Numerical Renormalization-Group Study of Particle-Hole Symmetry Breaking in Two-Channel Kondo Problem : Effect of Repulsion between Conduction Electrons and Potential Scattering

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Particle-hole symmetry breaking perturbation in two-channel pseudospin Kondo problem is studied by the numerical renormalization-group method. It is shown that the repulsion between conduction electrons at the impurity site and the single particle potential are the relevant perturbations against the conventional non-Fermi liquid fixed point. Although the repulsion (potential) with realistic strength prevents the overscreening of pseudospin, it induces in turn a real spin, which is also overscreened again. Thus the real spin susceptibility becomes anomalous contrary to the conventional two-channel Kondo problem.

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Multichannel Kondo problem has attracted much attentions in these years because of its anomalous non-Fermi liquid behavior. While the problem was originally discussed long ago as a generalized Kondo effect of magnetic impurity with orbital degeneracy, the two-channel Kondo problem has recently been revived in a proposal of quadrupolar Kondo effect as an origin of U-based heavy fermions. The two-level system interacting with conduction electrons was also recognized as a candidate for realization of two-channel Kondo model. The latter system has attracted much interest not only because it offers a model explaining anomalous transport properties of glassy metals but also it is expected to give a canonical model of strong coupling electron-phonon systems.

Although the two-channel Kondo problem has been fully solved by a variety of methods, there seems still to remain for us to clarify a reality of the model itself. As for relation with experiments, the pseudospin two-channel Kondo model gives anomalous behavior the self. As for relation with experiments, the pseudospin still to remain for us to clarify a reality of the model it-

We begin with the model Hamiltonian for the Wilson NRG calculation as follows:

\[ \frac{H_N}{D} = \Lambda^{(N-1)/2} \left\{ \sum_{m\sigma} \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n (f_{n,m\sigma}^\dagger f_{n+1,m\sigma} + \text{h.c.}) + H_{\text{int}} \right\}, \]  

(1)

where

\[ H_{\text{int}} = J \sum_{m\sigma\sigma'} f_{0,m\sigma}^\dagger \sigma \sigma' f_{0,m\sigma} \tau + V \sum_{m\sigma} f_{0,m\sigma}^\dagger f_{0,m\sigma} \]

\[ + \frac{U}{2} \sum_{mm'\sigma\sigma'} f_{0,m\sigma}^\dagger f_{0,m\sigma} f_{0,m'\sigma'}^\dagger f_{0,m'\sigma'}, \]

(2)

where the indices \( m \) and \( \sigma \) denote a label indicating channel 1, 2 and pseudospin \( \uparrow \), \( \downarrow \), respectively, \( \sigma \) is the Pauli matrix vector, and \( \tau \) is twice the operator of the impurity pseudospin of 1/2. The pseudospin stands for the charge polarization at the impurity site and two channels for two components of “real” spin of conduction electron. Here we have defined

\[ D \equiv \frac{1 + \Lambda^{-1}}{2} \tilde{D}, \quad J \equiv \frac{1}{1 + \Lambda^{-1}} \tilde{J}, \]

\[ U \equiv \frac{8}{1 + \Lambda^{-1}} \tilde{U}, \quad V \equiv \frac{4}{1 + \Lambda^{-1}} \tilde{V}, \]

(3)

where \( 2\tilde{D} \) denotes the bandwidth of conduction electrons, \( \tilde{J} \) the exchange interaction between conduction electrons.
and impurity pseudospin, $\tilde{V}$ the potential at impurity site, and $\tilde{U}$ the repulsion between conduction electrons at impurity site [20]. Hereafter we set $D = 1$, i.e., the energy levels are scaled by $D$ and ignore $\Lambda$-dependence in $\xi_n$, i.e., $\xi_n = 1$, because $\xi_n \rightarrow 1$ for large $n$.

