \langle\langle d_{\sigma};\, d^{+}_{\sigma}\rangle\rangle^{\eta}_{E}$ of the non-equilibrium retarded, advanced and lesser Green functions of QD, $f_{\beta}(E)$ is the Fermi distribution function in the β^{th} lead, and $\boldsymbol{\Gamma}^{\beta}(E)$ describes a contribution to the half-width of the dot level due to tunneling through the β^{th} barrier and takes the form $\boldsymbol{\Gamma}^{\beta}_{\sigma}(E) = 2\pi\sum_{k} V_{k\beta\sigma} V^{*}_{k\beta\sigma} \delta(E - \varepsilon_{k\beta\sigma})$.

In this paper we assume that $\boldsymbol{\Gamma}^{\beta}_{\sigma}(E)$ is constant within the electron band, $\boldsymbol{\Gamma}^{\beta}_{\sigma}(E) = \boldsymbol{\Gamma}^{\beta}_{\sigma} = \text{const}$ for $-D \le E \le D$ and $\boldsymbol{\Gamma}^{\beta}_{\sigma}(E) = 0$ otherwise, where D denotes the electron bandwidth of the metallic electrode.

1.2. Equation of motion method

The EOM for the QD Green function $G^{r}_{\sigma\sigma}(E)$ can be written in form

$$[E - \varepsilon_{\sigma} - \Sigma^{r}_{0\sigma}(E)]G^{r}_{\sigma\sigma}(E) = 1 + UG^{(2)r}_{\sigma\sigma}(E)\,, \tag{3}$$

where $G^{(2)r}_{\sigma\sigma}(E) \equiv \langle\langle d_{\sigma} n_{\bar{\sigma}};\, d^{+}_{\sigma}\rangle\rangle^{\eta}_{E}$ is the second-order QD Green function, $\Sigma^{r}_{0\sigma}(E)$ is the self-energy in the absence of Coulomb interactions and describes the coupling to the electrodes, are defined as

$$\Sigma^{r}_{0\sigma}(E) = \sum_{\beta = L,R} \Gamma^{\beta}_{\sigma}\left(P\int \frac{d\varepsilon}{2\pi}\frac{1}{E - \varepsilon} - \frac{i}{2}\right). \tag{4}$$

Equation (3) for the QD Green function $G^{r}_{\sigma\sigma}(E)$ contains the second-order QD Green function $G^{(2)r}_{\sigma\sigma}(E)$. Appling the EOM method to $G^{(2)r}_{\sigma\sigma}(E)$, second-order electrode-QD Green functions come out. The consecutive application of the EOM method to these Green functions lead to the higher-order Green functions. Therefore, we adopt the following decoupling approximation [3] to establish a closed set of equations.

$$\langle c_{k\beta\sigma_1}^{+} d_{\sigma} \rangle \approx 0$$
$$\langle c_{k\beta\sigma_1} c_{q\alpha\sigma_2} \rangle \approx 0$$
$$\langle\langle c_{k\beta\sigma_1} d_{\sigma_2}^{+} c_{q\alpha\sigma_3} ; d_{\sigma}^{+} \rangle\rangle_E \approx \delta_{\sigma_1\sigma_2} \langle c_{k\beta\sigma_1} d_{\sigma_2}^{+} \rangle \langle\langle c_{q\alpha\sigma_3} ; d_{\sigma}^{+} \rangle\rangle_E + \delta_{\sigma_2\sigma_3} \langle d_{\sigma_2}^{+} c_{q\alpha\sigma_3} \rangle \langle\langle c_{k\beta\sigma_1} ; d_{\sigma}^{+} \rangle\rangle_E$$
$$\langle\langle c_{k\beta\sigma_1} c_{q\alpha\sigma_2}^{+} d_{\sigma_3} ; d_{\sigma}^{+} \rangle\rangle_E \approx \delta_{\sigma_1\sigma_2} \langle c_{k\beta\sigma_1} c_{q\alpha\sigma_2}^{+} \rangle \langle\langle d_{\sigma_3} ; d_{\sigma}^{+} \rangle\rangle_E + \delta_{\sigma_2\sigma_3} \langle c_{q\alpha\sigma_2}^{+} d_{\sigma_3} \rangle \langle\langle c_{k\beta\sigma_1} ; d_{\sigma}^{+} \rangle\rangle_E \tag{5}$$

In fact, in the low temperature, such as $T << T_K$, the lead-lead correlation terms like $\langle c_{k\beta\sigma} c_{q\alpha\sigma}^{+} \rangle$ have appeared logarithm.

