Phase evolution of the two-dimensional Kondo lattice model near half-filling

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Abstract
Within a mean-field approximation, the ground state and finite temperature phase diagrams of the two-dimensional Kondo lattice model have been carefully studied as functions of the Kondo coupling $J$ and the conduction electron concentration $n_c$. In addition to the conventional hybridization between local moments and itinerant electrons, a staggered hybridization is proposed to characterize the interplay between the antiferromagnetism and the Kondo screening effect. As a result, a heavy fermion antiferromagnetic phase is obtained and separated from the pure antiferromagnetic ordered phase by a first-order Lifshitz phase transition, while a continuous phase transition exists between the heavy fermion antiferromagnetic phase and the Kondo paramagnetic phase. We have developed an efficient theory to calculate these phase boundaries. As $n_c$ decreases from the half-filling, the region of the heavy fermion antiferromagnetic phase shrinks and finally disappears at a critical point $n_c^* = 0.8228$, leaving a first-order critical line between the pure antiferromagnetic phase and the Kondo paramagnetic phase for $n_c^* < n_c$. At half-filling limit, a finite temperature phase diagram is also determined on the Kondo coupling and temperature ($J-T$) plane. Notably, as the temperature is increased, the region of the heavy fermion antiferromagnetic phase is reduced continuously, and finally converges to a single point, together with the pure antiferromagnetic phase and the Kondo paramagnetic phase. The phase diagrams with such triple point may account for the observed phase transitions in related heavy fermion materials.

Keywords: heavy-fermion phenomena, phase transitions, anti-ferromagnetics

(Some figures may appear in colour only in the online journal)
correlation may produce a heavy fermion antiferromagnetic phase (HFAFM) with coexisting AFM order and Kondo screening near half-filling [6–10]. The HFAFM has been observed in CeCoGe$_3$Si$_2$ [11] and Ce$_3$Pd$_2$Si$_6$ [7], etc. In Ce$_3$Pd$_2$Si$_6$, the HFAFM is observed within the magnetically ordered phase, indicating the separation of two transitions, i.e. the breakdown of Kondo screening effect and concomitant Fermi surface reconstruction (FSR) which happens between HFAFM and pure AFM, and the magnetic transition which occurs between HFAFM and KP phase [7]. However, studies of Hall coefficient and pressure effect in YbRh$_2$Si$_2$ have shown that the Kondo breakdown occurs precisely at the magnetic transition, while under Co and Ir doping, two transitions separate [8–10]. The Kondo breakdown also occurs away from the magnetic transition in CeIn$_3$ and CeRh$_1$.Co$_1$In$_6$ [12, 13].

To understand the behavior of the phase transitions in these materials, the corresponding parameter region and the features of the AFM phase, the HFAFM phase and the KP phase, these have been investigated within the framework of the Kondo lattice model (KLM) or Kondo Heisenberg lattice model, and intensively studied at zero temperature by mean-field approximation, variational Monte Carlo calculations, Gutzwiller approximation, etc [6, 14–24]. At the half-filling limit, reconstruction of the energy bands leads to an insulating state, and the ground state phases were computed with varying Kondo coupling [6, 14, 15]. Away from half-filling, the phase transitions are discussed by mean-field approximation on the Kondo Heisenberg lattice model, and the shift from offset-to-convergence between the Kondo breakdown and magnetic transition is proposed to be driven by the change of the Heisenberg exchange and the ratio of short and long-range hopping strength [10].

Actually, the ground state phases and their features are controlled by the Kondo coupling $J$, the electron occupation number $n_c$ and the electron hopping strength. However, the phase evolutions with these parameters have not been fully explored yet, particularly how these phases evolve with $n_c$ and long-distance electron hopping remains an open issue [5, 24]. As the Kondo lattice favors an AFM configuration near half-filling [4, 10], we focus on the experimental relevant region near half-filling, and study the possible coexistence of AFM and Kondo screening, then calculate the corresponding regions of HFAFM, AFM and KP phases on the $n_c$-$J$ plane. In order to deal with this issue, we adopt the slave-fermion mean-field technique on the KLM, and develop an efficient theory to calculate the phase boundaries between various phases. We show that the relative positions of Kondo breakdown and magnetic transition can be shifted by both $n_c$ and $J$, on the $n_c$-$J$ plane. As $n_c$ decreases, two transitions get closer and then coincide. This $n_c$-generated offset-to-convergence structure with a triple point in the phase diagram is related to the experimental observations of Ce$_3$Pd$_2$Si$_6$ and YbRh$_2$Si$_2$ under doping.

On the other hand, most of earlier works focused on the ground state, while detailed theoretical studies at finite temperatures are still lacking. In the case when the occupation number of the conduction electron $n_c$ is far away from half-filling, the coexisting phase of FM and Kondo screening has been investigated at finite temperatures and the phase diagram has been derived [25, 26]. Remarkably, the boundaries separating the various phases joint at a single point on the $J$-$T$ plane, so an interesting issue arises as to whether the half-filled Kondo lattice system possesses a similar feature in the finite temperature phase diagram. Therefore, we study the ground state and finite-temperature phase diagrams of the Kondo lattice model at and away from half-filling, attempting to give a detailed description of the evolution of the various phases with the Kondo coupling, the conduction electron occupation number, the electron hopping strength and temperature. To this end, a modified mean-field decoupling technique for the Kondo interaction is employed, then the phase diagrams are obtained as functions of $n_c$, $J$, $T$, and $T$. Our method turns out to give a compact description of the phase diagrams at both zero and finite temperatures.

