A nonmagnetic effective Hamiltonian of a frustrated tetrahedron Kondo model

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Abstract. We investigate a four-site impurity Kondo model with 1/2 spins locating on vertices of a tetrahedron, when the inter site superexchange interaction $J$ is much larger than band width $D$ of conduction electrons and magnetic Kondo coupling. In this case, four impurity spins form doubly-degenerate ground states and we derive their effective Hamiltonian induced by coupling with conduction electrons. Quadrupole moments of the ground states couple to those of conduction electrons. For particle-hole asymmetric case, we find that the model can be mapped to that with a pseudospin-1/2 impurity coupled with three-orbital conduction electrons with keeping U(1) charge conservation for each of the orbital.

1. Introduction
Frustration in condensed matter has been attracted much attention due to possible mechanism stabilizing spin liquid states without any symmetry breaking[1]. In the context of cluster impurity Kondo model, it has been shown that triangular cluster impurity configuration with antiferromagnetic interactions between the impurity spins leads to a stable non Fermi liquid (NFL) ground state on a basis of numerical renormalization group and boundary conformal field theory[2]. This contrasts with an unstable NFL state in a two-impurity Kondo model studied more than two decades ago[3], where there is no magnetic frustration between the impurity spins. This suggests that, exotic NFL states emerge and are stabilized, when antiferromagnetic Kondo interactions are switched on for localized spins on geometrically frustrated clusters.

In this paper, we construct an effective low-energy model in another fundamental cluster with frustrated geometry, a tetrahedron cluster, which has a possibility to realize NFL ground states. As in the case of triangular cluster, there remains nonmagnetic degeneracy in the ground state of tetrahedron cluster spins that antiferromagnetically interact with each other. We will concentrate on deriving an effective Hamiltonian that describes low-energy dynamics of this degenerate ground state interacting with conduction electrons by using symmetry argument and scaling approach[4].

2. Model
2.1. Hamiltonian
In this paper, we investigate a tetrahedron-impurity Kondo model, in which four spin-1/2 impurities are located on the vertices of a tetrahedron. They interact antiferromagnetically
to each other with Heisenberg coupling $J$ and also interact with conduction electrons via Kondo exchange coupling $J_K$:

$$
H = \int d\vec{k} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + J \sum_{i\neq j=1}^{4} \mathbf{S}_i \cdot \mathbf{S}_j + H_K
$$

(1)

$$
H_K = J_K \sum_{i=1}^{4} \mathbf{S}_i \cdot (\mathbf{s} \sigma') \int d\vec{k} d\vec{p} c_{k\sigma}^\dagger c_{p\sigma'} \exp[i(\vec{p} - \vec{k}) \cdot \vec{x}_i]
$$

(2)

where $\mathbf{S}_i (i = 1, 2, 3, \text{or } 4)$ and $c_{k\sigma}^\dagger$ represent the spin-1/2 operator at the site $i$ and the conduction electron creation operator with wavevector $\mathbf{k}$ and spin $\sigma$, and $\mathbf{s} = \sigma/2$, where $\tau^x$, $\tau^y$, and $\tau^z$ are the Pauli matrices. The intersite antiferromagnetic superexchange interaction $J > 0$ is set to the largest energy scale in this paper. A schematic picture of this model is shown in Fig. 1(a).

For later purposes, let us define the following conduction electron operators[5], which directly couple to the impurity spins:

$$
c_{k\sigma} = \int d\Omega_k c_{k\sigma} \exp(i\mathbf{k} \cdot \mathbf{x}_i),
$$

(3)

with $k = |\mathbf{k}|$ and $d\Omega_k$ is the angular integral in the $\mathbf{k}$-space. $c_{k\sigma}$’s, however, are not orthogonal with each other. An orthonormal set of conduction electron operators is obtained by using linear combinations of $c_{i\sigma}$ as

$$
c_{0\sigma} = N_{kA_1}^{-1} (c_{1\sigma} + c_{2\sigma} + c_{3\sigma} + c_{4\sigma})/2, \quad c_{a\sigma} = N_{kT_2}^{-1} (c_{1\sigma} - c_{2\sigma} + c_{3\sigma} - c_{4\sigma})/2,
$$

