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

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Particle-hole symmetry breaking perturbation in the two-channel pseudospin Kondo problem is studied by the numerical renormalization-group method. It is shown that the repulsion among conduction electrons at the impurity site and the single particle potential are relevant perturbations against the conventional non-Fermi-liquid fixed point. Although the repulsion (potential) with realistic strength prevents the overscreening of the 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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The multichannel Kondo problem has attracted much attention recently because of its anomalous non-Fermi-liquid behavior. While the problem was originally discussed long ago as a generalized Kondo effect with orbital degeneracy [1], the two-channel Kondo problem has been revived in a proposal of a quadrupolar Kondo effect as an origin of U-based heavy fermions [2]. The two-level system interacting with conduction electrons was also recognized as a candidate for realization of the two-channel Kondo model [3]. The latter system has attracted much interest not only because it offers a model explaining the anomalous transport properties of glassy metals [4,5] but also because it is expected to give a canonical model of strong coupling electron-phonon systems [6–8].

Although the two-channel Kondo problem has been fully solved by a variety of methods [9–15], it seems still to remain for us to clarify the reality of the model itself [16]. In the magnetic two-channel Kondo model, proposed quite recently for Ce^{3+} [17], it is a straightforward conclusion that the magnetic susceptibility shows non-Fermi-liquid behavior. In the pseudospin two-channel Kondo model, where primarily the susceptibility of the pseudospin (i.e., that of charge polarization) shows anomalous behavior, it is not clear whether or not the real spin susceptibility exhibits non-Fermi-liquid behavior. However, it is suggested that the system $Th_{1-x}U_xRu_2Si_2$, which shows a c-axis logarithmically divergent magnetic susceptibility, can be explained by the quadrupolar Kondo effect in tetragonal symmetry [16,18]. However, it might make sense to investigate the possibility that such magnetic anomalies are related to the appearance of localized real spins in a more general sense. For instance, a repulsion between conduction electrons at the impurity site, which was neglected in the above pseudospin models [19], is expected to prevent overscreening [20] and to induce a real spin.

The purpose of this paper is to examine the effect of such a repulsion on the two-channel Kondo model by the numerical renormalization-group (NRG) method [21,22]. It is shown that the fixed point Hamiltonian is described not only by the conventional exchange coupling J^* but also by an impurity potential V^*, to which the repulsive interaction $\tilde{U}$ is renormalized; namely, the single particle potential $\tilde{V}$ is also a relevant perturbation. The competition between the exchange coupling and the repulsion or the impurity potential induces the degrees of freedom of channels (i.e., real spin) and leads to the pseudospin singlet ground state for realistic strengths of $\tilde{U}$ or $\tilde{V}$. It is the particle-hole symmetry breaking that causes such competition. The overscreening of the induced real spin again makes the real spin susceptibility anomalous, contrary to the conventional pseudospin two-channel Kondo problem without $\tilde{U}$ and $\tilde{V}$.

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

$$\frac{H_N}{D} = \Lambda^{(N-1)/2}\left\{\sum_{m\sigma}\sum_{n=0}^{N-1}\Lambda^{-n/2}\xi_n(f^\dagger_{n,m\sigma}f_{n+1,m\sigma} + \text{H.c.}) + H_{\text{int}}\right\}, \tag{1}$$

where

$$H_{\text{int}} = J\sum_{m\sigma\sigma'} f^\dagger_{0,m\sigma'}\boldsymbol{\sigma}_{\sigma'\sigma}f_{0,m\sigma}\cdot\boldsymbol{\tau} + V\sum_{m\sigma} f^\dagger_{0,m\sigma}f_{0,m\sigma} + \frac{U}{2}\sum_{mm'\sigma\sigma'}^{m\sigma\neq m'\sigma'} f^\dagger_{0,m\sigma}f_{0,m\sigma}f^\dagger_{m'\sigma'}f_{0,m'\sigma'}, \tag{2}$$

