Kondo lattice model with a direct exchange interaction between localized moments

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We study the Kondo lattice model with a direct antiferromagnetic exchange interaction between localized moments. Ferromagnetically long-range ordered state coexisting with the Kondo screening shows a continuous quantum phase transition to the Kondo singlet state. We obtain the value of the critical point where the magnetizations of the localized moments and the conduction electrons vanish. The magnetization curves yield a universal critical exponent independent of the filling factors and the strength of the interaction between localized moments. It is shown that the direct exchange interaction between localized moments introduces another phase transition from an antiferromagnetic ordering to a ferromagnetic ordering for small Kondo exchange interaction. We also explain the local minimum of the Kondo temperature in recent experiments.

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I. INTRODUCTION

Interaction between itinerant electrons and localized moments in the Kondo regime is described by the s-f mixing and the polarization terms in the Kondo lattice model. The polarization term induces a RKKY type magnetic correlation, while the s-f mixing causes demagnetization. The magnetic correlation is dependent on the filling factor; ferromagnetic for low filling and antiferromagnetic around half filling. As the interaction between the conduction electrons and the localized moments increases, the phase evolves to the Kondo singlet phase. In particular, for half-filled case, the phase transition has been shown continuous and the value of critical point has been obtained\textsuperscript{2,3,4,5}.

In reality, however, the direct exchange interactions between localized moments should be included for a more comprehensive understanding. The Kondo exchange interaction, $J_K$, between the conduction electrons and the localized moments invokes the effective exchange interaction between the localized moments, the RKKY interaction $J_{\text{RKKY}} \sim |J_K|^2$. In the present study, in addition to the RKKY interaction, we introduce a direct antiferromagnetic exchange interaction between localized moments. In the ferromagnetic Kondo lattice model for manganites, its effects have been widely investigated in\textsuperscript{2,3,4,5}. In this study, we aim to address the effect of antiferromagnetic exchange interaction, $J_{\text{af}}$, on the phase diagram and on the critical behavior of Kondo lattice model (KLM) for low filling cases by calculating the density of states in a mean field level.

First of all, we investigate the magnetizations of both the lattice magnetic moments $\mu'$ and the conduction electrons $\mu$ for various filling factors and various values of $J_{\text{af}}$. The magnetic moments $\mu'$ and $\mu$ show qualitatively different behaviors; $\mu'$ falls monotonously from its maximum value as $J_K$ increases, whereas $\mu$ starts from zero, passes through a local maximum, and falls to zero at the same point as $\mu'$ does. Near the critical point, the magnetization curves show characteristic behaviors of continuous phase transition. The critical behavior of the magnetizations shows a universal exponent independent of the filling factor and the strength of exchange interaction $J_{\text{af}}$ such that $\mu'(\mu) \sim (J_K - J_c)^{1/2}$ with the critical point $J_c$. There emerge two mean fields. The first one, $x$, represents the mean field of the s-f mixing and the other field, $B$, the magnetic correlation between localized moments. As $J_K$ increases, the $x$ field increases whereas the $B$ field decreases, which indicates a phase transition from the magnetically ordered state to the Kondo state. Calculated values of the mean fields $x$ and $B$ explain consistently the physical situation such as the existence of phase transition between the ferromagnetic ordered state and the Kondo singlet state.

A notable feature of the present calculation is the existence of a new antiferromagnetic state at small Kondo exchange interaction especially for low filling factors. The s-f mixing field, $x$, is generally believed to be a monotonously increasing function of $J_K$\textsuperscript{6,7,8}. However, for very small $J_K$, we find a local minimum of $x$ field. It is accompanied by suppression of the $B$ field, which is the precursor of a transition to another magnetic order, an antiferromagnetic phase. A recent experiments on CeRu$_2$Ge$_2$ by Siullow et al\textsuperscript{9} and on CeAgSb$_2$ by Sidorov et al\textsuperscript{10} can be explained in connection with the anomalous behavior of the $x$ field and the $B$ field.

II. COEXISTENCE OF MAGNETIC ORDERING AND KONDO SCREENING

The magnetic correlation and the s-f mixing process are the two competing orders in the KLM. The Doniach diagram\textsuperscript{11} shows that the former has dominant effect for small $J_K$ while the latter for large $J_K$. The Kondo exchange model includes the s-f mixing term and the polarization term in the Kondo interaction to describe the competing orders. The polarization term give rise to the RKKY interaction\textsuperscript{12}.

