Kondo Hamiltonian for a triplet impurity as a bridge between Fermi and non-Fermi-liquid physics

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A connection between competing Fermi and non-Fermi-liquid states is studied by a Kondo Hamiltonian for a triplet impurity, keeping cubic symmetry in mind. A uniaxial anisotropy stabilizes either state, corresponding to a local field in the two-channel Kondo model, which reflects on the local charge redistribution in the singlet-doublet configuration of the impurity. The numerical renormalization group and SU(2) group theoretical analyses show that the critical point is described by threefold degenerate terms of the two-channel Kondo Hamiltonian, one of which derives the non-Fermi-liquid state and the other two lead to the Fermi liquid.

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I. INTRODUCTION

Since the first theory presented by Kondo,[1] the problem of a single magnetic impurity coupled to conduction electrons has been studied extensively as one of the important issues of strongly correlated electron systems. The singlet formation by electron coupling with a local moment is the essence of this physics and the low temperature properties can be understood within the framework of the Fermi liquid (FL) theory. Beyond the initial solution, the Kondo physics has been extended to various cases such as orbitally degenerate impurities embedded in metals, lattice versions for heavy fermion systems and recently developed artificial devices called quantum dots.[2–4]

Among the advanced Kondo problems, multichannel cases have been studied frequently, associated with nontrivial solutions unexpected for a single channel.[5] These are well known as the overscreening Kondo effects characterized by the logarithmic or power-law divergence of the temperature T dependent magnetic susceptibility $\chi(T)$ and specific heat coefficient $\gamma(T)$ of an impurity.[6] For another intriguing case, much theoretical interest has been attracted by the two-impurity Kondo problem where the self-screening of antiferromagnetically coupled interimpurities competes with the Kondo screening of each impurity.[7–9] If particle-hole symmetry is not broken, there is a critical point separating the two phases, at which the low temperature properties are not FL-like. As an extended version, theories of the two-impurity, two-channel case reported a critical line in the complicated phase diagram.[10,11] While the details of non-Fermi-liquid (NFL) properties are elucidated by a lot of theories, it is not still clear why such an abnormal liquid state is stabilized against FL. In general, it may be believed that NFL states are so unstable that they can emerge exceptionally in an extremely narrow parameter space with respect to Kondo couplings, local fields, anisotropic perturbations, etc.; most of the region is dominated by a FL phase. In fact, NFL stability conditions are more restricted than FL in the above multichannel and two-impurity cases.

To prove that the appearance of NFL states is not exceptional and is possible in a real system, we showed examples of competing FL and NFL phases.[12–14] One of the keys to the competition is almost degenerate energy levels of the impurity lowest-lying states. A singlet-doublet configuration is the most appropriate candidate that is expected for Pr^{3+} or U^{4+} ions in the f^2 configuration. Another key is orbitally degeneracy of conduction electrons that plays an important role in the hybridization with localized orbitals such as f electrons. Due to the strong spin-orbit coupling in f-electron systems, an impurity with large angular momentum gives rise to quadrupolar exchange interaction and other multipolar types between the impurity states and conduction electrons in addition to spin (dipolar) exchange. Thus, the variety of exchange leads to the FL vs NFL competition.

A critical point separating the FL and NFL stability regions is considered to be due to a highly symmetric exchange interaction on an impurity. If the configuration of the impurity state can be controlled by an experiment, competing FL and NFL states are observable. Suppose the competition occurs in a tetragonal metal, there must be a critical point that reflects such higher symmetry as cubic one. It is expected in a cubic metal that both FL and NFL states can be derived, for instance, by applying pressure that deviates the system from the cubic symmetry.