(4)

$$
c_{b\sigma} = N_{kT_2}^{-1} (c_{1\sigma} - c_{2\sigma} - c_{3\sigma} + c_{4\sigma})/2, \quad c_{c\sigma} = N_{kT_2}^{-1} (c_{1\sigma} + c_{2\sigma} - c_{3\sigma} - c_{4\sigma})/2,
$$

(5)

where $N_{kA_1} = k^2[1 + 3\sin(kA_1)]$ and $N_{kT_2}^2 = k^2[1 - \sin(kA_1)/kA_0]$ with $a_0 = |\mathbf{x}_1 - \mathbf{x}_2|$. Note that $c_{0\sigma}$ and $c_{i\sigma}$ ($l = a, b, \text{or } c$) are basis sets of $A_1$ and $T_2$ representations in $T_2$ point group symmetry, respectively. For later purposes, we define the coefficients in Eqs. (4) and (5) as $c_{0\sigma} = \sum_i f_{0i} c_{i\sigma}/N_{kA_1}$, $c_{a\sigma} = \sum_i f_{ai} c_{i\sigma}/N_{kT_2}$ and similarly for $b$ and $c$. Using these bases, the Hamiltonian (2) is rewritten as

$$
H_K = \sum_{\sigma \sigma'} \int d\vec{k} d\vec{p} \left[J_0 \mathbf{S}_0 \cdot \mathbf{s}_{\sigma \sigma'} c_{0\sigma}^\dagger c_{\sigma'} + J_1 \mathbf{S}_1 \cdot \sum_{l=a,b,c} c_{l\sigma}^\dagger c_{l\sigma'} \mathbf{s}_{\sigma \sigma'} + J_2 \sum_{l=a,b,c} \left|\varepsilon^{lmm}\right| \left(S_l \cdot \mathbf{s}_{\sigma \sigma'} c_{lm\sigma}^\dagger c_{n\sigma'} + \text{h.c.}\right) \right],
$$

(6)

where $J_0 = J_K N_{a_1}^2/2$, $J_2 = J_K N_{a_2}^2 N_{A_1}/2$, and $J_1 = J_3 = J_K N_{T_2}^2/2$, and $\varepsilon^{lmm}$ is the antisymmetric tensor with $\varepsilon^{abc} = 1$. We have approximate $N_{kA_1,T_2} \sim N_{kF,A_1,T_2} = N_{A_1,T_2}$ with $k_F$ being the Fermi wave number. $\mathbf{S}_i (l = 0, a, b, \text{and } c)$ are given as $\mathbf{S}_i = \sum_j f_{ji} \mathbf{S}_j$. Here, $\mathbf{S}_0 (\mathbf{S}_{a,b,c})$ is $A_1 (T_2)$ representation as in Eqs. (4) and (5). The conduction electron kinetic-energy part in the Hamiltonian (1) is approximated as

$$
\int d\vec{k} c_{k\sigma}^\dagger c_{k\sigma} \simeq \int d\vec{k} \sum_{l=0,a,b,c,d} \epsilon_{kl} c_{l\sigma}^\dagger c_{k\sigma} = H_c,
$$

(7)

since only these four components directly couple with impurity spins. We further approximate $\epsilon_{kl} \sim v_F (k - k_F)$, where $v_F$ indicates the velocity at Fermi energy. The density of states of conduction electrons are set to constant $\rho$ from $-D_\infty = -\lambda D$ to $D$ as shown in Fig. 1(b). Note that the case $\lambda \neq 1$ represents a conduction electron band without particle-hole symmetry.
2.2. Ground states and low-energy states of four local spins