The conserved quantities of the Hamiltonian $H_N$, (4), are the total number of conduction electrons $Q$, the real spin $j$ and the total pseudospin $S$, defined as follows:

\begin{equation}
Q_N = \sum_{m} \sum_{n=0}^{N} \sum_{\sigma} (f_{n,m,\sigma}^\dagger f_{n,m,\sigma} - 1/2),
\end{equation}

\begin{equation}
J_N = \frac{1}{2} \sum_{\sigma} \sum_{n,m'} f_{n,m',\sigma}^\dagger \sigma_{m'} f_{n,m,\sigma} \equiv \sum_{\sigma} \tilde{j}_N^\sigma, \tag{5}
\end{equation}

\begin{equation}
S_N = \frac{1}{2} \sum_{\sigma} \sum_{n,m} f_{n,m,\sigma}^\dagger \sigma_{m} f_{n,m,\sigma} + \tau \equiv \sum_{m} \tilde{s}_N^m + t. \tag{6}
\end{equation}

Since both the repulsion $U$ and the potential $V$ breaks the particle-hole symmetry unless $3U/2 + V = 0$, the degenerate eigenstates denoted by $\pm Q$ are split in general. In our calculations, we have used $\Lambda = 3$ and retained low lying energy states up to 300 states at each step as bases for constructing new quadruple states.

First we have investigated the case $U = V = 0$ and verified that the same energy levels as the work of Pang and Cox [10] are reproduced. Next we have investigated the case $U \neq 0$. The flow diagram of level of low lying states for $J = 2.0$ and $U = 1.6$ is shown in Fig. 1. The solid (dotted) lines are for even (odd) iterations. Each level is labelled by $(Q, j, S)$. The ground state of the fixed point is pseudospin doublet $(S = 1/2)$, which is expected for the case where the exchange coupling is stronger than the repulsion. In Fig. 2 the flow diagram for $J = 1.0$ and $U = 2.0$ is shown. The ground state is now pseudospin singlet $(S = 0)$, because the repulsion $U$, larger than exchange coupling $J$ and the hopping $D = 1$, prohibit the overscreening. It is noted that the ground state is still degenerate due to degrees of freedom of channel, i.e., $j = 1/2$. It is remarked that the position of energy levels at the fixed point in Fig. 1 and Fig. 2 exactly coincide with each other while the nature of ground state is different. As discussed later, the quantum numbers specifying each levels in Fig. 1 are in a certain relation with those in Fig. 2.

The nature of ground states for various coupling constants $J$, $U$ and $V = 0$ are shown in Fig. 3. The closed circles stand for the ground state with $S = 0$, while the open circles $S = 1/2$. The line dividing two types of ground state is drawn by estimating the coupling constants which give the same energies of these two types of ground state. It is noted that the boundary line flatten as $J \rightarrow 0$ and has a constant slope for $J_{\geq 1}$. We can understand this result as follows. The energy gains for overscreening formation at the impurity $(n = 0)$ site are both due to the exchange energy $J$ and the kinetic energy associated with the transfer $D$ between 0- and 1-site, while the energy loss arises through the repulsion $U$ between overscreened conduction electrons. On the other hand, for singlet formation, the energy gain is due to avoiding the repulsion $U$ while the energy loss is due to the exchange coupling $J$ and the kinetic energy $D$. Consequently, the boundary line is roughly determined by the condition $U \sim \max(J, D)$. Namely, for $\tilde{U} > \tilde{J}/8$ and $\tilde{D}/4$, the ground state becomes a pseudospin singlet. It is noted that the ground state is expected to belong to that of $S = 0$ for a realistic value of $U$ and $\tilde{J}$.

Now we discuss about properties of the fixed point. The fixed point Hamiltonian $H^*$ is described as

\begin{equation}
H^* = \sum_{n=0}^{\infty} \frac{\Lambda - n/2}{n} (f_{n}^\dagger f_{n} + h.c.) + H_{\text{int}}^*,
\end{equation}

\begin{equation}
H_{\text{int}}^* = 4J^* (s_1^0 + s_2^0) \cdot t + \alpha^* (s_1^0 + s_2^0)^2 + \beta^* (j_1^0 + j_2^0)^2 + V^* Q_0 + \epsilon, \tag{7}
\end{equation}

where $H_{\text{int}}^*$ has the same symmetry as $H_{\text{local}}$ in (1), the effective couplings $J^*$, $\alpha^*$, $\beta^*$, and $V^*$ may depend on the initial couplings in general, and $\epsilon$ is a constant energy shift. If we set $J^* = J$, $\alpha^* = \beta^* = -U$, $V^* = 3U/2 + V$, and $\epsilon = 3U + 2V$, $H_{\text{int}}^*$ becomes equivalent to $H_{\text{local}}$ in (1).