To grasp the essential features of this physics, in this paper, we present a Kondo model for a local triplet and investigate the effect of deviation from cubic symmetry introducing a uniaxial field. We previously studied NFL behavior due to a crystal-field triplet.[15] The leading relevant operator with the scaling dimension $1/6$ is expected to govern low temperature properties in cubic systems such as Pr or U based compounds. Due to a uniaxial anisotropic field that separates the triplet into a singlet and a doublet, either FL or NFL state can be stabilized by multiorbital exchange interaction of conduction electrons with the local moment. When the doublet is dominant, the stabilized state is exactly mapped to the NFL derived from the two-channel Kondo effect. Here, we first describe the FL vs NFL competition controlled by the uniaxial field. Then, we examine the vicinity of the critical point to pursue what determines their stability.

The numerical renormalization group (NRG) method[16] is the most powerful tool for such complex impurity problems. This quantitative approach to a critical point guides us to find a hidden symmetry of the critical-point Hamiltonian using a group theoretical method. In our case, the SU(2) Lie algebra is very useful. We show that the relevant part is mapped to a combination of SU(2) forms of two-channel Kondo Hamiltonian. On the basis of the reduced Hamiltonian, one can find clearly what derives either FL or NFL with a local field.

The paper is organized as follows. In Sec. II, the Kondo model is presented for an impurity in the singlet-triplet configuration controlled by the uniaxial local field. The FL vs NFL competition is explained by the detailed NRG analysis in the vicinity of the critical point. In Sec. III, the critical-point Hamiltonian is reconstructed from an analogy between the cubic point and SU(2) groups. It is found that both FL and NFL stabilized by the uniaxial field is closely related to the two-channel Kondo effect. The paper closes with concluding remarks in Sec. IV.

II. MODEL AND NUMERICAL RENORMALIZATION GROUP ANALYSIS

Let us begin with a Kondo model describing a local singlet-doublet configuration coupled to conduction electrons.[15] Their orbital channels considered here are fourfold degenerate, expressed by a 3/2 pseudospin operator. The model Hamiltonian is written as

$$H=\sum_{km}\varepsilon_k c_{km}^\dagger c_{km}+\Delta(S_z^2-2/3)$$
$$+\sum_{kk'mm'}c_{km}^\dagger c_{k'm'}\sum_{X=S,Q}J_X(\boldsymbol{X}^{\mathrm{c}})_{mm'}\cdot\boldsymbol{X}. \tag{1}$$

Here, the first term is the kinetic energy of conduction electrons with wave number k and pseudospin m $(=3/2,1/2,-1/2,-3/2)$. The electron creation (annihilation) is represented by the fermion operator $c_{km}^\dagger$ (c_{km}). The second term expresses a uniaxial anisotropic field coupling to a local triplet represented by an $S=1$ pseudospin. The positive (negative) Δ lowers the $S_z=0$ singlet denoted by $|0\rangle$ ($S_z=\pm1$ doublet denoted by $|\pm\rangle$), keeping the center of their gravity. The last term in Eq. (1) consists of dipolar exchange ($\boldsymbol{S}^c\cdot\boldsymbol{S}$) and quadrupolar exchange ($\boldsymbol{Q}^c\cdot\boldsymbol{Q}$) interactions with the positive coupling constants J_S and J_Q, respectively, between the $S^c=3/2$ electrons and the local $S=1$ spin. For the local moment, the quadrupole operator $\boldsymbol{Q}$ has five components defined by the $S=1$ components,

$$\{Q_u,Q_v,Q_{yz},Q_{zx},Q_{xy}\}=\{(2S_z^2-S_x^2-S_y^2)/\sqrt{3},S_x^2-S_y^2,S_yS_z$$
$$+S_zS_y,S_zS_x+S_xS_z,S_xS_y+S_yS_x\}. \tag{2}$$