II. Model and mean-field treatment

We consider the spin-$1/2$ Kondo lattice model on a two-dimensional square lattice with $N$ sites,

$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} (c_{\mathbf{k}, \sigma} \mathcal{H}_1 + c_{\mathbf{k}, \sigma}^\dagger) + J \sum_i S_i \cdot S_{\text{m}},$$

(1)

where $c_{\mathbf{k}, \sigma}$ is the dispersion of conduction electrons, which interact with local moments through antiferromagnetic Kondo exchange $J > 0$, and $\mu$ denotes the chemical potential. $S_i = \frac{1}{2} \sum_{\alpha, \beta} \sigma_{\alpha, i} \sigma_{\beta, i}$ with $\sigma$ being the Pauli matrix, represents the spin density for conduction electrons, while the local moments can be written in the slave-fermion representation as $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha, \beta} \sigma_{\alpha, i} \sigma_{\beta, i}$, which is subject to the restriction $\sum_{\mathbf{i}} f_{\mathbf{i}} f_{\mathbf{i}} = 1$ imposing by a Lagrangian term $\frac{1}{2} \lambda \left( \sum_{\mathbf{i}} f_{\mathbf{i}} f_{\mathbf{i}} - 1 \right)$. The Kondo interaction can be decomposed into

$$J \sum_i S_i \cdot S_{\text{m}} = - \frac{3J}{8} \sum_i \left( c_{\mathbf{i}, f_{\mathbf{i}, \uparrow} + c_{\mathbf{i}, f_{\mathbf{i}, \downarrow}} (f_{\mathbf{i}, \uparrow} f_{\mathbf{i}, \downarrow} + f_{\mathbf{i}, \downarrow} f_{\mathbf{i}, \uparrow}) \right) + \frac{J}{8} \sum_i \left( c_{\mathbf{i}, f_{\mathbf{i}, \uparrow} - c_{\mathbf{i}, f_{\mathbf{i}, \downarrow}} (f_{\mathbf{i}, \uparrow} f_{\mathbf{i}, \downarrow} - f_{\mathbf{i}, \downarrow} f_{\mathbf{i}, \uparrow}) \right)$$

(2)

where the first term represents the singlet hybridization between conduction electrons and slave fermions and the three other terms describe the triplet pairings. This expression captures SU(2) invariance of the Kondo coupling. In contrast, in previous mean-field studies, the Kondo exchange was decomposed into longitudinal and transverse parts [6, 14]: $J \mathbf{S}_i \cdot \mathbf{S}_{\text{m}} = J S_{i, \uparrow} S_{i, \downarrow} + \frac{J}{2} (S_{i, \uparrow}^2 + S_{i, \downarrow}^2 + S_{i, \uparrow} S_{i, \downarrow})$. As we can see below, our treatments give more reliable results and compact phase diagrams at both zero and nonzero temperatures.

In order to describe the antiferromagnetism in the Kondo lattice model, two AFM order parameters

$$J \sum_i S_i \cdot S_{\text{m}} = - \frac{3J}{8} \sum_i \left( c_{\mathbf{i}, f_{\mathbf{i}, \uparrow} + c_{\mathbf{i}, f_{\mathbf{i}, \downarrow}} (f_{\mathbf{i}, \uparrow} f_{\mathbf{i}, \downarrow} + f_{\mathbf{i}, \downarrow} f_{\mathbf{i}, \uparrow}) \right) + \frac{J}{8} \sum_i \left( c_{\mathbf{i}, f_{\mathbf{i}, \uparrow} - c_{\mathbf{i}, f_{\mathbf{i}, \downarrow}} (f_{\mathbf{i}, \uparrow} f_{\mathbf{i}, \downarrow} - f_{\mathbf{i}, \downarrow} f_{\mathbf{i}, \uparrow}) \right)$$

(2)
\( m_f = \frac{1}{2} \sum_{\sigma} (f_i^\dagger f_{i\sigma}) e^{iQ \cdot \mathbf{R}}, m_c = -\frac{1}{2} \sum_{\sigma} (c_{i\sigma}^\dagger c_{i\sigma}) e^{iQ \cdot \mathbf{R}} \)

are introduced to decouple the longitudinal term in Kondo interaction [6], where \( Q = (\pi, \pi) \) is the AFM vector, explicitly,

\[
J \sum_i S_i^+ \cdot S_i^z = \frac{1}{2} J \sum_{i, \sigma, \sigma'} \sigma c_{i\sigma}^\dagger c_{i\sigma'} f_{i\sigma'}^\dagger f_{i\sigma} c_{i\sigma} \approx -\frac{1}{2} J m_c \sum_{\sigma} f_{i\sigma} c_{i\sigma}^\dagger e^{iQ \cdot \mathbf{R}} + \frac{1}{2} J m_f \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} e^{iQ \cdot \mathbf{R}} + NJm_m f.
\]

Then the staggered magnetization is expressed by \( M = m_f - m_c \). Other AFM orders may also exist (e.g. with \( Q = (0, \pi) \) or \( (\pi, 0) \)), however, they have higher energies than the \( (\pi, \pi) \) phase at least near half-filling, so these phases are not considered in our calculations.

To characterize the Kondo screening in the presence of AFM long-range order, two different hybridization parameters on each magnetic sublattice A and B have to be introduced [6, 24],

\[
V_1 = \langle c_{iA}^\dagger f_{iB} \rangle, \\
V_2 = \langle c_{iB}^\dagger f_{iA} \rangle.
\]

The conventional hybridization parameter is expressed as

\[
V_1 = \frac{1}{2} (V_1 + V_2) = \frac{1}{2} (c_{iA}^\dagger f_{iB} + c_{iB}^\dagger f_{iA}) = \frac{1}{2} \sum_{\sigma} \langle c_{i\sigma}^\dagger f_{i\sigma} \rangle,
\]

while the staggered hybridization parameter is defined by

\[
V_2 = \frac{1}{2} (V_1 - V_2) = \frac{1}{2} (c_{iA}^\dagger f_{iA} - c_{iB}^\dagger f_{iB}) = \frac{1}{2} \sum_{\sigma} \langle c_{i\sigma}^\dagger f_{i\sigma} \rangle,
\]

which requires the breaking of particle-hole symmetry of the conduction electrons, i.e. \( n_c = 1 \), or \( t' = 0 \). It is seen that the singlet channel hybridizes the \( c \)- and \( f \)-fermions with the same wave vector, while the longitudinal exchange brings a momentum transfer \( Q \) within both \( c \)- and \( f \)-fermions (see equation (4)), resulting in the staggered triplet channel. The singlet and triplet hybridizations in Kondo interaction (equation (2)) can be estimated by Hartree–Fock approximation using \( V_1 \) and \( V_2 \), respectively. The local Lagrangian constraint is replaced by a uniform one: \( \lambda = \lambda \).