As we mentioned before, the antiferromagnetic superexchange interaction $J$ is the largest energy scale in the system. Let us first examine the energy spectrum and the eigenstates for the isolated tetrahedron. Since the superexchange interaction term in the Hamiltonian (1) becomes $2JS_0^2 + \text{constant}$, the ground state of a tetrahedron impurity is a nonmagnetic doublet, i.e., the eigenvalue of the total spin $S(=2S_0)$ $S = 0$, which is $E$ representation in $T_d$ point group. The wavefunctions for these two states are given as

$$|e_1\rangle = \frac{1}{\sqrt{2}}(1 + i \hat{I}) \left( |\uparrow\uparrow\uparrow\uparrow\rangle - |\downarrow\downarrow\downarrow\downarrow\rangle \right),$$

$$|e_2\rangle = \frac{1}{\sqrt{3}}(1 + i \hat{I}) \left( |\uparrow\uparrow\uparrow\downarrow\rangle - \frac{1}{2} \left( |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle \right) \right),$$

where $|\sigma_1\sigma_2\sigma_3\sigma_4\rangle$ represents a state with the $z$-component of spin $\sigma_i(=\uparrow$ or $\downarrow)$ at site $i$ and $\hat{I}$ is the spin inversion operator.

The first excited states are $T_2$ multiplet with the total spin $S = 1$, i.e., nine-fold degenerate states and the energy gap is $J$. The wavefunctions of $T_2$ states are given as

$$|0\rangle_a = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\uparrow\uparrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle \right), |0\rangle_b = \frac{1}{\sqrt{2}} \left( |\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle \right), |0\rangle_c = \frac{1}{\sqrt{2}} \left( |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle \right),(10)$$

$$|\uparrow\downarrow\rangle = \sum_i f_i S^-_i |\uparrow\uparrow\uparrow\uparrow\rangle, \quad |\downarrow\uparrow\rangle = - \sum_i f_i S^+_i |\downarrow\downarrow\downarrow\downarrow\rangle,$$

where $|S,\ell\rangle$ is a $T_2$ state with the $z$-component of spin $S_z$ and orbital index $\ell = a, b, \text{ or } c$. There is also an $S = 2$ excited state with the excitation energy $3J$, but it is not relevant to our discussion in the following, because of vanishing matrix element of $S_0$ and $S_l(l = a, b, \text{ and } c)$ between the ground states and the second excited states. The matrix elements of $S_l$ between the ground and the first excited states are finite, while those of $S_0$ vanishes since the ground states are spin singlet. We show the nonvanishing matrix elements in Table 1.

3. Effective Hamiltonian

3.1. Symmetry

Now, we derive an effective Hamiltonian describing interactions between nonmagnetic $E$ states and conduction electrons. Since the ground state is doublet, we can express any operators projected to these two states in terms of the Pauli matrices. Relevant operators in this paper are $\tau^x = |e_1\rangle\langle e_2| + |e_2\rangle\langle e_1|$ and $\tau^z = |e_1\rangle\langle e_1| - |e_2\rangle\langle e_2|$, which form two-dimensional $E$ representation and represent quadrupole moment of the ground states, or alternatively scalar chirality of the ground state[6], when we employ the complex representation for the $E$ state: $|e_1\rangle \pm i|e_2\rangle|/\sqrt{2}$.
Table 1. List of nonvanishing matrix elements between the ground states and first excited states \( \langle S_z \mid S_{z'} \pm \mid e_1 \rangle \) (i = 1, or 2; l, l' = 0, a, b, or c). \( S^z_l \) is defined as in a usual manner \( S^z_l = S^z_1 \pm i S^y_l \). Elements not shown are all zero.

| \( \langle S_z \mid S_{z'}^\pm \mid e_1 \rangle \) | \( \langle S_z \mid S_{z'}^\pm \mid e_2 \rangle \) |
|---------------------------------|---------------------------------|
| \( \langle 0 \mid a \mid S_{z_1}^\pm \mid e_1 \rangle = \langle 0 \mid b \mid S_{z_1}^\pm \mid e_1 \rangle \) | \( \frac{1}{\sqrt{2}} \) |
| \( \langle \uparrow \mid a \mid S_{z_1}^\pm \mid e_1 \rangle = \langle \uparrow \mid b \mid S_{z_1}^\pm \mid e_1 \rangle \) | -1 |
| \( \langle \downarrow \mid a \mid S_{z_1}^- \mid e_1 \rangle = \langle \downarrow \mid b \mid S_{z_1}^- \mid e_1 \rangle \) | 1 |