Similarly, for the conduction electrons, $\boldsymbol{Q}^c$ is constructed from the $S^c=3/2$ operators. This Kondo Hamiltonian (1) for $\Delta=0$ can be directly derived from an Anderson Hamiltonian with a cubic symmetry, where valence fluctuations are restricted between an $O_h\Gamma_7$ doublet and a Γ_5 (Γ_4 also holds) triplet for the f^1 and f^2 configurations, respectively.[15] In this case, the Γ_8 partial waves of conduction electrons hybridize with the f orbitals. The Γ_5 and Γ_8 representations can be exactly mapped to $S=1$ and $S^c=3/2$, respectively. Although the uniaxial anisotropy affects not only the impurity states

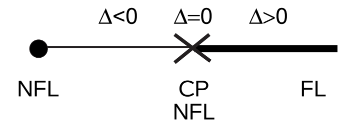

FIG. 1. Diagram of the stability regions of the FL and NFL states separated by the critical point (CP) in the single parameter Δ line. The NFL for $\Delta<0$ is independent of Δ, represented by the single solid circle $(\Delta\to-\infty)$. The Δ (>0) dependent FL is represented by the bold line.

but also the cubic forms of effective exchange interaction terms, it just modifies quantitative properties.

The NRG calculation performed here follows our previous study for the $\Delta=0$ case. We extend it to the range $-10^{-2}<\Delta<10^{-2}$ in the unit of the bandwidth and focus on the vicinity of the critical point. There are three types of zero temperature states (see Fig. 1).

(a) NFL in the $\Delta<0$ regime. The low-lying energy spectrum is completely same with that of the two-channel Kondo case. This is less dependent on Δ when both J_S and J_Q are fixed. For the small coupling constants, broken particle-hole symmetry is negligibly small.

(b) *Critical-point* NFL at $\Delta=0$. The low-lying energy spectrum contains triplet levels, which differs from the two-channel Kondo case. Their distinction appears clearly in $\chi(T)$ and $\gamma(T)$ as low $T\to0$: $\sim T^{-2/3}$ for $\Delta=0$, whereas $\sim-\log T$ for $\Delta<0$. The particle-hole symmetry is broken by the quadrupolar exchange interaction that is the most relevant since a finite J_Q leads to this NFL for $J_s=0$.[15]

(c) FL in the $\Delta>0$ regime. The quasiparticle excitation energies depend strongly on Δ, indicating that the excited doublet $|\pm1\rangle$ is combined with the lowest singlet $|0\rangle$ through the Kondo effect. This situation can be described by a free electron model with an effective local potential that consists of two terms.[13] One gives rise to an uniform shift of fourfold degenerate $S^c=3/2$ energy levels and the other splits them to the $m=\pm3/2$ and $m=\pm1/2$ levels. The latter represents a Γ_1 quadrupolar field with D_{4h} symmetry. This field couples to the conduction electrons as $V_Q^*\Sigma_m(5/4-m^2)c_{km}^\dagger c_{km}$. Here, V_Q^* is an effective coupling constant defined at the FL fixed point.

Figure 2 shows Δ dependence of the singlet-doublet charge distribution at $T=0$, represented by the doublet weight N_{doublet}. Here, the NRG data are given for the fixed $1.5J_S=3J_Q=0.1$ in the unit of the bandwidth. Since $|0\rangle$ and $|\pm\rangle$ are degenerate at $\Delta=0$, N_{doublet} takes 2/3. In the FL phase $(\Delta>0)$, it decreases continuously with increasing Δ and then approaches zero asymptotically as $\Delta\to\infty$ at which the local excited doublet is neglected completely and the free electron states are obtained. In the vicinity of $\Delta=0$, it is found that $(2/3-N_{\mathrm{doublet}})$ is proportional to $|\Delta|\log|\Delta|$. This behavior resembles a local spin field effect for the two-channel Kondo model where a crossover from NFL to FL takes place.[17] This FL state is characterized by a phase shift δ that is dependent on the local field h: $(\pi/4-\delta)\propto|h|\log|h|$ as $h\to0$.[17] In our case, for small coupling constants J_S and J_Q, the FL energy spectrum can be reproduced by only V_Q^* that follows almost the same Δ dependence with N_{doublet}, as shown in Fig. 2. Note that the