Though such a mean-field treatment, the model Hamiltonian is written in the momentum space by the matrix form

\[
\mathcal{H} = N\varepsilon_0 + \sum_{\mathbf{k}, \sigma} \Phi_{\mathbf{k}\sigma} \mathcal{H}_{\mathbf{k}\sigma} \Phi_{\mathbf{k}\sigma},
\]

where the superscript represents the summation of \( \mathbf{k} \) restricted in the magnetic Brillouin zone (MBZ) with boundaries \( |k_x \pm k_y| = \pi \). A four-component Nambu operator has been used as \( \Phi_{\mathbf{k}\sigma} = (c_{\mathbf{k}\sigma} e^{i\mathbf{Q}\cdot\mathbf{R}} + d_{\mathbf{k}\sigma} e^{-i\mathbf{Q}\cdot\mathbf{R}})^T \), and the constant term is given by \( \varepsilon_0 = \frac{1}{2} (3V_c^2 - V_t^2) + Jm_m m_f - \lambda \). The Hamiltonian matrix is given by

\[
\mathcal{H}_{\mathbf{k}\sigma} = \begin{pmatrix}
\epsilon_k - \mu & \frac{1}{2} J m_f \sigma & -3J V_c & \frac{1}{4} J V_c \\
\frac{1}{2} J m_f \sigma & \epsilon_k + \mu & \frac{1}{4} J V_c & -3J V_c \\
-3J V_c & \frac{1}{4} J V_c & \lambda & \frac{1}{2} J m_m \\
\frac{1}{4} J V_c & -3J V_c & \frac{1}{2} J m_m & \lambda
\end{pmatrix}
\]

where \( \epsilon_k = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y \) is the tight-binding dispersion of conduction electrons with nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping strength \( t \) and \( t' \), respectively. For the general case of conduction electron filling, the quasiparticle excitation spectra can not be derived analytically, and we have to perform numerical calculations. However, at half-filling, particle-hole symmetry can help to simplify the related calculations.

### III. Zero-temperature phase diagram at half-filling

We first discuss the half-filling limit with only NN hopping \( t \). In this case, the particle-hole symmetry guarantees \( \lambda = \mu = 0 \). Moreover, the staggered hybridization disappears as \( V_1 = 0 \). Further discussions including the influence of \( n_c \) and NNN hopping \( t' \) will be given in the following sections. The NN hopping between conducting electrons leads to the dispersion \( \epsilon_k = -2t(\cos k_x + \cos k_y) \), satisfying the relation \( \epsilon_{k+Q} = -\epsilon_k \). For convenience, we define \( V = -\frac{3}{2} V_c \), then the analytic formulas for the four branches of dispersions \( E_k^\pm \) and \( -E_k^\pm \) are obtained by diagonalizing \( \mathcal{H}_{\mathbf{k}\sigma} \), with

\[
E_k^\pm = \frac{1}{2\sqrt{2}} (\Lambda_k \pm \sqrt{\Lambda_k^2 - \Gamma_k^2}),
\]

where

\[
\Lambda_k = \epsilon_k^2 + \frac{1}{4} J^2 (m_m^2 + m_f^2) + \frac{1}{2} J^2 V_c^2,
\]

\[
\Gamma_k = \sqrt{\frac{3}{2} m_c \epsilon_k^2 + \frac{1}{4} J^4 (m_m m_f + V_c^2)^2},
\]

with the relation

\[
E_k^+ + E_k^- = \sqrt{\Lambda_k + \Gamma_k} \equiv E_k.
\]

At zero temperature, two lower branches of spectrums \( E_k^\pm \) lying below the Fermi level are full occupied, giving rise to an insulating heavy fermion state. Two higher branches \( E_k^\pm \) above the Fermi level give no contribution to the ground
state energy, therefore the ground state energy density is evaluated as
\[
E_{g}^{\text{HAFAFM}} = \frac{2}{3} J V^2 + J m_c m_f - \frac{1}{N} \sum_{k} E_k,
\]
with the summation of \(k\) running over the entire Brillouin zone. The mean-field parameters are determined by minimizing \(E_{g}^{\text{HAFAFM}}\) with respect to \(m_c, m_f\) and \(V\), yielding the self-consistent equations
\[
\frac{J}{4N} \sum_{k} E_k = \frac{m_c}{3(m_f - m_c)},
\]
\[
\frac{J^3}{8N} (m_c m_f + V^2) \sum_{k} E_k^{-1} = \frac{2m_f - 3m_c}{3(m_f - m_c)},
\]
\[
\frac{3J}{2N} \sum_{k} \frac{e_k^2}{E_k^{-1}} = 1 + m_f/m_c.
\]

In the whole coupling range, the pure AFM phase and KP phase should also be examined, then the stable ground state phase corresponds to the phase with lowest energy. When \(m_c = m_f = 0\), the energy density of KP phase is obtained by
\[
E_{g}^{\text{KP}} = \frac{2}{3} J V^2 - \frac{1}{N} \sum_{k} \sqrt{\varepsilon_k^2 + J^2 V^2},
\]
where \(V\) is determined by
\[
\frac{3}{8N} \sum_{k} \frac{1}{E_k^{-1}} = 4/3.
\]
For the pure AFM phase with \(V = 0\), the conduction electrons and the local moments are decoupled, resulting in the dispersions
\[
E_k^\pm = \pm \sqrt{\varepsilon_k^2 + \frac{1}{2} J^2 m_f^2}
\]
for the conduction electrons and
\[
E_k^\pm = \pm \frac{1}{2} J m_f
\]
for the local moments, respectively. By performing similar self-consistent calculations, the energy for AFM phase is found to be
\[
E_{g}^{\text{AF}} = -\frac{1}{N} \sum_{k} \sqrt{\varepsilon_k^2 + J^2 V^2/16},
\]
with order parameters \(m_f = 1/2\) and \(m_c = \frac{J}{8N} \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + J^2 V^2/16}}\).