where the indices m and σ denote a label indicating channel and pseudospin, respectively, $\boldsymbol{\sigma}$ is the Pauli matrix vector, and $\boldsymbol{\tau}$ is that for the impurity pseudospin. Our exchange Hamiltonian (2) is written in terms of the local pseudospin degrees of freedom. In the case of the quadrupolar Kondo effect, for instance, these are local quadrupolar degrees of

freedom, while the magnetic index of the conduction electrons serves as a channel index. Here we have defined

$$D \equiv \frac{1 + \Lambda^{-1}}{2}\tilde{D}, \qquad J \equiv \frac{1}{1 + \Lambda^{-1}}\tilde{J},$$

$$U \equiv \frac{8}{1 + \Lambda^{-1}}\tilde{U}, \qquad V \equiv \frac{4}{1 + \Lambda^{-1}}\tilde{V}, \qquad (3)$$

where $2\tilde{D}$ denotes the bandwidth of conduction electrons, $\tilde{J}$ the exchange interaction between conduction electrons and the impurity pseudospin, $\tilde{V}$ the potential at the impurity site, and $\tilde{U}$ the repulsion among the conduction electrons at the impurity site [23]. Hereafter we set $D = 1$; i.e., the energy levels are scaled by D and ignore Λ dependence in ξ_n, i.e., $\xi_n = 1$, because $\xi_n \to 1$ for large n.

The conserved quantities of the Hamiltonian H_N, (1), are the total number of conduction electrons Q, the real spin j, and the total pseudospin S, defined as follows:

$$Q_N = \sum_m \sum_{n=0}^{N} \sum_\sigma (f^\dagger_{n,m\sigma} f_{n,m\sigma} - 1/2), \qquad (4)$$

$$\mathbf{j}_N = \frac{1}{2} \sum_\sigma \sum_{n=0}^{N} \sum_{mm'} f^\dagger_{n,m'\sigma} \boldsymbol{\sigma}_{m'm} f_{n,m\sigma} \equiv \sum_\sigma \mathbf{j}^N_\sigma, \qquad (5)$$

$$\mathbf{S}_N = \frac{1}{2}\left[\sum_m \sum_{n=0}^{N} \sum_{\sigma\sigma'} f^\dagger_{n,m\sigma'} \boldsymbol{\sigma}_{\sigma'\sigma} f_{n,m\sigma} + \boldsymbol{\tau}\right]$$

$$\equiv \sum_m \mathbf{s}^N_m + \mathbf{t}. \qquad (6)$$

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

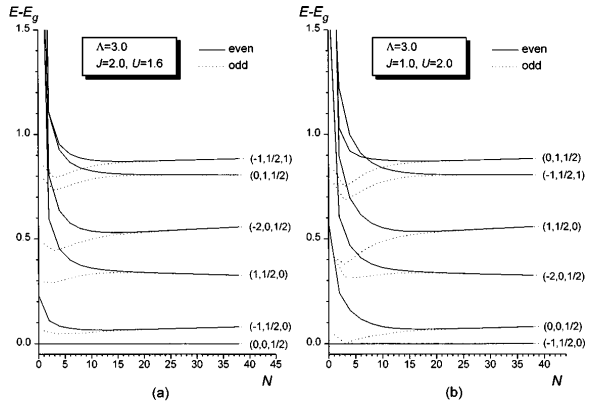

FIG. 1. The flow diagram for (a) $J = 2.0$, $U = 1.6$, $V = 0$ and (b) $J = 1.0$, $U = 2.0$, $V = 0$.