As for the conduction electron part, operators consisting of two fermion operators with \( E \) representation are the most relevant and can couple with the impurity. It turns out that there is only one such \( E \) representation for the conduction electron part, which is given as

\[
\int dk dp \sum_{\sigma} \frac{1}{\sqrt{3}} [c_{k\sigma}^\dagger c_{p\sigma} - c_{k\sigma} c_{p\sigma}^\dagger - 2c_{k\sigma}^\dagger c_{k\sigma} c_{p\sigma}] + 2 \int dk dp \sum_{\sigma} [c_{k\sigma}^\dagger c_{p\sigma} - c_{k\sigma} c_{p\sigma}^\dagger].
\] (12)

Thus, taking into account trivial potential scattering terms in \( A_1 \) and \( T_2 \) sectors, the effective interactions in low-energy sector should be

\[
H_{\text{eff}}^{\text{K}} = g \int dk dp \sum_{\sigma} \left[ \tau^x \frac{1}{\sqrt{3}} \left( c_{k\sigma}^\dagger c_{p\sigma} + c_{k\sigma} c_{p\sigma}^\dagger - 2c_{k\sigma}^\dagger c_{k\sigma} c_{p\sigma} \right) + \tau^y \left( c_{k\sigma}^\dagger c_{p\sigma} - c_{k\sigma} c_{p\sigma}^\dagger \right) \right] + V_0 \int dk dp \sum_{\sigma} c_{k\sigma}^\dagger c_{p\sigma} + V_1 \int dk dp \sum_{\sigma} \sum_{l=a,b,c} c_{k\sigma}^\dagger c_{l\sigma} c_{p\sigma}. \]

(13)

Note that operator \( \tau^y \) does not appear, since \( \tau^y \) belongs to \( A_2 \) representation and there is no such representation in conduction electron part as far as we consider quadratic operators of fermions. The effective interaction (13) is purely nonmagnetic and all the terms break particle-hole symmetry \((c_{k\sigma}^\dagger \leftrightarrow \sigma c_{k\sigma})\), which is not broken in the magnetic Kondo couplings in \( H_K \). Thus, the particle-hole asymmetry in the conduction electron band \( \lambda \neq 1 \) is essential to realize the model (13)[7]. Since there is no magnetic terms in the effective Hamiltonian (13), which is present in the original interactions (2), the magnetic interactions play a role of “source” of the nonmagnetic interactions. It is noted that emergent \( U(1) \otimes U(1) \otimes U(1) \) symmetry is present in the effective model (13), which corresponds to the charge conservation of each conduction electron orbital. Such an emergent charge conservation was also found in the NFL state in triangular Kondo model[2].

3.2. Renormalization group equations

Let us demonstrate how the model (13) is generated in the low-energy sector of the tetrahedron Kondo model (1). Here, we employ a renormalization group method[4] rather than perturbation theory in terms of \( 1/J \). Following the discussion in Ref. [4], we can derive one-loop renormalization group equations for this system. We take into account the virtual scattering processes in the second order in \( H_K + H_{\text{eff}}^{\text{K}} \), in which conduction electrons near the Fermi surface are scattered into the band edge within the width \( \delta D \) and \( \lambda \delta D \) as shown in Fig. 1(b). Initially,
the parameters $g$, $V_0$ and $V_1$ are all zero. They are generated by the second order processes of the magnetic interactions $J$'s in Eq. (6). Since we project out all the excited states, the magnetic couplings are not renormalized. Owing to the selection rule, the possible virtual states are $T_2$ states and the matrix elements are given in Table 1. The renormalization group equations are, indeed, trivial because of no renormalization in magnetic exchange interactions and commutativity in the conduction electron part of the effective Hamiltonian (13):