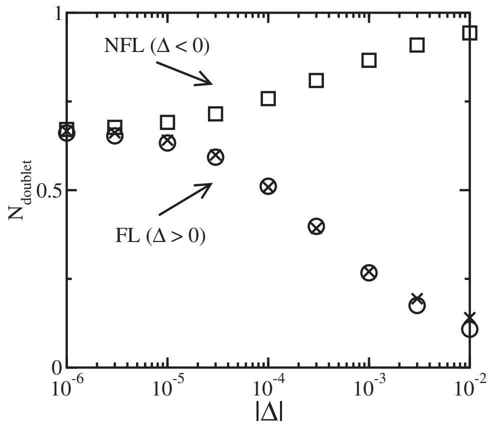

FIG. 2. Anisotropic field Δ dependence of the singlet-doublet charge distribution at the zero temperature represented by the doublet weight N_{doublet}. The circle and square symbols are the data for the FL case and for the NFL, respectively. The former are almost coincident with the cross ones for the local quadrupolar field V_Q^* normalized by $1.5V_Q^*(\Delta \to 0^+)$ here. This $\Delta \to 0^+$ limit corresponds to a phase shift $\delta = \pi/4$ in the FL state.

strong enhancement of the local quadrupolar field V_Q^* with decreasing Δ is due to the existence of the critical point. In the NFL phase ($\Delta<0$), ($N_{\mathrm{doublet}}-2/3$) shows the similar behavior to that for FL, obeying $|\Delta|\log|\Delta|$ near $\Delta=0$. The different points from the FL case are that the change of N_{doublet} does not reflect on the NFL energy spectrum and the local singlet $|0\rangle$ contribution is negligible.

III. CRITICAL POINT HAMILTONIAN

As mentioned above, the FL state for $\Delta>0$ is related to the two-channel Kondo case. This implies that essential features of both FL and the critical-point NFL can be understood on the basis of the two-channel Kondo model. Next, we analyze the triplet impurity Kondo Hamiltonian (1) for $\Delta=0$ using SU(2) Lie algebra to elucidate how to derive both FL and NFL from the critical point.

In each line of Table I, one spin operator and two of quadrupole operators in Eq. (2) satisfy the commutation relation $[\tau_\alpha, \tau_\beta] = i\varepsilon_{\alpha\beta\gamma}\tau_\gamma$ ($\alpha, \beta, \gamma = 1,2,3$). There are two kinds of groups denoted by the superscripts $X=A,B$. Here, τ_α^{Xi} and $\tau_\alpha^{Xi,c}$ are for $S=1$ and for $S^c=3/2$, respectively. They are also classified by quantized $i=x,y,z$ axes. In $\tau_1^{Xx,c}$, $\tau_2^{Xy,c}$, and $\tau_3^{Xz,c}$, a new operator T_j^c ($j=x,y,z$) represents the Γ_4 octupole defined as

$$T_j^c = \frac{5}{2}(S_j^c)^3 - \frac{1}{2}[3S^c(S^c+1)-1]S_j^c. \tag{3}$$

The appearance of an octupole is due to the spin size $\geqslant 3/2$. For each (Xi) group, the scalar product $\boldsymbol{\tau}^c \cdot \boldsymbol{\tau}$ gives an isotropic exchange form

$$\bar{H}_{Xi} = \sum_{\alpha=1,2,3} \tau_\alpha^{Xi,c}\tau_\alpha^{Xi}, \quad X=A,B, \quad i=x,y,z. \tag{4}$$

Combination of all the $\bar{H}_{Xi}$ terms leads to a cubic symmetric form of exchange Hamiltonian,

TABLE I. Spin and quadrupole operators. In each line, they satisfy the SU(2) Lie algebra, classified into two groups named X ($=A,B$) below. Here, i ($=x,y,z$) represents a quantized axis. The components τ_α^{Xi} and $\tau_\alpha^{Xi,c}$ ($\alpha=1,2,3$) are derived from the $S=1$ and $S^c=3/2$ spin operators, respectively.