The nature of ground states for various coupling constants J, U, and $V = 0$ are shown in Fig. 2. The closed circles stand for the ground state with $S = 0$ and while the open circles with $S = 1/2$. The line dividing the two types of ground states is drawn by estimating the coupling constants which give the same energies of these two types of ground states. It is noted that the boundary line flattens as $J \to 0$ and has a constant slope for $J \gtrsim 1$. We can understand this result as follows. The energy gains for overscreening formation at the impurity ($n = 0$) site are due to both the exchange energy J and the kinetic energy associated with the transfer D between the 0 and 1 sites, while the energy loss arises through the repulsion U between overscreened conduction electrons. 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

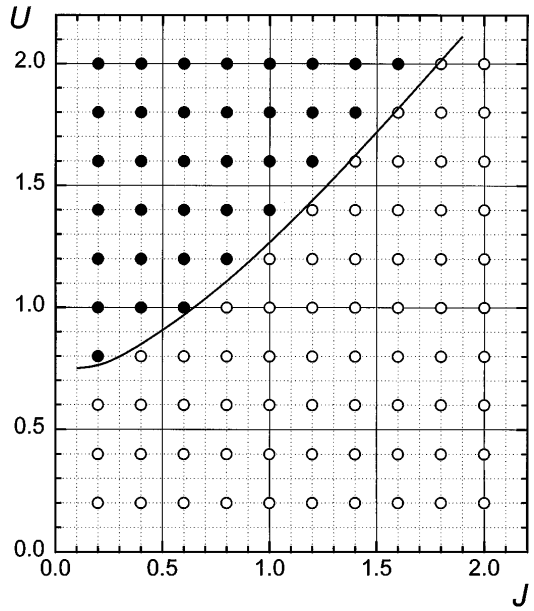

FIG. 2. The nature of ground states for various sets of coupling constants of J, U, and $V = 0$ in the unit D.

noted that the ground state is expected to belong to that of $S = 0$ for a realistic value of $\tilde{U}$ and $\tilde{J}$.

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

$$H^* = \sum_{n=0}^{\infty} \Lambda^{-n/2}(f_{n+1}^{\dagger} f_n + \text{H.c.}) + H_{\text{int}}^*,$$
$$H_{\text{int}}^* = 4J^*(\mathbf{s}_1^0 + \mathbf{s}_2^0)\cdot\mathbf{t} + \alpha^*(\mathbf{s}_1^0 + \mathbf{s}_2^0)^2 + \beta^*(\mathbf{j}_{\uparrow}^0 + \mathbf{j}_{\downarrow}^0)^2 + V^* Q_0 + \epsilon, \quad (7)$$

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

Since the energy of low lying excited states at the fixed point is mainly determined by H_{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 I. It is noted that the effective exchange coupling J^* is independent of the initial coupling U (including $U = 0$), and α^* and β^* are always zero. In the case (d), there is particle-hole symmetry so that the fixed point is the same as in 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

$$H_{\text{int}}^* = J^*(\mathbf{s}_1^0 + \mathbf{s}_2^0)\cdot\mathbf{t} + V^* Q_0 \qquad (J^* = 0.20). \quad (8)$$

The J, U dependence of V^* with $V = 0$ is shown in Fig. 3. 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 $f(J, U, V = 0) = \text{const}$. Especially, for $V^* = J^* = 0.20$, the "flow line" becomes equivalent to the boundary line shown in Fig. 2, because the first excitation energy is zero for these couplings.

In order to investigate the ω and T dependences of the susceptibility, let (Q, j, S) be (Q_D, j_D, S_D) for $V^* = V_D^* < 0.20$, where the ground state is a pseudospin doublet $(S = 1/2)$, and (Q_S, j_S, S_S) for $V^* = V_S^* > 0.20$ where

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) $(0.2, 0.4, -0.6)$.