$$\frac{\partial g}{\partial D} = \frac{\sqrt{3}f(D, \lambda, J)}{3} \left( \rho J_2^2 - \rho J_3^2 \right),$$

$$\frac{\partial V_0}{\partial D} = \frac{3f(D, \lambda, J)}{4} \rho J_2^2,$n

$$\frac{\partial V_1}{\partial D} = f(D, \lambda, J) \left( \frac{\rho J_2^2}{4} + \frac{\rho J_3^2}{2} \right),$$

$$\frac{\partial J_0}{\partial D} = \frac{\partial J_1}{\partial D} = \frac{\partial J_2}{\partial D} = \frac{\partial J_3}{\partial D} = 0,$$ (17)

where $f(D, \lambda, J) = \frac{D(1-\lambda)^2}{(D+J)(AD+J)} \sim (1-\lambda)/J$ for $J \gg D$. The scaling stops when the coupling constant $|g(D^*)| \sim D^*$ and $D^*$ is given as $D^* \simeq D\alpha/(1+\alpha) \simeq \alpha D$ with $\alpha = \sqrt{3}\rho[(1-\lambda)(J_2^2 - J_3^2)]/(8J)$ for $J \gg D \gg |\rho|J_2^2 - J_3^2|$. Since $A_1$ component of conduction electrons is decoupled in the effective Hamiltonian (13), we can concentrate on the $T_2$ components hereafter.

Now, we have obtained the effective coupling constant $g$ and $V_1$ in the effective Hamiltonian (13). Next, in order to capture physical picture of the effective model, we consider strong coupling limit, where the conduction electron kinetic part $H_c$ can be neglected. Diagonalizing the effective Hamiltonian (13), we obtain various ground states as shown in Fig. 2. Each state is characterized by the occupation numbers in $T_2$ conduction electrons $n_l \equiv \int dk \sum_{\sigma} n_{kl\sigma}$: $(n_a, n_b, n_c)$ and the ground state energy is given as $-|g|\sqrt{\frac{3}{2}} \sqrt{(n_a - n_b)^2 + (n_b - n_c)^2 + (n_c - n_a)^2} + V_1(n_a + n_b + n_c)$ . Except for the lines $|g| = \pm \sqrt{3}V_1/2$, the ground states are nonmagnetic. The states $|0,0,0\rangle$ and $|2,2,2\rangle$ are both doublet, where orbital degeneracy of $E$ states remains, i.e., $(0,0,0)|e_1\rangle$ and $(0,0,0)|e_2\rangle$, while $|2,2,0\rangle$ and $|2,0,0\rangle$ are both orbital triplet. Here, for example, $|2,0,0\rangle$ means the three states: $(2,0,0)$, $(0,2,0)$ and $(0,0,2)$. In the cases of $|2,0,0\rangle$ and $|2,0,0\rangle$ ground states, further step renormalization generates effective interactions, in which residual degrees of freedom couple to the pair hopping processes between different orbitals of conduction electrons. Further analysis of this effective model is now in progress by using boundary conformal field theory[8]. The high symmetry present in the effective model also enables us to carry out an efficient numerical renormalization group calculations in the model with three orbital degrees of freedom. The results support the present one and will be published elsewhere[8].

4. Summary and perspective
In summary, we have discussed an effective Hamiltonian of a tetrahedron Kondo model for $J \gg J_K$. The point group symmetry restricts the type of Kondo coupling between conduction electrons and degenerate impurity $E$ states. Particle-hole asymmetry also plays an important role to realize the Kondo-like effective model. In the effective model, conduction electrons in each orbital are not scattered into different orbitals by scatterings due to the impurity. This means U(1) charge for each of the conduction electron orbital conserves during scattering processes. Detailed analyses of the fixed point and possible fixed points for $J_K \gg J$ are now in progress.
We also study a tetrahedron Anderson impurity model by using continuous time quantum Monte Carlo method and results will be published elsewhere[9].
Figure 2. Ground state phase diagram of $H_{\text{eff}}$ at the scale $\sim D^*$. 

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