The comparison of the ground state energies for AFM, HFAFM and KP phases is demonstrated in figures 1(a) and (b). As expected, the competition between ordering of local moments and Kondo screening leads to a coexisting solution in the intermediate Kondo coupling range \(J_1 < J < J_2\) [6], while the pure AFM phase and the KP phase exist in the regions \(J < J_1\) and \(J > J_2\), respectively. The derived staggered magnetization \(M = m_f - m_c\) and Kondo screening strength \(V\) are given in figure 2(a) as functions of the Kondo coupling \(J\). In the HFAFM phase, the fluctuations of local spins caused by Kondo screening effect suppress the AFM order, while the staggered magnetic order brings a rapid decrease of the Kondo screening strength. Both \(M\) and \(V\) vary continuously on the phase boundaries. \(J_1\) and \(J_2\) correspond to the lower boundary of the Kondo screening with order parameters \(m_c = 0, m_f = 0, V \to 0\), and the upper boundary of the AFM state with \(m_c = -0, m_f = 0, V \to 0\), respectively. The limit \(V \to 0\) can be replaced by setting \(V = 0\) in the self-consistent equations equation (14), because the denominators of the integral functions are always nonzero, leading to the numerical results \(J_1 = 3.1498t, m_f = 0.5, m_c = 0.2735\). To calculate \(J_2\), we can simply set \(m_c = 0, m_f = 0\) in the integrals in equation (14) because \(E_k = \frac{g}{2} \left( \varepsilon_k^2 + J^2 c^2 V^2 \right)\) and \(\Gamma_k = \frac{1}{2} J^2 c^2 V^2\) are both gapped. To keep \(m_f/m_c\) as a constant, we obtain the numerical solutions \(J_2 = 3.4161t, V = 0.5853\).

As noticed, the energy of HFAFM phase \(E_{g}^{\text{HAFAFM}}\) is tangent to \(E_{g}^{\text{AF}}\) on the edge \(J_1\), and to \(E_{g}^{\text{KP}}\) at \(J_2\), respectively, implying that the Kondo lattice system undergoes second-order phase transitions on both phase boundaries. The coexistence of AFM and Kondo screening in the Kondo lattice systems has been reported previously at zero temperature [6, 10, 14]. Though the proposed phase boundaries \(J_1\) and \(J_2\) are slightly different from our results, the main physical pictures remain the same. This inconsistency comes from differing mean-field
decoupling procedures. In the earlier studies [6, 14], the Kondo exchange was decomposed directly into longitudinal term and transversal part, then they were approximated by mean-field decoupling. While in this work, the singlet and triplet hybridizations between itinerant electrons and local moments are considered at the same level in the beginning. Therefore, our method can be generalized straightforwardly to deal with the case away from half-filling and with hopping beyond NN, as will be discussed in the following.

IV. Finite temperature phase diagram at half-filling

At finite temperatures $T > 0$, the existence of thermal fluctuations may shift the parameter region of the HFAFM phase. For simplicity and without loss of generality, we consider the half-filling case $n_e = 1$ with $t' = 0$. Since in this situation, the mean-field Hamiltonian has been diagonalized with the spectrum $E^c_k$ and $-E^f_k$, the free energy density $F^\text{HFAFM}$ can be calculated via the partition function, leading to the result (in the following we set the Boltzmann constant $k_B = 1$)

$$F^\text{HFAFM} = \frac{2}{3} JV^2 + J m_f - \frac{2T}{N} \sum_{k,\pm} \ln[2 \cosh(E^c_k/2T)].$$  \hspace{1cm} (17)

It is easy to verify the equivalence of the ground state energy and above free energy at the zero-temperature limit. The mean-field parameters are determined by minimizing $F^\text{HFAFM}$, then the self-consistent equations are derived as

$$\frac{4}{3J} = \frac{1}{N} \sum_{k,\pm} F^c_k \left[ 1 \pm \frac{2 \Lambda_k - J^c(m,m_f + V^2)}{2 \sqrt{\Lambda_k^2 - 1^2}} \right],$$

$$\frac{2m_c}{J} = \frac{1}{N} \sum_{k,\pm} F^c_k \left[ m_f \pm \frac{2 \Lambda_k m_f - J^c m_f(m,m_f + V^2)}{2 \sqrt{\Lambda_k^2 - 1^2}} \right],$$

$$\frac{1}{N} \sum_{k,\pm} F^c_k \left[ m_c \pm \frac{\Lambda_k m_c - J^c m_f(m,m_f + V^2) - 2m_c^2 \epsilon_k}{\sqrt{\Lambda_k^2 - 1^2}} \right] = \frac{2m_f}{J},$$  \hspace{1cm} (18)

where $F^c_k = \frac{1}{4\epsilon_k} \tanh(E^c_k/2T)$. In order to draw the phase diagram on the $J$-$T$ plane, the free energies of the pure AFM and KP phase should also be calculated.

The free energy of the KP phase is given by

$$F^\text{KP} = \frac{2}{3} JV^2 - \frac{2T}{N} \sum_{k,\pm} \ln[2 \cosh(E^c_k/2T)],$$  \hspace{1cm} (19)

with $E^c_k = \frac{1}{2} \sqrt{\epsilon_k^2 + J^c V^2/2 \pm \epsilon_k \sqrt{\epsilon_k^2 + J^c V^2}}$, and the equation for $V$:  \hspace{1cm} (20)

$$\frac{4}{3J} = \frac{1}{4N} \sum_{k,\pm} \tanh(E^c_k/2T) \left( 1 \pm \frac{|\epsilon_k|}{\sqrt{\epsilon_k^2 + J^c V^2}} \right).$$

As $T$ approaches Kondo temperature $T_K$, $V \to 0$, then $E^c_k \to |\epsilon_k|$, $E^c_k \to 0$, therefore $T_K$ of the KP phase is determined by

$$4 \frac{J}{3} = \frac{1}{2N} \sum_{\epsilon_k} \tanh(|\epsilon_k|/2T_K).$$  \hspace{1cm} (21)