Since the energy of low lying excited states at the fixed point are mainly determined by $H_{\text{int}}^*$, we can determine the parameters $J^* \sim \epsilon$ in (7) so as to reproduce the low lying energy levels at $N = 39$. The results for the initial parameters, $(J, U, V)$, (a) $(0.5, 0.0, 0.0)$, (b) $(2.0, 1.6, 0.0)$, (c) $(1.0, 2.0, 0.0)$ and (d) $(0.2, 0.4, -0.6)$ are shown in Table 1. It is noted that the effective exchange coupling, $J^*$ is independent of the initial coupling $U$ (including $U = 0$), and $\alpha^*$ and $\beta^*$ are always zero. In the case (d), there is the particle-hole symmetry so that the fixed point is the same as the case (a) where $U = V = 0$. The character of the fixed point is determined mainly by the effective impurity potential $V^*$ which depends on the initial couplings $J$, $U$ and $V$, i.e. $V^* = f(J, U, V)$. Consequently, the effective interaction at the fixed point can be written as

\begin{equation}
H_{\text{int}} = J^* (s_1^0 + s_2^0) \cdot t + V^* Q_0, \quad (J^* = 0.20). \tag{8}
\end{equation}

$J$, $U$-dependence of $V^*$ with $V = 0$ is shown in Fig. 4. It is noted that $V^*$ increases (decreases) as $U$ ($J$) increases. From this effective interaction, the “flow lines” for scaling in parameter space are obtained from $f(J, U, V = 0) = \text{constant}$. Especially, for $V^* = J^* = 0.20$, the “flow line” becomes equivalent to the boundary line shown in Fig. 3. because the first excitation energy is zero for these couplings.

In order to investigate $\omega$ and $T$ dependence of susceptibility, let $(Q, j, S)$ be $(Q_D, j_D, S_D)$ for $V^* = V_D^* < 0.20$,
where the ground state is pseudospin doublet ($S = 1/2$), and $(Q_S,j_S,S_S)$ for $V^* = V_S^* > 0.20$ where the ground state is pseudospin singlet ($S = 0$). For each low lying excited states, we can find the relations, $Q_S = -Q_D - 1$, $j_S = S_D$, and $S_S = j_D$. If we set $V_S^* = 2J^* - V_D^*$, the low lying excited energies at the fixed point for each parameters are the same as easily seen by means of the effective interaction $\tilde{U}$. A prime example is the relation between Fig. 1 and Fig. 2 as mentioned above. According to this coincidence, the coincidence of energy levels occurs after 20 iterations. From this coincidence, it is expected that $\omega$ and $T(\omega/D,T/D < \Lambda^{-20/2})$ dependence of the susceptibility of real spin (channel) for $V_D^*$ coincide with those of the pseudospin for $V_S^* = 2J^* - V_D^*$ and vice versa. This is a new aspect of two-channel Kondo problem which has not been recognized so long as the conventional model without the repulsion and the potential scattering ($U = V = 0$) had been investigated.

