Phase Diagram of the Two-Channel Kondo Lattice

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The phase diagram of the two-channel Kondo lattice model is examined with a Quantum Monte Carlo simulation in the limit of infinite dimensions. Commensurate (and incommensurate) antiferromagnetic and superconducting states are found. The antiferromagnetic transition is very weak and continuous; whereas the superconducting transition is discontinuous to an odd-frequency channel-singlet and spin-singlet pairing state.

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Introduction. A number of Heavy Fermion materials display highly unusual superconductivity (HFSCs) \(^{[1]}\). It seems unlikely that conventional superconductivity coexists with the strong local Coulomb correlations necessary to enhance the electronic mass. Indeed, the specific heat makes it clear pairing is between the heavy electrons (with order 100-1000-fold mass enhancement).

The strong coulomb correlations present no problem for unconventional superconducting order parameters with either spatial \(^{[2]}\) or temporal nodes (so called “odd-frequency pairing”) \(^{[3]}\). Such an interpretation is supported by two sets of data: (i) power laws observed in physical properties below the superconducting transition \(^{[1]}\), which contrast with the activated behavior of the conventional (nodeless) s-wave order of, e.g., aluminum; (ii) the complex superconducting phase diagrams of UPt\(_3\) and U\(_{1-x}\)Th\(_x\)Be\(_{13}\) (and possibly UBe\(_{13}\) itself, for which the penetration depth displays evidence of a secondary transition) \(^{[1]}\). The superconductivity can coexist with antiferromagnetism, which is usually commensurate, as in UPt\(_3\), URu\(_2\)Si\(_2\), UPd\(_2\)Al\(_3\), and UNi\(_2\)Al\(_3\) \(^{[1]}\), or compete with it as in CeCu\(_2\)Si\(_2\) \(^{[3]}\). Finally, at least in UBe\(_{13}\) \(^{[10]}\) and CeCu\(_2\)Si\(_2\) \(^{[3]}\), the superconductivity arises in a normal state which is clearly not described as a Fermi liquid. In each of these materials above \(T_c\) the linear specific heat rises with decreasing temperature, the resistivity is approximately linear in \(T\), and the residual resistivity at \(T_c\) is high (typically 80-100 \(\mu\) - \(\Omega\)-cm in the best samples of UBe\(_{13}\)).

In this paper, we provide the first calculations of the phase diagram for the two-channel Kondo lattice in infinite spatial dimensions. We find second order antiferromagnetic and first order odd frequency superconducting phase transitions. Coexistence of commensurate (and incommensurate) antiferromagnetism with superconductivity is in principle possible. We present several possible routes to account for the multiple superconducting phases observed in real materials. Taken together with the non-Fermi liquid (NFL) paramagnetic phase discussed in previous publications \(^{[12]}\), and earlier suggestions that the two-channel lattice may describe UBe\(_{13}\) and other heavy fermion systems \(^{[8]}\), our work establishes the two-channel Kondo lattice model as possessing the key ingredients needed to explain heavy fermion superconductivity.

Motivation A possible model for some heavy fermion compounds is the two-channel Kondo lattice which consists of two identical species of non-interacting electrons antiferromagnetically coupled to an adjacent lattice of spin 1/2 Kondo moments \(^{[8]}\). This model displays Non-Fermi liquid behavior because of the overcompensation of the Kondo spins by the conduction electrons, first pointed out in the single site two-channel model by Nozières and Blandin \(^{[11]}\) where extended screening clouds form which retain a spin 1/2 character. As a result, the paramagnetic state is degenerate and the excitation spectrum non-Fermi liquid like. This overscreening results in an interchannel pairing mechanism \(^{[8]}\) in the two-channel impurity problem which tends to favor spin-singlet channel-singlet odd frequency superconducting fluctuations \(^{[8]}\). For the lattice, we find that this overscreening generates novel antiferromagnetic superexchange between the Kondo spins which, taken together with the RKKY exchange, favors antiferromagnetism in the lattice model close to half filling of the bands. The nature of the resulting superconducting and magnetic transitions, as well as the competition between them, is the subject of this manuscript.