For the pure AFM phase, the corresponding free energy density is written as

$$F^\text{AF} = \frac{J m_f}{N} - 2T \ln[2 \cosh(E^c_k/2T)] - \frac{2T}{N} \sum_{k,\pm} \ln[2 \cosh(E^c_k/2T)],$$  \hspace{1cm} (22)

with the self-consistent equations for the AFM order parameters:

$$m_c = \frac{J m_f}{N} \sum_{k,\pm} \tanh(E^c_k/2T) = 0,$$

$$m_f = \frac{1}{2} \tanh(Jm_f/4T) = 0.$$  \hspace{1cm} (23)

When $T$ approaches the Néel temperature $T_N$, $m_f, m_c \to 0$, then $E^c_k \to |\epsilon_k|, E^f_k \to 0$, thus the equation determining $T_N$ is derived as

$$\frac{32T_N}{J^2} = \frac{1}{N} \sum_{k,\pm} \tanh(|\epsilon_k|/2T_K).$$  \hspace{1cm} (24)

In order to derive the finite-temperature phase diagram, the free energies of the AFM phase, the KP phase and the HFAFM phase are compared. In figure 1(c), the free energies of the three phases are calculated at temperature $T = 0.2t'$, and are plotted in a narrow range of Kondo coupling strength $J$, in which the three phases have close free energies. It can be seen that the HFAFM phase is stable in the coupling range $J_1 < J < J_2$, as it exhibits lowest free energy, and the AFM and KP phase occur in the coupling region $J < J_1$ and $J > J_2$, respectively. The phase boundaries $J_1$ and $J_2$ now vary with temperature, and are crucial to determine the phase diagram on the $J$-$T$ plane. Alternatively, we can consider the characteristic temperature separating HFAFM phase with AFM phase as a function of $J$. On this boundary, $V$ approaches zero, so it appears as the Kondo temperature $T_K$ in HFAFM phase. Using equation (18), the equations determining $T_K$ are reduced to

$$\frac{4}{3J} = \frac{1}{N} \sum_{k,\pm} \tanh(E^c_k/2T_K) \left[ 1 \pm \frac{2 \Lambda_k - J^f m_f}{2 \sqrt{\Lambda_k^2 - 1^2}} \right] = 0,$$

$$\frac{m_c}{J} = \frac{m_f}{N} \sum_{k,\pm} \tanh(E^c_k/4T_K) = 0,$$

$$2m_f = \tanh(Jm_f/4T_K).$$  \hspace{1cm} (25)

where $\Lambda_k = \frac{\epsilon_k^2 + J^f (m^2 + m_f^2)}{2}$, $\Gamma_k = Jm_c \sqrt{\epsilon_k^2 + \frac{1}{4} J^f m_f^2}$, $E^c_k = \sqrt{\epsilon_k^2 + J^f m_f^2}/4$, and $E^f_k = Jm_f/2$.

On the boundary between HFAFM phase and KP phase, the AFM order vanishes, so this phase boundary line corresponds to the Néel temperature $T_N$. On this edge, $m_f/m_c$ remains finite. The self-consistent equations determining $T_N$ with varying $J$ are simplified to
The reduction $\epsilon_k$ at $J_N$ and $T_N$ are Néel temperature and Kondo temperature, respectively. Three phases converge to a single point on the $J$-$T$ plane.

$$\frac{4}{3J} = \frac{1}{N} \sum_{k} \frac{\tanh(E_k/2T_N)}{4E_k^+} \left[ 1 \pm \frac{|\epsilon_k|}{\sqrt{\epsilon_k^2 + J^2V^2}} \right],$$

$$\frac{2}{J} = \frac{1}{N} \sum_{k} \frac{\tanh(E_k/2T_N)}{4E_k^+} \left[ \gamma \pm 2\Lambda_k \gamma - J^2V^2 \right],$$

$$\frac{2\gamma}{J} = \frac{1}{N} \sum_{k} \frac{\tanh(E_k/2T_N)}{4E_k^+} \left[ 1 \pm \frac{\Lambda_k - J^2V^2/2 - 2\epsilon_k^+}{\sqrt{\Lambda_k^2 - 1/\gamma}} \right],$$

(26)

where $\Lambda_k = \epsilon_k^2 + J^2V^2/2$, $\Gamma_k = J^2V^2/2$, $E_k^+ = \frac{1}{2J} \sqrt{\epsilon_k^2 + J^2V^2} + \frac{1}{2J} \sqrt{\epsilon_k^2 + J^2V^2}$, and $\gamma = m_1/m_2$.

The critical lines $T_K$, $T_N$, $T'_K$ and $T'_N$ (which are all calculated as functions of $J$) necessary to determine the finite-temperature phase diagram at half-filling can be illustrated in figure 3. Both the Kondo temperature and Néel temperature show two distinct parts. In the weak Kondo coupling region, the Néel temperature first increases from zero to a maximal value $T_N = 0.238t$ at $J = 2.85t$, then diminishes rapidly down to zero at a critical Kondo exchange $J_2 = 3.4161t$. The reduction of $T_N$ in the intermediate coupling region is due to the spin fluctuations caused by the Kondo screening effects in the HFAFM phase. For the Kondo temperature in the KP phase, it grows rapidly with increasing $J$ from $T_K = 0.238t$ at $J = 2.85t$, while inside the HFAFM phase, it shows a steep reduction down to zero from $J = 2.85t$ to $J_1 = 3.1498t$. The HFAFM phase exists in the narrow region between $T'_K$ and $T'_N$, which contracts continuously as the temperature rises, then finally disappears.

Notably, the four lines intersect each other at $J = 2.85t$, $T = 0.238t$, showing that the AFM phase, the KP phase and the HFAFM phase converge to a single point on the $J$-$T$ plane, similar to that reported in the case of far away from half-filling, where the ferromagnetism and Kondo screening can coexist [25, 26]. This feature of the phase diagram is similar to that derived by dynamic mean-field theory [2]. In fact, the HFAFM phase deduced by previous mean-field treatments [6, 14] does not converge together with the AFM and KP phase to a single point in the phase diagram, in contrast, the HFAFM phase diminishes as temperature rises, and disappears inside the AFM and KP phase. Therefore, we believe our mean-field decoupling of the Kondo interaction provides more convenient and reliable description of KLM than previous used methods. However, the existence of this convergent point still deserves further verification beyond simple mean-field treatments.