This remarkable aspect can be seen more vividly by investigating the spectral weight of the dynamical susceptibilities for real spin of conduction electrons at the impurity site, $\chi''_j(\omega)$, and for the impurity pseudospin, $\chi''_{j'}(\omega)$. They are calculated by the method of ref. [1] as shown in Figs. 1 and 2. It is noted that, in the presence of the repulsion $U$, $\chi''_j(\omega)$ shows the non-Fermi liquid behavior with $\lim_{\omega \rightarrow 0} \chi''_j(\omega)$ being finite, while without the repulsion it shows Fermi liquid one with $\chi''_j(0) = 0$. However, if we set $3U/2 + V = 0$, the similar calculations show that $\chi''_j(0) = 0$. Namely, it is the particle-hole symmetry breaking that gives $\chi''_j(\omega)$’s the non-Fermi liquid behaviors. The potential $V^*$ shifts the number of conduction electrons at the impurity site from one in each channel, though the exchange works to hold the overscreening formation. This competition induces the degrees of freedom of channel (i.e., real spin). It is also overscreened again by conduction electrons with two channels, i.e., pseudospin degrees of freedom. Thus the real spin susceptibility becomes anomalous due to the potential $V^*$ which breaks the particle-hole symmetry. The case $V^* < 0$ is understood as $V^* > 0$ by particle-hole transformation. Since the degrees of freedom of pseudospin, however, are not perfectly vanished, pseudospin susceptibility is anomalous for any strength of the repulsion including $U = 0$.

In summary, the low lying excited states at the fixed point of pseudospin two-channel Kondo model with the particle-hole symmetry breaking perturbations are described not only by the exchange $J^*$ but also the impurity potential $V^*$. For $|V^*| > 0.20$, i.e., $U > J/8$ and $D/4$, realistic values, a pseudospin singlet ground state is realized in contrast with the pseudospin doublet ground state which is realized in the conventional two-channel Kondo problem. The spectral weight of the dynamical susceptibility of the real spin shows the non-Fermi liquid behavior because of the overscreening of the real spin. Thus, it is expected that the magnetic non-Fermi liquid behaviors observed in some compounds are understood by the particle-hole symmetry breaking perturbation, which induces the degrees of freedom of the real spin.

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an isotropic one by renormalization-evolution as will be
discussed elsewhere; so that we confine ourselves to
discussing the case of isotropic repulsive interaction in (2).

FIG. 1. The flow diagram for $J = 2.0, U = 1.6$ and $V = 0$. Each level is labelled by $(Q, j, S)$, where $Q$, $j$, and $S$ are the total number of electrons, the real spin, and the total pseudospin, respectively. The solid (dotted) lines are for even (odd) iterations. The ground state is a pseudospin doublet.

FIG. 2. The flow diagram for $J = 1.0, U = 2.0$ and $V = 0$. The ground state is a pseudospin singlet. The degeneracy of the ground state is due to degrees of freedom of channel, i.e., $j = 1/2$.

FIG. 3. The nature of ground states for various sets of coupling constants of $J$, $U$ and $V = 0$ in the unit $D$. The open circles are for the ground state with pseudospin doublet $S = 1/2$, while the closed circles the ground state with pseudospin singlet $S = 0$. The line dividing two phases of, $S = 0$ and $S = 1/2$, is drawn by inspection.

FIG. 4. $J$, $U$-dependence of the effective impurity potential, $V^*$, with $V = 0$ at the fixed point.

FIG. 5. $\omega$ dependence of imaginary part of local real spin susceptibility $\chi''_j(\omega)$.

FIG. 6. $\omega$ dependence of imaginary part of impurity pseudospin susceptibility $\chi''_{t}(\omega)$.

| $(J,U,V)$  | $J^*$ | $\alpha^*$ | $\beta^*$ | $V^*$ | $\epsilon$ |
|------------|-------|------------|-----------|-------|-----------|
| (a) (0.5,0,0,0,0) | 0.20  | 0          | 0         | 0     | 0.80      |
| (b) (2.0,1.6,0,0) | 0.20  | 0          | 0         | 0.12  | 0.80      |
| (c) (1.0,2.0,0,0) | 0.20  | 0          | 0         | 0.28  | 0.88      |
| (d) (0.2,0.4,-0.6) | 0.20  | 0          | 0         | 0     | 0.80      |

TABLE I. Effective couplings, $J^* \sim \epsilon$, which make a reproduction of the energy levels at $N = 39$ for the initial parameters, $(J,U,V)$, (a) (0.5,0,0,0,0), (b) (2.0,1.6,0,0), (c) (1.0,2.0,0,0), and (d) (0.2,0.4,-0.6).