$X=A,B$ $i=x,y,z$	τ_1^{Xi} $\tau_1^{Xi,c}$	τ_2^{Xi} $\tau_2^{Xi,c}$	τ_3^{Xi} $\tau_3^{Xi,c}$
Az	$Q_v/2$ $Q_v^c/2\sqrt{3}$	$Q_{xy}/2$ $Q_{xy}^c/2\sqrt{3}$	$S_z/2$ $2(S_z^c-T_z^c/3)/5$
Ax	$S_x/2$ $2(S_x^c-T_x^c/3)/5$	$Q_{yz}/2$ $Q_{yz}^c/2\sqrt{3}$	$(\sqrt{3}Q_u+Q_v)/4$ $(\sqrt{3}Q_u^c+Q_v^c)/4\sqrt{3}$
Ay	$Q_{zx}/2$ $Q_{zx}^c/2\sqrt{3}$	$S_y/2$ $2(S_y^c-T_y^c/3)/5$	$(\sqrt{3}Q_u-Q_v)/4$ $(\sqrt{3}Q_u^c-Q_v^c)/4\sqrt{3}$
Bz	Q_{zx} $Q_{zx}^c/2\sqrt{3}$	Q_{yz} $Q_{yz}^c/2\sqrt{3}$	S_z $(S_z^c+4T_z^c/3)/5$
Bx	S_x $(S_x^c+4T_x^c/3)/5$	Q_{xy} $Q_{xy}^c/2\sqrt{3}$	Q_{zx} $Q_{zx}^c/2\sqrt{3}$
By	Q_{xy} $Q_{xy}^c/2\sqrt{3}$	S_y $(S_y^c+4T_y^c/3)/5$	Q_{yz} $Q_{yz}^c/2\sqrt{3}$

$$H_{\mathrm{cubic}} = \sum_{X=A,B} J_X \sum_{i=x,y,z} \bar{H}_{Xi} = \sum_{i=x,y,z} \frac{1}{5}\left[(J_A+J_B)S_i^c + \frac{1}{3}(-J_A + 4J_B)T_i^c\right]S_i + \frac{\sqrt{3}}{12}(J_A+4J_B)\sum_{j=yz,zx,xy} Q_j^c Q_j + \frac{\sqrt{3}}{8}J_A \sum_{k=u,v} Q_k^c Q_k, \tag{5}$$

where the positive J_A and J_B are introduced as independent antiferromagnetic coupling constants. When $J_A=8J_B$ is satisfied, the quadrupolar exchange interaction becomes highly symmetric, expressed by ($\boldsymbol{Q}^c \cdot \boldsymbol{Q}$), as given in Eq. (1).

We next show that $\bar{H}_{Az}$ is expressed by the two-channel Kondo type of exchange form $\Sigma_\mu c_{\mu\sigma}^\dagger c_{\mu\sigma'}(\boldsymbol{\sigma}/2)_{\sigma\sigma'} \cdot \boldsymbol{S}$, where μ ($=1,2$) and σ ($=\uparrow,\downarrow$) represent channel and pseudospin, respectively. The Clebsch–Gordan method gives the 3×3 matrix expression as

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad S_+ = S_-^\dagger = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \tag{6}$$

for the $S=1$ spin, where $S_\pm = S_x \pm iS_y$. In the same manner, the $S^c=3/2$ operators are expressed by the 4×4 matrices as

$$S_z^c = \frac{1}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, \quad S_+^c = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{7}$$