	(J, U, V)	J^*	α^*	β^*	V^*	ϵ
(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

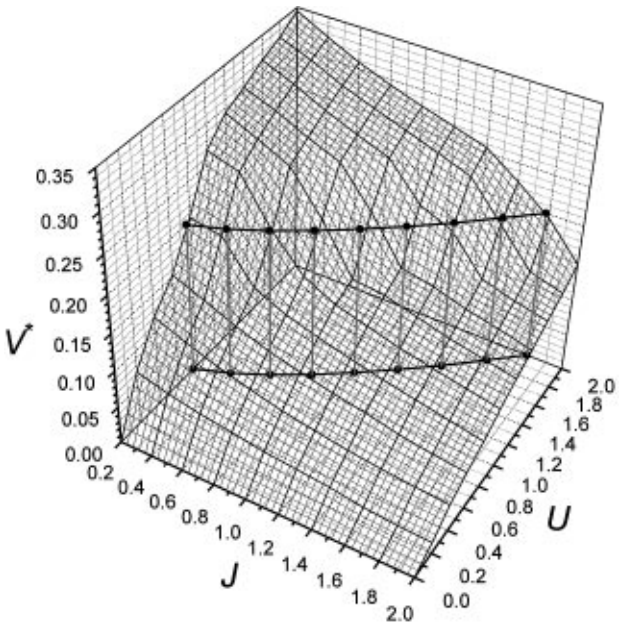

FIG. 3. J, U dependence of the effective impurity potential, V^*, with $V = 0$ at the fixed point.

the ground state is a pseudospin singlet ($S = 0$). For each of the 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 parameter are the same, as easily seen by means of the effective interaction (8). A prime example is the relation between Figs. 1(a) and 1(b) as mentioned above. According to this example, the coincidence of energy levels occurs after 20 iterations. From this coincidence, it is expected that the ω and T $(\omega/D, T/D < \Lambda^{-20/2})$ dependence of the susceptibility of the *real spin* (channel) for V_D^* coincide with those of the pseudospin for $V_S^* = 2J^* - V_D^*$, which has been known as anomalous [11], and vice versa. This is a new aspect of the two-channel Kondo problem which was not recognized as long as the conventional model without repulsion and potential scattering ($U = V = 0$) had been investigated, though the possibility of a diverging channel susceptibility has been suggested from another point of view [24,25]. This dual nature implies that when the impurity spin is magnetic the pseudospin susceptibility should be anomalous, together with the real spin susceptibility.

This remarkable aspect can be seen more vividly by investigating the spectral weight of the dynamical susceptibilities for the real spin of conduction electrons at the impurity site, $\chi_j''(\omega)$, and for the impurity pseudospin, $\chi_t''(\omega)$. They are calculated by the method of Ref. [11] as shown in Fig. 4. It is noted that, in the presence of the repulsion U, $\chi_j''(\omega)$ shows non-Fermi-liquid behavior with $\lim_{\omega\to 0}\chi_j''(\omega)$ being finite, while without the repulsion it shows Fermi-liquid behavior with $\chi_j''(0) = 0$. However, if we set $3U/2 + V = 0$, similar calculations show that $\chi_j''(0) = 0$; namely, it is the particle-hole symmetry

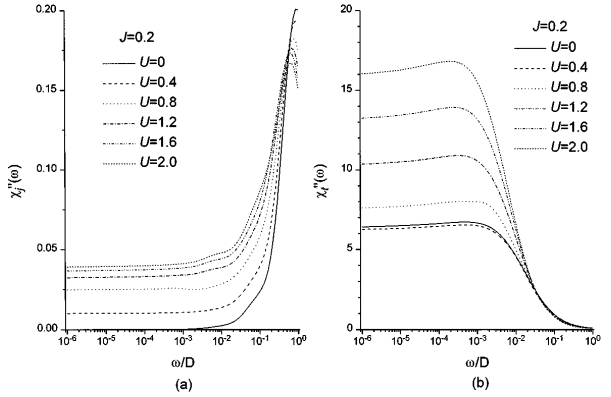

FIG. 4. ω dependence of the imaginary part of (a) local real spin susceptibility $\chi_j''(\omega)$ and (b) impurity pseudospin susceptibility $\chi_t''(\omega)$.

breaking that gives $\chi_j''(\omega)$ non-Fermi-liquid behavior. 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 the channel (i.e., real spin). It is also overscreened again by conduction electrons with two channels, i.e., pseudospin degrees of freedom [26]. 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, have not perfectly vanished, the pseudospin susceptibility is anomalous for any strength of the repulsion including $U = 0$. It is noted that the enhancement of U actually enhances the pseudospin susceptibility despite the crossover of the ground state.