Integrating out the fast mode in the action including the Kondo interaction may produce the effective RKKY interaction term in the Hamiltonian\textsuperscript{13} with the interac-
tion strength dependent on the Kondo interaction and the cutoff frequency. In this study, however, we consider the case that the RKKY interaction is implicitly included in the polarization term of the Kondo Hamiltonian. Instead we introduce the direct antiferromagnetic exchange interaction between the localized moments whose strength we treat as independent parameter. For ferromagnetic Kondo lattice model for manganites, where the interaction between the conduction electrons and the localized electrons is ferromagnetic, the effect of the direct exchange interaction between localized moments has already been studied. Here, various antiferromagnetic phases appear, even though the antiferromagnetic exchange interaction is much weaker than that of the Hund coupling.

The Hamiltonian $H = H_0 + V_K + V_H$ with the Kondo interaction $V_K$ and the interaction between localized moments $V_H$ is written by

$$ H_0 = \sum_{k, \sigma} \epsilon_k c_{k, \sigma}^\dagger c_{k, \sigma} + \sum_{i, \sigma} E_0 f_{i, \sigma}^\dagger f_{i, \sigma} \tag{1} $$

$$ V_K = -J_K \sum_i \left( S_1 \cdot S_i - \frac{1}{4} n_{f,i} n_{c,i} \right) \tag{2} $$

$$ V_H = -\frac{1}{2} J_{af} \sum_{i, a} \left( S_i \cdot S_{i+a} - \frac{1}{4} n_{f,i} n_{f,i+a} \right), \tag{3} $$

where $\sigma$ represents spin, $a$ a unit vector connecting the nearest neighbors, and $E_0$ the energy of the localized level. $J_K(<0)$ is the antiferromagnetic Kondo exchange interaction and $J_{af}(<0)$ the antiferromagnetic exchange interaction between localized moments. $c_{k, \sigma}^\dagger$ is the creation operator for conduction electrons with wave vector $k$, $f_{i, \sigma}^\dagger$ for localized electrons at cite $i$, $n_{c,i} = \sum_{\sigma} c_{i, \sigma}^\dagger c_{i, \sigma}$, and $n_{f,i} = \sum_{\sigma} f_{i, \sigma}^\dagger f_{i, \sigma}$.

Using the Stratonovich-Hubbard transformation and the identities, $S_1 = \frac{1}{2} c_{1, \sigma}^\dagger c_{1, \sigma}$ and $S_i = \frac{1}{2} f_{i, \sigma}^\dagger f_{i, \sigma}$, with Pauli matrices $\sigma$, the interaction terms are represented by $V_K = H_1 + H_2 - (J_K/2) \sum_i x_i^2$ and $V_H = H_3 + H_4 - (J_{af}/4) \sum_i x_i^2$, where

$$ H_1 = \frac{J_K}{2} \sum_{i, \sigma} x_i (f_{i, \sigma}^\dagger c_{1, \sigma} + c_{1, \sigma}^\dagger f_{i, \sigma}) \tag{4} $$

$$ H_2 = \frac{J_K}{2} \sum_{i, \sigma} \left[ f_{i, \sigma}^\dagger f_{1, \sigma} - (c_{1, \sigma}^\dagger c_{i, \sigma}) \right] + (c_{1, \sigma}^\dagger c_{i, \sigma}) f_{i, \sigma} \tag{5} $$

$$ H_3 = \frac{J_{af}}{4} \sum_{i, a, \sigma} y_i (f_{i, \sigma}^\dagger f_{i+a, \sigma} + f_{i+a, \sigma}^\dagger f_{i, \sigma}) \tag{6} $$

$$ H_4 = \frac{J_{af}}{4} \sum_{i, a, \sigma} \left[ f_{i, \sigma}^\dagger f_{i, \sigma} f_{i+a, \sigma} - (c_{1, \sigma}^\dagger c_{i, \sigma}) f_{i+a, \sigma} \right] \tag{7} $$

where $x_i$ and $y_i$ are the mean fields representing the s-f mixing and the magnetic correlation between localized moments respectively. Hereafter, we consider the uniform case such that $x_i = x$ and $y_i = y$.