Then, these equations lead to the following matrices for the Az group in Table I:

$$\tau_1^{Az} = \frac{1}{2} Q_v = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{8}$$

$$\tau_2^{Az} = \frac{1}{2} Q_{xy} = \frac{1}{2} \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \tag{9}$$

and

$$\tau_1^{Az,c} = \frac{1}{2\sqrt{3}} Q_v^c = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{10}$$

$$\tau_2^{Az,c} = \frac{1}{2\sqrt{3}} Q_{xy}^c = \frac{1}{2} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \tag{11}$$

$$\tau_3^{Az,c} = \frac{2}{5}\left(S_z^c - \frac{1}{3} T_z^c \right) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{12}$$

One can find that $\boldsymbol{\tau}^{Az}$ is regarded as a $S=1/2$ spin operator within the subspace of $|+\rangle$ and $|-\rangle$ for the local $S=1$ states. For the corresponding $S^c=3/2$ conduction electrons, the m components are mapped to channel μ and pseudospin σ degrees of freedom as $(3/2, 1/2, -1/2, -3/2) \rightarrow (1\uparrow, 2\uparrow, 1\downarrow, 2\downarrow)$ for $\boldsymbol{\tau}^{Az,c}$. By applying the same procedure to the Bz group in Table I, it is shown that $\bar{H}_{Bz}$ is of the two-channel Kondo type as well. In this case, $\boldsymbol{\tau}^{Bz}$ is represented by a local $S=1$ spin and the $m \rightarrow (\mu, \sigma)$ correspondence for $\boldsymbol{\tau}^{Bz,c}$ is given by $(3/2, 1/2, -1/2, -3/2) \rightarrow (1\uparrow, 1\downarrow, 2\uparrow, 2\downarrow)$.

The two-channel $S=1$ Kondo effect by $\bar{H}_{Bz}$ stabilizes an FL state due to complete compensation of the local spin by the conduction electrons, while the overscreening $S=1/2$ case by $\bar{H}_{Az}$ leads to an NFL, as mentioned in Sec. II.[5] The same argument holds for $\bar{H}_{Xx}$ and $\bar{H}_{Xy}$. The NRG study demonstrated the relevance of the quadrupolar exchange interaction in Eq. (5) leading to the two-channel $S=1/2$ Kondo effect in the vicinity of the critical point at $\Delta=0$. This means that the relevant exchange for $\Delta \neq 0$ is described by the A group Hamiltonian $H_A = J_A(\bar{H}_{Ax} + \bar{H}_{Ay} + \bar{H}_{Az})$ in H_{cubic}.

We next argue the stability of FL vs NFL considering a uniaxial anisotropy effect on each term $H_{Ai} \equiv J_A \bar{H}_{Ai}$ $(i=x,y,z)$. For this purpose, we introduce the unitary matrices U_{Ai} and U_{Ai}^c that transform the quantized z axis to the $i=x,y$ axis via the following equations:

$$(U_{Ai})^{-1} \tau_3^{Ai} U_{Ai} = \tau_3^{Az}, \quad (U_{Ai}^c)^{-1} \tau_3^{Ai,c} U_{Ai}^c = \tau_3^{Az,c}, \tag{13}$$

respectively, where

$$U_{Ax} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -1 & 0 \end{pmatrix}, \quad U_{Ay} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \\ -1 & 1 & 0 \end{pmatrix}, \tag{14}$$

and

$$U_{Ax}^c = \frac{1}{4} \begin{pmatrix} a_+ & 1 & a_- & -1 \\ -a_- & 1 & a_+ & 1 \\ 1 & a_- & -1 & a_+ \\ -1 & a_+ & -1 & -a_- \end{pmatrix},$$

$$U_{Ay}^c = \frac{1}{4} \begin{pmatrix} a_+ & 1 & -a_- & 1 \\ -a_- & 1 & a_+ & 1 \\ -1 & -a_- & -1 & a_+ \\ 1 & -a_+ & 1 & a_- \end{pmatrix}. \tag{15}$$