The staggered magnetization $M$ and the Kondo hybridization parameter $V$ are calculated as functions of $J$ for given temperatures, illustrated in figure 2(b), and as functions of $T$ but constant $J$, demonstrated in figure 4. On the edge between the AFM and HFAFM phases (denoted by $J_1$ in figure 2 and $J'_2$ in figure 4(b)), $M$ varies continuously showing a kink, then decreases and approaches zero on the upper edge $J_2$ or $T'_N$; while on the boundary between the HFAFM and KP phases ($J_2$ in figure 2 and $T'_N$ in figure 4(b)), the Kondo screening strength $V$ also varies continuously with a kink and then decreases and disappears when approaching the lower edge ($J_1$ or $T'_K$). The suppression of AFM order and Kondo screening by each other in the HFAFM phase is owing to the competition between them. At non-zero temperatures, magnetic order in a pure 2D system is prohibited by Mermin–Wagner theorem. However, a small inter-plane coupling between the lattice layers will be sufficient to stabilize the magnetic order at low temperatures. Since the mean-field method adopted here is not sensitive with small inter-plane coupling, our finite-temperature results can still be qualitatively applied to real 3D systems.

V. Ground-state phase diagram close to half-filling

In the above sections, the HFAFM phase is studied in the half-filling case with only NN hopping $t$ among conduction electrons, and the system is in an insulating phase. While away from half-filling or with NNN hopping $t'$ or beyond, the system no longer possesses particle-hole symmetry, thus in addition to the singlet hybridization $V_s$, the triplet hybridization $V_t$ between
the conduction electrons and local moments plays an important role. Consequently, the system may possess enriched phase transitions and phase diagram. In contrast to the mean-field methods in earlier works [6, 14], the optimized mean-field decoupling we employed here can be naturally generalized to include the influence of \( n_c \) and \( t' \), and various phases and phase transitions between them can be discussed explicitly.

In the general case, the quasiparticle spectrums of the HFAFM phase have to be derived by diagonalizing \( \mathcal{H}_{k} \) (equation (9)) numerically, and the unitary transformation between the quasiparticles and \( c \)-\( f \) fermions can also be obtained through this computation. The self-consistent equations for the HFAFM phase are derived by the definitions of mean-field parameters \( V_c, V_f, m_c, m_f \), and by fitting the number of \( c \) and \( f \) fermions to \( n_c \) and 1 per site, respectively:

\[
\begin{align*}
V_c &= \frac{1}{2N} \sum_{k,\sigma} \langle c_{k\sigma} f_{k\sigma} \rangle, \\
V_f &= \frac{1}{2N} \sum_{k,\sigma} \sigma \langle c_{k\sigma} f_{k\sigma+Q\sigma} \rangle, \\
m_c &= \frac{1}{2N} \sum_{k,\sigma} \sigma \langle c_{k\sigma} c_{k+Q\sigma} \rangle, \\
m_f &= \frac{1}{2N} \sum_{k,\sigma} \sigma \langle f_{k\sigma} f_{k+Q\sigma} \rangle, \\
1 &= \frac{1}{2N} \sum_{k,\sigma} \langle f_{k\sigma} c_{k\sigma} \rangle.
\end{align*}
\tag{27}
\]

The expected values in the above equations can be expressed in terms of the matrix elements of the unitary transformation. These equations are solved iteratively until convergence is reached, then the energy of the HFAFM phase is obtained by summing the excitations below the Fermi level. For pure AFM phase and KP phase, since the analytic spectrums exist, these two phases can be solved by minimizing their ground-state energies. In the AFM phase, the conduction electrons and \( f \)-fermions are decoupled, with \( \lambda = 0 \), \( m_f = 1/2 \), causing smooth dispersions \( E_{d} = \pm \frac{1}{2} J_m c \) of local spins.

In order to determine the phase boundaries among the HFAFM phase, AFM phase and KP phase, we have to develop an efficient theory. Considering when \( J \rightarrow J_2 \), the parameters \( m_f, m_c, V_f \rightarrow 0 \), the quasiparticle spectrums of HAFM phase can be expressed by two parts: one is the function of \( V_f, \lambda, \mu \), and the other can be perturbed in the first-order of \( m_f, m_c, V_f \). To do this, we rewrite the mean-field Hamiltonian to the form

\[
\mathcal{H} = N\epsilon_0 + \sum_{k,\sigma} \Phi_{k\sigma}^{+} \mathcal{H}_{k} \Phi_{k\sigma},
\tag{28}
\]

the operators are redefined as \( \Phi_{k\sigma} = (c_{k\sigma}, f_{k\sigma}, c_{k+Q\sigma}, f_{k+Q\sigma})^{T} \), and the Hamiltonian matrix

\[
\mathcal{H}_{k} = \begin{pmatrix}
\epsilon_k - \mu & -\frac{3}{4} J_V & -\phi J_{m}\sigma \frac{1}{2} J_{m}\sigma & -\frac{3}{4} J_{V}\sigma \\
-\frac{3}{4} J_{V}\sigma & \lambda & -\frac{1}{2} J_{m}\sigma & -\frac{3}{4} J_{V}\sigma \\
\phi J_{m}\sigma & \frac{1}{2} J_{m}\sigma & \epsilon_k - \mu & -\frac{3}{4} J_{V}\sigma \\
-\frac{3}{4} J_{V}\sigma & -\frac{1}{2} J_{m}\sigma & -\frac{3}{4} J_{V}\sigma & \lambda
\end{pmatrix}
\equiv \begin{pmatrix}
\Lambda_k & \sigma B_k \\
\sigma B_k & \Lambda_{k+Q}
\end{pmatrix},
\tag{29}
\]