The application of this approximation leads to the EOM for $G_{\sigma\sigma}^{(2)r}(E)$:

$$(E - \varepsilon_{\sigma} - U - \Sigma_{03\sigma}^{r}) G_{\sigma\sigma}^{(2)r} = \langle n_{\overline{\sigma}} \rangle - (\widetilde{P}_{\sigma} - \widetilde{\widetilde{P}}_{\sigma}) - [\Sigma_{1\sigma}^{r} + \Sigma_{0\sigma}^{r} (\widetilde{P}_{\sigma} - \widetilde{\widetilde{P}}_{\sigma}) + (\widetilde{Q}_{\sigma} - \widetilde{\widetilde{Q}}_{\sigma})] G_{\sigma\sigma}^{r} \tag{6}$$

where

$$\begin{aligned}
\widetilde{P}_{\sigma}(E) &= i \int \frac{d\varepsilon}{2\pi} \frac{1}{E + \varepsilon - \varepsilon_{\sigma} - \varepsilon_{\overline{\sigma}} - U + i\hbar/\tau_{\overline{\sigma}}} F_{\overline{\sigma}}(\varepsilon) \cdot \\
&\quad \cdot \left[G_{\overline{\sigma}\overline{\sigma}}^{r}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{r}(\varepsilon) + \widetilde{\Sigma}_{3\sigma}^{r}(E)) - G_{\overline{\sigma}\overline{\sigma}}^{a}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{a}(\varepsilon) + \widetilde{\Sigma}_{3\sigma}^{r}(E)) \right] \\
\widetilde{\widetilde{P}}_{\sigma}(E) &= i \int \frac{d\varepsilon}{2\pi} \frac{1}{E - \varepsilon - \varepsilon_{\sigma} + \varepsilon_{\overline{\sigma}} + i\hbar/\tau_{\overline{\sigma}}} F_{\overline{\sigma}}(\varepsilon) \cdot \\
&\quad [G_{\overline{\sigma}\overline{\sigma}}^{r}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{r}(\varepsilon) - \widetilde{\widetilde{\Sigma}}_{3\sigma}^{r}(E)) - G_{\overline{\sigma}\overline{\sigma}}^{a}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{a}(\varepsilon) - \widetilde{\widetilde{\Sigma}}_{3\sigma}^{r}(E))] \\
\widetilde{Q}_{\sigma}(E) &= i \int \frac{d\varepsilon}{2\pi} \frac{1}{E + \varepsilon - \varepsilon_{\sigma} - \varepsilon_{\overline{\sigma}} - U + i\hbar/\tau_{\overline{\sigma}}} F_{\overline{\sigma}}(\varepsilon) \cdot \\
&\quad \cdot \left[G_{\overline{\sigma}\overline{\sigma}}^{r}(\varepsilon) \Sigma_{0\overline{\sigma}}^{r}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{r}(\varepsilon) + \widetilde{\Sigma}_{3\sigma}^{r}(E)) - G_{\overline{\sigma}\overline{\sigma}}^{a}(\varepsilon) \Sigma_{0\overline{\sigma}}^{a}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{a}(\varepsilon) + \widetilde{\Sigma}_{3\sigma}^{r}(E)) \right] \\
\widetilde{\widetilde{Q}}_{\sigma}(E) &= i \int \frac{d\varepsilon}{2\pi} \frac{1}{E - \varepsilon - \varepsilon_{\sigma} + \varepsilon_{\overline{\sigma}} + i\hbar/\tau_{\overline{\sigma}}} F_{\overline{\sigma}}(\varepsilon) \cdot \\
&\quad \cdot \left[G_{\overline{\sigma}\overline{\sigma}}^{r}(\varepsilon) \Sigma_{0\overline{\sigma}}^{r}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{r}(\varepsilon) - \widetilde{\widetilde{\Sigma}}_{3\sigma}^{r}(E)) - G_{\overline{\sigma}\overline{\sigma}}^{a}(\varepsilon) \Sigma_{0\overline{\sigma}}^{a}(\varepsilon) (\Sigma_{0\overline{\sigma}}^{a}(\varepsilon) - \widetilde{\widetilde{\Sigma}}_{3\sigma}^{r}(E)) \right]
\end{aligned} \tag{7}$$