In summary, the low lying excited states at the fixed point of the pseudospin two-channel Kondo model with particle-hole symmetry breaking perturbations are described not only by the exchange J^* but also by the impurity potential V^*. For $|V^*| > 0.20$, i.e., $\tilde{U} > \tilde{J}/8$ and $\tilde{D}/4$, 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 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 can be understood by the particle-hole symmetry breaking perturbation, which induces degrees of freedom of the real spin.

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[1] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).
[2] D. L. Cox, Phys. Rev. Lett. **59**, 1240 (1987); J. Magn. Magn. Mater. **76 & 77**, 53 (1988).
[3] A. Muramatsu and F. Guinea, Phys. Rev. Lett. **57**, 2337 (1986).
[4] M. Blume, V. J. Emery, and A. Luther, Phys. Lett. **33A**, 46 (1970).
[5] K. Vladár and A. Zawadowski, Phys. Rev. B **28**, 1564 (1983).
[6] P. W. Anderson and C. C. Yu, in *Proceedings of the International School of Physics "Enrico Fermi,"* edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, Amsterdam, 1985), p. 767; C. C. Yu and P. W. Anderson, Phys. Rev. B **29**, 6165 (1984).
[7] T. Matsuura and K. Miyake, J. Phys. Soc. Jpn. **55**, 29 (1986); **55**, 610 (1986).
[8] M. D. Núñez-Regueiro, J. M. Lopez-Castillo, and C. Ayache, Phys. Rev. Lett. **55**, 1931 (1985).
[9] D. M. Cragg, P. Lloyd, and P. Nozières, J. Phys. C **13**, 803 (1980).
[10] H. B. Pang and D. L. Cox, Phys. Rev. B **44**, 9454 (1991).
[11] O. Sakai, Y. Shimizu, and N. Kaneko, Physica (Amsterdam) **186–188B**, 323 (1993).
[12] N. Andrei and C. Destri, Phys. Rev. Lett. **52**, 364 (1984).
[13] A. M. Tsvelik and P. B. Wiegmann, J. Stat. Phys. **38**, 125 (1985).
[14] V. J. Emery and S. Kivelson, Phys. Rev. B **46**, 10 812 (1992).
[15] P. Coleman, L. Ioffe, and A. M. Tsvelik, Report No. COND-MAT/9504006.
[16] D. L. Cox, Physica (Amsterdam) **186–188B**, 312 (1993).
[17] See T. S. Kim and D. L. Cox, Phys. Rev. Lett. **75**, 1622 (1995), and references therein.
[18] See, for example, for $Th_{1-x}U_xRu_2Si_2$, H. Amitsuka and T. Sakakibara, J. Phys. Soc. Jpn. **63**, 736 (1994).
[19] Such a repulsion has already been taken into account at the level of the "Anderson" model for the magnetic two-channel Kondo problem.
[20] K. Miyake, H. Kusunose, and O. Narikiyo, J. Phys. Soc. Jpn. **62**, 2553 (1993).
[21] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[22] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).
[23] Since the Coulomb repulsion works most effectively between conduction electrons with the same polarization, the repulsion is anisotropic in pseudospin space. However, the anisotropic interaction is shown to flow into an isotropic one by renormalization evolution as will be discussed elsewhere, so we confine ourselves to discussing the case of isotropic repulsive interaction in (2).
[24] A. W. W. Ludwig and I. Affleck, Phys. Rev. Lett. **67**, 3160 (1991).
[25] D. L. Cox and A. E. Ruckenstein, Phys. Rev. Lett. **71**, 1613 (1993).
[26] Such a possibility is suggested in Ref. [16] from a general point of view on group theoretical arguments.