Here, $H_1$ describes the Kondo scattering and $H_2$ the polarization of the conduction electrons by the localized moments. $H_2$ gives the magnetic ordering through the RKKY interaction between localized moments. The competition between $H_1$ and $H_2$ is previously studied. $H_3$ comes from the transverse part of the direct exchange interaction $V_H$ in Eq. 3 and can be represented in k-space

$$ H_3 = B \sum_{k, \sigma} \epsilon_k f_{k, \sigma}^\dagger f_{k, \sigma}, \tag{8} $$

where $B = -zy J_{af}/2D$ and $\epsilon_k = -(D/z) \sum_a \cos k \cdot a$ with coordination number $z$. This term gives the localized moments a small band width $2BD$. $H_4$ is the term polarizing the nearest neighbor localized moments.

In order to describe the critical behavior near the critical point, we consider the coexistence of the magnetic ordering and the Kondo screening. Calculating magnetizations of the localized moments and the conduction electrons for various filling factors and various $J_{af}$, we obtain the phase boundaries and the critical exponent. In this case we have the relations such that

$$ \langle c_{1, \sigma}^\dagger c_{1, \sigma} \rangle = \frac{1}{2} (n + \mu), \quad \langle c_{1, \sigma}^\dagger c_{1, \sigma} \rangle = \frac{1}{2} (n - \mu), \tag{9} $$

$$ \langle f_{i, \sigma}^\dagger f_{i, \sigma} \rangle = \frac{1}{2} (1 - \mu'), \quad \langle f_{i, \sigma}^\dagger f_{i, \sigma} \rangle = \frac{1}{2} (1 + \mu'), \tag{10} $$

where $\mu (\mu')$ is the magnetization of s (f) electrons in the spin-down (spin-up) direction and $n$ is the filling factor. Since the Kondo exchange interaction $J_K$ is antiferromagnetic, we expect that $\mu$ and $\mu'$ have the same sign.

With these equations the Green’s function for the f-electrons and the c-electrons corresponding to the Hamiltonian $H$ can be obtained as follows,

$$ G_{ff}(\omega) = \sum_k \left[ \omega \pm is - E_0 - B \epsilon_k - \frac{1}{4} J_K (n + \mu) - \frac{1}{4} \frac{z J_{af}}{D} (1 - \mu') - \frac{J_{af}^2 x^2}{D (\omega \pm is - \epsilon_k - \frac{1}{4} J_K (1 - \mu'))} \right]^{-1}, \tag{11} $$

$$ G_{cf}(\omega) = \sum_k \left[ \omega \pm is - \epsilon_k - \frac{1}{4} J_K (1 - \mu') - \frac{1}{4} \frac{z J_{af}}{D} (n + \mu) - \frac{J_{af}^2 x^2}{D (\omega \pm is - E_0 - B \epsilon_k - \frac{1}{4} J_K (n + \mu) - \frac{1}{4} \frac{z J_{af}}{D} (1 - \mu'))} \right]^{-1}. \tag{12} $$

For the spin down case, the quantities such as $G_{ff}(\omega)$ can be simply obtained by substituting $\mu \rightarrow -\mu$ and $\mu' \rightarrow -\mu'$. The above Green’s functions can be arranged to be written as follows,

$$ G_{ff}(\omega) = \sum_k \left[ \frac{P_{ff}(\omega) \pm is - \epsilon_k}{Q_{ff}(\omega) \pm is - \epsilon_k} \right], $$

$$ G_{cf}(\omega) = \sum_k \left[ \frac{P_{cf}(\omega) \pm is - \epsilon_k}{Q_{cf}(\omega) \pm is - \epsilon_k} \right], $$

where $P_{ff}(\omega)$ and $Q_{ff}(\omega)$ are the polynomials of $\omega$.
Using the expressions obtained for $P^\uparrow(\omega)$ and $\rho^\uparrow(\omega)$ in fashion. Since we can readily show $\rho^\uparrow(\omega)$, here we use the flat band for the conduction electrons, $\rho^\uparrow(\omega) = \Im G^\uparrow(\omega)$, can be obtained by solving the equations