Using the Bogoliubov transformation

\[
\begin{pmatrix}
\epsilon_k - \mu \\
\phi J_{m}\sigma
\end{pmatrix}
= U_{k} \begin{pmatrix}
\alpha_k \\
\beta_k
\end{pmatrix} = \begin{pmatrix}
V_{k} - v_{k} \\
v_{k}
\end{pmatrix} \begin{pmatrix}
\alpha_k \\
\beta_k
\end{pmatrix}
\tag{30}
\]

with \( u_k^2 + v_k^2 = 1 \), the block diagonal parts \( \Lambda_k \) and \( \Lambda_{k+Q} \) are diagonalized:

\[
U_{k}^{+} \mathcal{H}_{k} U_{k} = \text{diag}(E_{k+Q}, E_{k+Q}, E_{k+Q}^\prime, E_{k+Q}^\prime) \equiv \Lambda_k, \quad U_{k+Q}^{+} \mathcal{H}_{k+Q} U_{k+Q} = \text{diag}(E_{k+Q}, E_{k+Q}, E_{k+Q}^\prime, E_{k+Q}^\prime) \equiv \Lambda_{k+Q},
\]

where the dispersions are functions of \( V_f, \lambda, \mu \), and are equal to the spectrums in the KP phase:

\[
E_{k+Q}^0 = \frac{1}{2} \left[ \epsilon_k - \mu + \lambda \pm \sqrt{(\epsilon_k - \mu - \lambda)^2 + 9J_f^2 V_f^2} \right].
\tag{31}
\]

Constructing a global zero-order unitary transformation with the Bogoliubov transformation

\[
M_k = \begin{pmatrix}
U_k & 0 \\
0 & U_{k+Q}
\end{pmatrix},
\]

this acts on the Hamiltonian matrix leading to

\[
M_k^{T} \mathcal{H}_{k} M_k = \begin{pmatrix}
\Lambda_k & \sigma \mathcal{D}_k \\
\sigma \mathcal{D}_k^T & \Lambda_{k+Q}
\end{pmatrix},
\tag{33}
\]

The off-diagonal elements hybridize the zero-order eigenstates with each other, hence bring corrections to the four dispersions \( E_{k+Q}\) and \( E_{k+Q} \), with \( E_{k+Q} = E_{k+Q}^0(V_f, \lambda, \mu) + E_{k+Q}^1(m_c, m_f, V_f) \), where \( E_{k+Q}^1 \) are easily obtained by these off-diagonal elements using perturbation theory. To the second order of \( m_c, m_f, V_f \), the ground-state energy density near \( J_2 \) can be divided into two parts as \( E_g^{\text{HAFM}} = E_g^0(V_f, \lambda, \mu) + E_g^1(m_c, m_f, V_f) \), where

\[
\begin{align*}
E_g^0 &= \frac{2}{N} \sum_{k} \theta(-E_{k+Q}^0)E_{k+Q}^0 + \frac{3}{2} J_f V_f^2 - \lambda + \mu m_c, \\
E_g^1 &= \frac{2}{N} \sum_{k} \theta(-E_{k+Q}^0)E_{k+Q}^1 + \frac{1}{2} J_f + m_c m_f.
\end{align*}
\tag{34}
\]

Minimization of \( E_g^0 \) with respect to \( V_f, \lambda, \mu \) gives rise to three self-consistent equations, while differentiating \( E_g^1 \) with \( m_c, m_f, V_f \) produces three other equations. At \( J_2 \), \( (m_c, m_f, V_f) \rightarrow 0 \), but \( m_c m_f, V_f m_f, V_f \) remain finite. Solving the six equations, \( J_2 \), and the value of \( V_f, \lambda, \mu \), \( m_c \), \( m_f \), \( V_f \) on this boundary are calculated.

In figure 5, the energies of the pure AFM phase, the HFAFM phase and the KP phase are plotted with varying \( J \), and the derived critical Kondo coupling \( J_1 \) between AFM and HFAFM phases on which the two phases have equal energy has been given as a function of \( n_c \) and \( t' \) in figure 6. At half-filling, the pure AFM phase is separated with the HFAFM phase by a second-order phase transition at \( J_1 \), and on this boundary, \( M \) varies continuously, while \( V_f \) and \( V_i \) approach zero, see figure 7(a). For \( n_c < 1 \), the transition at \( J_1 \) changes to a first-order one, as indicated by the kink in \( E_g \) (figure 5(b)) and the discontinuity of \( M, V_f \) and \( V_i \) at \( J_1 \) (figure 7(b)). Note that \( V_f \) and \( V_i \) remain finite at \( J_1 \) for \( n_c < 1 \). At \( J_2 \), a second-order phase transition between HFAFM and KP takes place, as seen by the tangency of ground state energy at \( J_2 \) in figure 5. \( E_g, V_f, V_i, M \) all vary continuously with \( J \) at \( J_2 \), at which \( V_f \)
and M approach zero. Moreover, the NNN hopping $t'$ can shift both boundaries. We find a sudden jump of $J_{c1}$ from $n_c = 1$ to $n_c < 1$ (see figure 6). To understand this feature, we plot $M$, $V_s$ and $V_t$ along $J_{c1}$ as functions of $n_c$ (note that $J_{c1}$ varies with $n_c$), it can be seen that $M$ varies discontinuously at $n_c = 1$ (see figure 8), this leads to a discontinuous change of $E_{g_{HFAFM}}$, causing the sudden jump of $J_{c1}$ at $n_c = 1$. This character may attribute to the change of the order of the phase transition at $J_{c1}$, i.e. from first to second order when $n_c$ is reduced from 1. Only $J_{c2}$ represents a real phase transition, because at this boundary the staggered magnetization $M$ vanishes from AFM to KP. The spectrums and Fermi surface structures of these three phases are shown in figure 9. The conduction electrons and local moments are completely decoupled in the pure AFM phase, leading to a hole-like Fermi surface around $(\pi/2, \pi/2)$ at $t'/t = 0.1$, which consists of only the conduction electrons and the Luttinger volume equals $n_cS_F$, where $S_F$ is the area of Brillouin zone; while in the HFAFM phase, the hybridization of conduction electrons and local moments constructs a hole-like Fermi surface around $(0, 0)$ and $(\pi, \pi)$ points, with Fermi surface volume $n_cS_F$. The change of Fermi surface topology between AFM and HFAFM phase indicates a first-order Lifshitz transition at $J_{c1}$. For the KP phase, a hole-like Fermi surface exists around $(\pi, \pi)$, with Fermi surface volume $n_cS_F$ containing both $c$- and $f$-fermions.