$$\begin{aligned}
\widetilde{\Sigma}_{i\sigma}^{r}(E) &= \sum_{\beta} \int \frac{d\varepsilon}{2\pi} \Gamma_{\overline{\sigma}}^{\beta} A_{\beta}^{(i)}(\varepsilon) \frac{1}{E + \varepsilon - \varepsilon_{\sigma} - \varepsilon_{\overline{\sigma}} - U + i\hbar/\tau_{\overline{\sigma}}} \\
\widetilde{\widetilde{\Sigma}}_{i\sigma}^{r}(E) &= \sum_{\beta} \int \frac{d\varepsilon}{2\pi} \Gamma_{\overline{\sigma}}^{\beta} A_{\beta}^{(i)}(\varepsilon) \frac{1}{E - \varepsilon - \varepsilon_{\sigma} + \varepsilon_{\overline{\sigma}} + i\hbar/\tau_{\overline{\sigma}}}
\end{aligned} \tag{8}$$

$$\Sigma_{i\sigma}^{r}(E) = \widetilde{\Sigma}_{i\sigma}^{r}(E) + \widetilde{\widetilde{\Sigma}}_{i\sigma}^{r}(E) \tag{9}$$

where $i = 1, 3$, $A_{\beta}^{(1)}(\varepsilon) = f_{\beta}(\varepsilon)$ and $A_{\beta}^{(3)}(\varepsilon) = 1$. $F_{\sigma}(\varepsilon)$ denotes pseudo-equilibrium distribution function and is defined as

$$F_{\sigma}(\varepsilon) = \frac{\Gamma_{\sigma}^{L} f_L(\varepsilon) + \Gamma_{\sigma}^{R} f_R(\varepsilon)}{\Gamma_{\sigma}^{L} + \Gamma_{\sigma}^{R}} \tag{10}$$

In [5] equilibrium distribution function $f(\varepsilon)$ instead of the pseudo-equilibrium one appears, because they used the fluctuation-dissipation theorem that is valid for the equilibrium state in order to calculate the correlation terms $\langle A^{+}B \rangle$. We derive equation (6) unlike ref. 5. First, we remember that the correlation terms $\langle A^{+}B \rangle$ is related to the lesser Green functions $\langle\langle B; A^{+} \rangle\rangle_E^{<}$ with

$$\langle A^+B\rangle = -i\int\frac{dE}{2\pi}\langle\langle B;\, A^+\rangle\rangle_E^< \tag{11}$$

Next we adopt the EOM method for lesser Green functions $\langle\langle B;\, A^+\rangle\rangle_E^<$, and then the emerging term $G_{\sigma\sigma}^<(E)$ from that is derived as

$$G_{\sigma\sigma}^<(E) = -F_\sigma(\varepsilon)[G_{\sigma\sigma}^r(E) - G_{\sigma\sigma}^a(E)] \tag{12}$$

by using the Ng *ansatz* [6]. We regard that equation(12) would be the generalization of the fluctuation-dissipation theorem for the pseudo-equilibrium formalism.

Equation (3) and (6) form the closed set of equations and from those QD retarded Green function $G_{\sigma\sigma}^r(E)$ is given by

$$G_{\sigma\sigma}^r = \frac{E-\varepsilon_\sigma - \Sigma_{03\sigma}^r - U[1-\langle n_{\bar\sigma}\rangle + (\tilde{P}_\sigma - \tilde{\tilde{P}}_\sigma)]}{(E-\varepsilon_\sigma-\Sigma_{0\sigma}^r)(E-\varepsilon_\sigma - U - \Sigma_{03\sigma}^r) + U[\Sigma_{1\sigma}^r + \Sigma_{0\sigma}^r(\tilde{P}_\sigma - \tilde{\tilde{P}}_\sigma) + (\tilde{Q}_\sigma - \tilde{\tilde{Q}}_\sigma)]} \tag{13}$$

The DOS for electrons in QD is defined by

$$\mathrm{DOS}_\sigma(E) = -\frac{1}{\pi}\mathrm{Im}\, G_{\sigma\sigma}^r(E) \tag{14}$$

and the expression (2) is written as follows using the Ng *ansatz* [6].