$$P^\uparrow(\omega) = \frac{1}{2D} \left[ \int_0^\Omega \sqrt{\Omega^2 + B J^2 x^2} \right]$$

$$P^\downarrow(\omega) = \frac{1}{2D} \left[ 1 - \int_0^\Omega \sqrt{\Omega^2 + B J^2 x^2} \right]$$

where $\Omega^\uparrow(\omega) = (1 - B)\omega - \frac{1}{4} J((n + \mu) - (1 - \mu')B)$

$$- E_{0\uparrow} = - \frac{1}{4} z J_{ad}(1 - \mu')$$

The band edges can be obtained by solving the equations $-D < g^\uparrow(\omega) < D$ and $-D < h^\uparrow(\omega) < D$. Using the expressions obtained for $g^\uparrow(\omega)$ and $h^\uparrow(\omega)$,

$$g^\uparrow(\omega) = \frac{1}{2B} \left[ (1 + B)\omega - \frac{1}{4} J((n + \mu) - (1 - \mu')B) - E_{0\uparrow} - \frac{1}{4} z J_{ad}(1 - \mu') + \sqrt{\Omega^2 + J^2 x^2} \right]$$

$$h^\uparrow(\omega) = \frac{1}{2B} \left[ (1 + B)\omega - \frac{1}{4} J((n + \mu) + (1 - \mu')B) - E_{0\uparrow} - \frac{1}{4} z J_{ad}(1 - \mu') - \sqrt{\Omega^2 + J^2 x^2} \right]$$

we get for $\omega^\uparrow$

$$\omega_1^\uparrow = \frac{1}{2} \left[ \omega_a - (1 + B)D \right]$$

$$\omega_2^\uparrow = \frac{1}{2} \left[ \omega_b - (1 + B)D \right]$$

$$\omega_3^\uparrow = \frac{1}{2} \left[ \omega_a + (1 + B)D \right]$$

$$\omega_4^\uparrow = \frac{1}{2} \left[ \omega_b + (1 + B)D \right]$$

where $\omega_a = \frac{1}{4} J((n + \mu) + (1 - \mu')) + E_{0\uparrow} + \frac{1}{2} z J_{ad}(1 - \mu')$ and $\omega_b = \frac{1}{4} J((n + \mu) - (1 - \mu')) + E_{0\uparrow} + \frac{1}{2} z J_{ad}(1 - \mu')$. Here, we used the relation, $g_{f\sigma}(\omega) = g_{\sigma\sigma}(\omega) = g_{\sigma}(\omega)$, $h_{f\sigma}(\omega) = h_{\sigma\sigma}(\omega) = h_{\sigma}(\omega)$, and $\omega_{f\uparrow} = \omega_{\uparrow\uparrow}$ in.

### III. RESULTS AND DISCUSSIONS

The ferromagnetic magnetizations $\mu'$ and $\mu$ in presence of the Kondo screening can be obtained as a function of the Kondo exchange interaction $J_K$ by solving the self consistent equations, Eqs. (9) and (10), using the density of state, Eqs. (15) and (16). Eqs. (9) and (10) for spin up case are represented as

$$\frac{1 + \mu'}{2} = \frac{1}{1 - B} \int_{\Omega_{f\uparrow}}^{\Omega_{f\uparrow}} \tilde{\rho}_{f\uparrow}(\Omega) d\Omega$$

$$\frac{n - \mu}{2} = \frac{1}{1 - B} \int_{\Omega_{f\uparrow}}^{\Omega_{f\uparrow}} \tilde{\rho}_{c\uparrow}(\Omega) d\Omega.$$

From the above equations $\Omega_{f\uparrow}$ and $\Omega_{c\uparrow}$ can be evaluated by inserting the density of states from Eqs. (15) and (16). $\Omega_{f\uparrow}(E_f)$ and $\Omega_{c\uparrow}(\omega_{f\uparrow})$ can also be represented from Eq. (17). Solving the equations, $\Omega_{f\uparrow} = \Omega_{f\uparrow}(E_f)$ and $\Omega_{c\uparrow} = \Omega_{c\uparrow}(\omega_{f\uparrow})$, the magnetizations $E_{f\uparrow}$ and $E_{c\uparrow}$ can be given by