The constant $a_\pm$ equals $2 \pm \sqrt{3}$. Using $P_{Ai} = U_{Ai} U_{Ai}^c$, $\bar{H}_{Ai}$ $(i=x,y)$ is reduced to $P_{Ai} \bar{H}_{Az} P_{Ai}^{-1}$. As discussed above, H_{Ai} is expressed by the two-channel Kondo Hamiltonian as

$$H_{Ai} = J_A \sum_{\mu=1,2} \sum_{\substack{kk' \\ \sigma\sigma'}} c_{k\mu\sigma}^{(i)\dagger} c_{k'\mu\sigma'}^{(i)} \left(\frac{\boldsymbol{\sigma}}{2} \right)_{\sigma\sigma'} \cdot \boldsymbol{S}^{(i)}. \tag{16}$$

Here, the superscript (i) represents the quantized i axis. The exchange interaction is expressed by the Pauli matrix $\boldsymbol{\sigma}$ and local pseudospin-$1/2$ $\boldsymbol{S}^{(i)}$ operators restricted to the quantized i axis. Using U_{Ai} in Eq. (13), the $S^{(i)}$ doublet $|\pm_i\rangle$ states are related to the $S=1$ triplet in Eq. (1),

$$|\pm_z\rangle = |\pm\rangle,$$

$$|+_x\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle), \quad |-_x\rangle = |0\rangle,$$

$$|+_y\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle), \quad |-_y\rangle = |0\rangle. \tag{17}$$

The transformation by U_{Ai}^c for the conduction electrons is given by

$$\begin{pmatrix} c_{k1\uparrow}^{(i)} \\ c_{k2\uparrow}^{(i)} \\ c_{k1\downarrow}^{(i)} \\ c_{k2\downarrow}^{(i)} \end{pmatrix} = (U_{Ai}^c)^{-1} \begin{pmatrix} c_{k,3/2} \\ c_{k,1/2} \\ c_{k,-1/2} \\ c_{k,-3/2} \end{pmatrix} \quad (i=x,y). \tag{18}$$

The uniaxial anisotropy effect, corresponding to the second term in Eq. (1), is apparently different between for the quantized z and for its perpendicular (x,y) axes. Using $S_z^{(i)} = \pm 1/2$, this is expressed by

$$H_{\text{uniaxial}}^{(z)} = \frac{1}{3}[(|+_z\rangle\langle +_z|) + (|-_z\rangle\langle -_z|)] = \frac{4}{3}\Delta[S_z^{(z)}]^2, \tag{19}$$

$$H^{(i)}_{\text{uniaxial}} = \frac{1}{3}[(|+_i\rangle\langle+_i|) - 2(|-_i\rangle\langle-_i|)] = \Delta\left[-\frac{1}{6} + S^{(i)}_z\right] \quad (i=x,y). \tag{20}$$

The latter is interpreted as Zeeman-type splitting of the local $S^{(i)}=1/2$ $(i=x,y)$ doublet so that Δ for the quantized x and y axes means a local spin field in the exchange interaction for H_{Ax} and H_{Ay}, respectively.

First, let us discuss the $\Delta<0$ case where the NFL state is stabilized. This is described by only $[H_{Az}+H^{(z)}_{\text{uniaxial}}]$, which means that $(H_{Ax}+H_{Ay})$ is irrelevant. For the quantized z axis, the anisotropy lowers the energy of the local doublet, keeping its degeneracy, coupled to all the orbitals of conduction electrons by H_{Az}. For the quantized $i=x,y$ axis, on the other hand, the anisotropy lifts the degeneracy of the doublet states $|\pm_i\rangle$ in Eq. (17) coupled to the conduction electrons by H_{Ai}. Since the exchange coupling is weakened effectively for the latter, the perpendicular Hamiltonian term $(H_{Ax}+H_{Ay})$ does not gain the energy compared with H_{Az}. Thus, the uniaxial anisotropy effect for $\Delta<0$ favors the NFL state derived from H_{Az}.