We have calculated $J_{c1}$ and $J_{c2}$ as $n_c$ varies from 0.7 to 1. Notably, as $n_c$ decreases, $J_{c1}$ and $J_{c2}$ approach each other and finally intersect at $n_c^* = 0.8228$ for $t'/t = 0.1$, and at $n_c^* = 0.8301$, $J^* = 2.4604t$ for $t' = 0$, respectively. This result indicates that the HFAFM phase reduces with decreasing $n_c$ and finally disappears at a triple point. As $n_c$ decreases further, the AFM and KP phases are separated by a first-order transition at $J_c$, at which the AFM and KP phase shares equal energy. The ground state phase diagram of the KLM are summarized in figure 6 on the $n_c$-$J$ plane for given hopping parameter $t'/t = 0$ and 0.1. When $n_c > n_c^*$, the collapse of Kondo

![Figure 5](image5.png) Energies of AFM phase $E_{g_{AF}}$ (red lines), KP phase $E_{g_{KP}}$ (blue lines) and HFAFM phase $E_{g_{HFAFM}}$ (green lines) versus Kondo exchange $J$. All energies are in units of NN hopping $t$.

![Figure 6](image6.png) Ground-state phase diagram of KLM near half-filling. As $n_c$ is reduced, the collapse of Kondo screening at $J_{c1}$ and the magnetic transition at $J_{c2}$ get closer and finally converge. Thick and thin lines denote first and second order phase transitions, respectively.

![Figure 7](image7.png) Staggered magnetization $M$, Kondo hybridization $V_s$ and triplet hybridization $V_t$ as functions of Kondo coupling $J$.

![Figure 8](image8.png) Staggered magnetization $M$, singlet hybridization $V_s$ and triplet hybridization $V_t$ along $J_{c1}$ as functions of $n_c$ for HFAFM phase. At $n_c = 1$, $V_s$ and $V_t$ approach zero (see figure 7(a)), while on the triple point ($n_c^* = 0.8228$ for $t'/t = 0.1$), $M$ and $V_t$ disappear.
screening at \( J_1 \) and the magnetic transition occurring at \( J_2 \) separate. While \( n_e < n_e^* \), the Kondo screening collapses precisely at the magnetic transition point. Similar phase diagrams are also given by mean-field treatments, Gutzwiller approximation and variational Monte Carlo approach \([10, 15, 21]\). This offset-to-convergence process between Kondo breakdown and magnetic transition as \( n_e \) decreases may account for the experimental observations for CeIn\(_3\) and CeRh\(_1\)-Co,In\(_3\) \([12, 13]\), and for YbRh\(_2\)Si\(_2\) under Co and Ir doping or external pressure \([8, 9]\).

Near half-filling of conduction electrons, using similar treatments, we found that the FM phase has much higher energy than the AFM phase, therefore it is not included in the phase diagrams at least near half-filling. As \( n_e \) is further reduced, the FM phase may have comparable energy with the AFM phase, then the FM phase may appear in the phase diagram at \( n_e < 0.7 \). With small occupation number of conduction electrons, we have reported the phase diagrams in our previous papers \([25, 26]\). In order to give a global phase diagram with \( 0 < n_e < 1 \), the FM phase should be certainly carefully considered in the future calculations.

The triple point \((n_e^*, J^*)\) in our phase diagram can be shifted by \( t'/t \), so in our mechanism this offset-to-convergence transition can also be generated by varying \( t'/t \), similar to that proposed in \([10]\). Chemical or external pressure may simultaneously change \( t'/t \) and \( n_e \), so which path cut in our phase diagram corresponding to these experiments is not clear. Experimental studies of the existence of \( n_e^* \) may be particularly interesting. The KP phase possesses larger Fermi surface than AFM phases, consequently, the transition from AFM to KP at \( J_e \) when \( n_e < n_e^* \) may induce a abrupt change of Hall coefficient as in YbRh\(_2\)Si\(_2\), where the FSR was observed via Hall effect at the onset of magnetic transition \([9]\).

VI. Conclusion

In summary, we have performed an optimized mean-field decoupling and careful numerical computations of the Kondo lattice model near half-filling at both zero and finite temperatures. We decomposed the Kondo interaction into singlet and triplet hybridizations, and then estimated them by Hartree–Fock approximation. We also introduced the AFM orders of conduction electrons and local moments, to approximate the longitudinal term in the Kondo exchange. In addition to the pure AFM phase in weak Kondo coupling range and the Kondo paramagnetic phase in relatively strong coupling range, a distinct heavy-fermion antiferromagnetic phase with coexisting AFM order and Kondo screening arises in the intermediate Kondo exchange region, and the ground state phase diagram has been determined as function of the Kondo coupling, electron concentration and electron hopping. In particular, for the heavy-fermion antiferromagnetic phase, in addition to the conventional singlet hybridization, we found a finite staggered triplet hybridization between local moments and conduction electrons. We also develop an efficient method to calculate the phase boundaries. The characteristic parameters and Fermi surface structures of these phases and the phase transitions between them have been discussed explicitly. We have further found a mechanism explaining the offset-to-convergence process between Kondo breakdown and magnetic transition, which is driven by the decreasing of electron number \( n_e \). This mechanism may account for the separation of the two transitions in YbRh\(_2\)Si\(_2\) under doping, and the existence of the triple point \((n_e^*, J^*)\) in the phase diagram deserves deep experimental investigation. At half-filling limit, a finite-temperature phase diagram has been determined on \( J-T \) plane. As temperature rises, the region of the heavy-fermion antiferromagnetic phase diminishes continuously then finally converges to a single point, together with the pure AFM phase and KP phase, which may require further theoretical and experimental verification.

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H Li et al