$$E_{0\uparrow} = \frac{4 \Omega_{f\uparrow}^2 + (1 - B)^2(4BD^2 - J^2 x^2)}{-2(1 + B)\Omega_{f\uparrow} + (1 - B)\sqrt{\Omega_{f\uparrow}^2 - 16B^2D^2 + 4BJ^2x^2}}$$

$$E_{f\uparrow} = \frac{1}{1 - B} [\Omega_{f\uparrow} + E_{f\uparrow}]$$

The values of magnetizations, $\mu'$ and $\mu$, are obtained numerically. First, we fix the values of $x$ and $B$ for given values of $n$, $J_{ad}$, and $J_K$ and, then, solve the equations, $E_{f\uparrow} = E_{f\downarrow}$, and $E_{0\uparrow} = E_{0\downarrow}$, to obtain the values of magnetizations, $\mu'$ and $\mu$. From these values we calculate the total energy of the conduction electrons and localized moments. The total energy can be written as $E = \sum_{i} E_{i\uparrow}^{E_F} \omega[\mu_{f\sigma}(\omega) + \mu_{c\sigma}(\omega)] d\omega + E_{MF}$. $E_{MF}$ can be obtained from the Hamiltonians in Eqs. (3) and (4) with the mean values from Eqs. (9) and (10) and is given by

$$E_{MF} = -(1/2)J_K x^2 - BD^2/zJ_{ad} - (1/4)J_K (n + \mu') - (1/8)zJ_{ad}(1 - \mu'^2).$$

For appropriate ranges of $x$ and $B$ values, we repeat the above process and determine the values of $\mu'$ and $\mu$ at the minimum point of the total energy of the system.

In Fig. 1 we show the magnetization of the localized moments, $\mu'$, and of the conduction electrons, $\mu$, in ferromagnetic state when $J_{ad}/D = -0.001$. The magnetization curves clearly demonstrate existence of continuous
quantum phase transition. We observed that the critical values of the Kondo exchange interaction are higher for smaller values of filling factors, which is consistent with previous studies. However, there have been conflicting reports on the behavior of $\mu$. A recent Monte Carlo study showed existence of a local maximum in the $\mu$ curve, but its behavior for small values of $J_K$ was left uncertain. On the contrary, a more recent bond-operator mean-field study produced a monotonously decreasing behavior. Present study shows that the magnetization of conduction electrons $\mu$ starts to increase from zero and pass a local maximum before it falls to zero at the same points as those of $\mu'$. It is consistent with the Monte Carlo calculation and also clarifies the situation for small values of $J_K$.

Fig. 2 shows the behavior of $\mu'$ near the critical point for $n=0.2$ with various values of $J_{af}$. $J_{af}$ competes with the ferromagnetic correlation and, thus, makes the critical points slightly smaller as shown in Fig. 2. We observe that the critical points are dependent on the values of $J_{af}$ as well as the filling factors. Close study on the critical behaviors of $\mu'$ and $\mu$ clearly shows that the critical exponent has a universal value independent of the filling factor and $J_{af}$. The form is given by $(J_K - J_c)^{1/2}$ as shown in Fig. 3.

The mean field variable $x$ representing the s-f mixing is closely related to the Kondo temperature and the variable $B$ representing the correlation between localized spins is to the correlation temperature. The behaviors of $x$ and $B$ as functions of $J_K$ are plotted in Fig. 4(a). Fig. 4(a) shows that both $x$ and $B$ have higher values for higher filling factors, which is consistent with the study by Ruppenthal et al. The field $B$ is shown to behave in the opposite direction of $x$. This signifies that $B$ represents the magnetically ordered state competing with the Kondo singlet state.

The KLM with a direct exchange interaction between localized moments exhibits a qualitatively different behaviors from those without direct interaction between localized moments. The value of $x$ shows a local minimum as $J_K$ becomes quite small. This phenomenon is accompanied by the suppression of the $B$ field. This behavior indicates that the magnetic correlation becomes weak and another transition is being anticipated. The local minimum of $x$ is shown in Fig. 4(a) for various filling factors when $J_{af}/D = -0.001$ and for various values of $J_{af}$ when $n=0.35$ in (b), where the re-growth of $x$ is shown stronger for larger $|J_{af}|$.