On the contrary, the $\Delta>0$ effect stabilizes the FL state due to $[H_{Ax}+H^{(x)}_{\text{uniaxial}}]$ or $[H_{Ay}+H^{(y)}_{\text{uniaxial}}]$ against the NFL. In Eq. (1), the singlet $|0\rangle$ of the $S=1$ triplet states is energetically lowered. For H_{Az}, the $\Delta/3$ level shift of the doublet $|\pm\rangle$ increases the total energy, while the completely decoupled $|0\rangle$ does nothing. On the other hand, the $(H_{Ax}+H_{Ay})$ term contains exchange coupling to the stabilized $|0\rangle$. For this reason, $(H_{Ax}+H_{Ay})$ gains an advantage over H_{Az} energetically. Note that the excited doublet $|\pm\rangle$ participates in singlet formation of the ground state as well as the lowest singlet $|0\rangle$. For the quantized $i=x,y$ axis, for instance, the $S^{(i)}_z$ moment is coupled to the conduction electrons as $[c^{(i)\dagger}_{k\mu\uparrow}c^{(i)}_{k'\mu\uparrow}-c^{(i)\dagger}_{k\mu\downarrow}c^{(i)}_{k'\mu\downarrow}]S^{(i)}_z$. In Eq. (18), one can find that the $m=\pm3/2$ $(m=\pm1/2)$ components are dominant in the spin-up (spin-down) electrons. The splitting of the $S^{(i)}_z$ doublet by the anisotropy lifts the degenerate $m=\pm3/2$ and $m=\pm1/2$ states of conduction electrons. This is the origin of the local quadrupolar field V^*_Q that reflects on the phase shift characterizing the FL state, as shown by the NRG result.

IV. CONCLUDING REMARKS

In this paper, we connect the FL and NFL physics via the Kondo Hamiltonian for a triplet impurity as the critical point separating the FL and NFL phases. In our model presented here, the phase separation is controlled by a uniaxial field that splits the triplet into a singlet and a doublet. If the singlet (doublet) is lower lying, the FL (NFL) state is stabilized at low temperatures. As shown in Fig. 2, the local charge redistribution reveals how to connect the stabilized FL and NFL at the critical point. The NRG analysis shows the same feature with the FL-NFL crossover for the case of a local spin field effect in the two-channel Kondo model. With the help of the SU(2) Lie algebra, this analogy brings us an idea that the critical point with cubic symmetry is described by a combination of three two-channel Kondo Hamiltonian terms classified by the quantized axes. A uniaxial anisotropy of the local triplet lifts the threefold degeneracy, leading to the FL and NFL phase separation.

Since our theory is realistic, it encourages experiments to observe the competing FL and NFL states in a nearly cubic system. The idea can be tested for relevant quadrupoles of triplet ground states identified in PrB_6 where quadrupole ordering occurs at low temperatures.[18,19] Applying pressure is an interesting attempt, which lowers the crystal symmetry and suppress the quadrupole order to realize the Kondo effect discussed above. Since the Kondo effect is very sensitive to the crystal field, a small deviation from the cubic symmetry causes the competing FL and NFL physics. As another experimental application, dilution of Pr by La, which would be also important, is in progress.[20]

Finally, we comment on a possibility of FL vs NFL competition in a series of Pr based filled skutterudites PrT_4X_{12} (T=Fe, Ru, Os; X=P, As, Sb) with T_h point-group symmetry (without fourfold axes in O_h).[21] The Pr ion has the f^2 singlet-triplet configuration as the lowest-lying state.[22–24] The crystal-field energy splitting can be controlled by changing the surroundings of Pr, for instance, by partially substituting one element for another among the transition metal (T) or pnictogen (X) ions.[25] In the paramagnetic phase of $PrFe_4P_{12}$, Kondo-type behavior is observed.[26] It is expected that a good experimental adjustment of the Pr crystal-field configuration can derive the same type of FL vs NFL competition discussed in the present paper.[14] In this case, the FL state is dominated by the Pr singlet and the NFL is due to the Pr triplet.

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