$$I_\sigma = \frac{ie}{\hbar}\int\frac{dE}{2\pi}\frac{\Gamma_\sigma^L\Gamma_\sigma^R}{\Gamma_\sigma^L + \Gamma_\sigma^R}(G_{\sigma\sigma}^r - G_{\sigma\sigma}^a)[f_L(E) - f_R(E)]. \tag{15}$$

Equation (13) for the retarded Green function contains the mean occupation number of electron in QD, $\langle n_{\bar\sigma}\rangle$. This is given as follows:

$$\langle n_{\bar\sigma}\rangle = -i\int\frac{dE}{2\pi}G_{\sigma\sigma}^<(E) \tag{16}$$

2. Numerical Results

2.1. State density

Fig. 1 shows the height of the Kondo peak (value of DOS at the Fermi level) vs. temperature T/T_K .

As shown in Fig. 1, the approximation [2] is valid only for the high-temperature regime $T >> T_K$, but gives rise to the distorted result in the low-temperature regime $T << T_K$.

When the temperature decreases, there appears the Kondo peak in DOS near the Fermi level. The height of the peak increases with decreasing temperature. Furthermore, the height of the Kondo peak in the very low temperature $T << T_K$ approaches to the maximum 1.

This value reaches exactly to 1 at $T = 0$. The result agrees with NRG [9] and NCA [10] results.

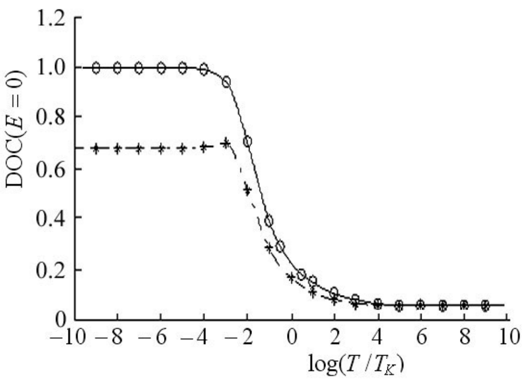

Fig. 1. The height of the Kondo peak vs. temperature
The solid and dashed lines are the result using the approximation [3] and [2] respectively.
$\varepsilon_0 = -0.6$, $U = 4$, $\Gamma_L = \Gamma_R = 0.1$, $D = 2$

2.2. Zero-bias conductance

Fig. 2 shows the zero-bias conductance vs. temperature T/T_K. The conductance follows the universal behavior in a fairly large range of temperatures. We point out that at very low-temperature $T/T_K << 1$ the universal curve has the expected Fermi-liquid behavior, while at higher temperature $T/T_K \approx 1$ the conductance is proportional to $\ln(T/T_K)$.

The dependence curve of the conductance on temperature is in agreement with results of NRG [11], non-crossing approximation method (NCA) [7] and non-equilibrium renormalized perturbation theory (NRPT) [8].

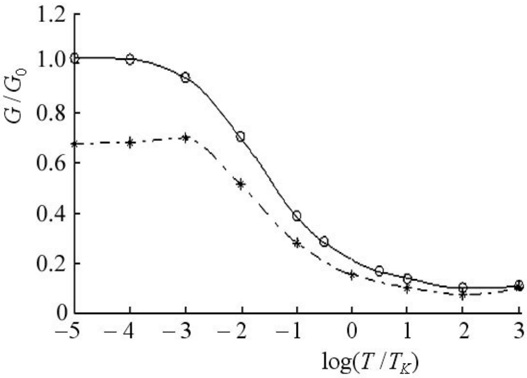

Fig. 2. The zero-bias conductance vs. temperature The solid and dashed lines are the result using the approximation [3] and [2] respectively.
$\varepsilon_0 = -0.6$, $U = 4$, $\Gamma_L = \Gamma_R = 0.1$, $D = 2$

Conclusion

In this paper, we study theoretically the non-equilibrium Kondo effect in the quantum dot within the whole range of temperature including the Kondo temperature by using the equation of motion method based on the non-equilibrium Green function techniques. We have taken account of the finite Coulomb correlation and the non-equilibrium effect by calculating the correlation terms emerged from the decoupling approximation using the equation of motion method for the lesser Green function. The numerical results are very good agreement with the results of numerical renormalization group (NRG), non-crossing approximation method (NCA) and non-equilibrium renormalized perturbation theory (NRPT), etc.[7, 8].

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