We have calculated the antiferromagnetic state energy and compared it with that of the ferromagnetic state. In Fig. 5 the phase boundary for the ferromagnetic state...
and the antiferromagnetic state is shown in the lower part of the figure. For low filling, the antiferromagnetic state become more favorable. As the value of $J_K$ increases, the transition to the Kondo singlet state follows as shown in Fig. 4. Similar phase boundary has been obtained previously by comparing the energy of the Kondo singlet state with that of the ferromagnetic state without Kondo scattering. Here, it should be noted that the present calculation is carried out when the ferromagnetism and the Kondo screening coexist.

This behavior explains the recent experiments on CeRu$_2$Ge$_2$ by Sillow et al. and on CeAgSb$_2$ by Sidorov et al.. In these experiments, the interaction between the localized moments, Ce, is ferromagnetic while the RKKY interaction is antiferromagnetic. Two consecutive phase transitions have been observed: a transition from the ferromagnetic phase to the antiferromagnetic phase followed by a transition to the Kondo singlet state as $J_K$ increases further. If we exchange the role of the antiferromagnetic interaction with that of the ferromagnetic interaction, we can explain the experiment in the present scenario, since here we have considered the antiferromagnetic interaction between f-electrons and the ferromagnetic RKKY interaction.

In the experiment on CeRu$_2$Ge$_2$, we observe suppression of the magnetic transition temperature near the critical point where the transition from one magnetic state to another magnetic state occurs. This corresponds to the suppression of the $B$ field in the present study. We can see in the experiments the local minimum of the Kondo temperature, $T_K$. In the experiment on CeRu$_2$Ge$_2$, we can only observe that the Kondo temperature resists going to zero as $J_K$ decreases. However, in the experiments on CeAgSb$_2$ and on CeRhIn$_5$, we clearly see the local minimum of the Kondo temperature. This local minimum has been conjectured to be caused by a certain mechanism competing with the Kondo effect. In the present theory, we show that the direct interaction between the localized moments competing with the Kondo scattering gives rise to the local minimum of the $x$ field and, thus, the Kondo temperature.

![FIG. 4: Plots for the mean field $x$ and $B$ (a) for various $n$ values when $J_{af}/D = -0.001$ and (b) for various values of $J_{af}/D$ when $n = 0.35$.](image)

![FIG. 5: Phase diagram for various $J_{af}$. The phase boundary for the antiferromagnetic state and the ferromagnetic state is shown in the lower part of the figure. The phase boundary for the ferromagnetic state and the Kondo singlet state is shown in the upper part for $J_{af}/D = 0$ and $J_{af}/D = -0.001$.](image)

**IV. CONCLUSION**

We have studied the KLM with an antiferromagnetic exchange interaction between localized moments for a general situation in which ferromagnetic correlation coexists with the Kondo screening. Calculating the magnetization of the localized moments and the conduction electrons as a function of the Kondo interaction for various filling factors and values of $J_{af}$, we obtained a continuous quantum phase transition from the ferromagnetic ordered state to the Kondo singlet state and the critical points where the magnetizations vanishes. Around the critical points, we obtained the critical exponent independent of the filling factor and the values of $J_{af}$ such that $\mu' (\mu) \sim (J_K - J_c)^{1/2}$.

Furthermore, we obtained the behavior of the mean fields, $x$ and $B$, corresponding to the Kondo scatter-
ing and the magnetic correlation respectively. As the Kondo interaction increases the value of $B$ decreases while $x$ increases, which explains existence of the Kondo singlet state at large value of $J_K$. On the contrary, as $J_K$ decreases, the value of $B$ increases while $x$ decreases. Hence, the enhanced magnetic correlation with suppressed Kondo screening leads the magnetically ordered state.

When $J_K$ is further reduced, the another phase transition from the antiferromagnetically ordered state to the ferromagnetically appears due to the $J_{af}$ interaction. Comparing the energy of the ferromagnetic state and the antiferromagnetic state, we obtain the phase boundary, which shows clearly that an antiferromagnetic state appears for low filling. The $x$ field exhibits a re-growth accompanied by the suppression of $B$. This phenomena is due to the $J_{af}$ interaction and is a precursor for the transition to the antiferromagnetically ordered state. Recent experiments\textsuperscript{10,11,17} can be explained through the present theory.

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