Model The Hamiltonian for the two-channel Kondo lattice is

\[
\begin{align*}
H &= J \sum_{i,\alpha} \mathbf{S}_i \cdot \mathbf{s}_{i,\alpha} - \frac{t^*}{2\sqrt{d}} \sum_{<ij>,\alpha,\sigma} \left( c_{i,\alpha,\sigma}^\dagger c_{j,\alpha,\sigma} + \text{h.c.} \right) \\
&\quad - \mu \sum_{i,\alpha,\sigma} c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma},
\end{align*}
\]

where \(c_{i,\alpha,\sigma}^\dagger \) (\(c_{i,\alpha,\sigma} \)) creates (destroys) an electron on site \(i\) in channel \(\alpha = 1, 2\) of spin \(\sigma\), \(\mathbf{S}_i\) is the Kondo spin on site \(i\), and \(\mathbf{s}_{i,\alpha}\) are the conduction electron spin operators for site \(i\) and channel \(\alpha\). The sites \(i\) form an infinite-dimensional hypercubic lattice. Hopping is limited to nearest neighbors with hopping integral \(t \equiv t^*/2\sqrt{d}\); the scaled hopping integral \(t^*\) determines the energy unit and
is set equal to one \((t^* = 1)\). Thus, on each site the Kondo spin mediates an interaction between the two different channels. This problem is non-trivial, and for the region of interest in which \(J > 0\) and \(T \ll J, t^*\) it is describable only with non-perturbative approaches. Clearly some simplifying method which allows for a solution of the lattice problem in a non-trivial limit is necessary.

**Formalism and Simulation.** Such a method was proposed by Metzner and Vollhardt [13] who observed that the renormalizations due to local two-particle interactions become purely local as the coordination number of the lattice increases. A consequence is that the solution of most standard lattice models may be mapped onto the solution of a local correlated system coupled to an effective bath that is self-consistently determined. We refer the reader to recent reviews for further details and references on the method [14].

In order to solve the remaining impurity problem, we use the Kondo impurity algorithm of Fye and Hirsch [15], modified to simulate the two-channel problem [16]. We simulated the model for a variety of fillings and values of the magnetic exchange \(J\) \((0 < N \leq 1\) for \(J = 0.75, 0.625, 0.5, 0.4\)). Error bars on measured quantities are less than 6\% for the results presented here. A sign problem was also encountered in the QMC process. It becomes severe for large \(J\) and also for low fillings since lower temperatures are required to access the physically interesting regime. This precludes a systematic study of the model with \(J > 0.8\) and filling \(N < 0.5\).

Both one and two-particle properties are natural products of the QMC simulation. To calculate the spin susceptibility, it was necessary to measure the local three-by-three matrix of the susceptibility including both the Kondo spin and conduction band spin fluctuations. This may then be inverted to calculate the associated irreducible vertex function and the corresponding lattice susceptibility in the usual way [17].

The situation for the superconductivity is a bit more complicated. Since there are no charge fluctuations involving the Kondo spin degree of freedom, only the two conduction channels contribute to the pair-field susceptibility. We can then look for pairing instabilities in singlet and triplet channels for both spin and channel spin. Motivated by the result for the impurity model [13] we have restricted our attention to interchannel and inter-spin particle-particle diagrams as shown in Fig. 1. It is possible to make two independent combinations of these diagrams \(\chi_{\pm}(i \omega_n, i \omega_m) = \chi_{11}(i \omega_n, i \omega_m) \pm \chi_{12}(i \omega_n, i \omega_m)\), from which we construct a quartet of spin and channel, singlet and triplet pair-field susceptibilities given by

\[
P_{SsCs} = T \sum_{nm} f_- (i \omega_n) \chi_- (i \omega_n, i \omega_m) f_- (i \omega_m) \quad (2)
\]

\[
P_{StCt} = T \sum_{nm} f_+ (i \omega_n) \chi_+ (i \omega_n, i \omega_m) f_+ (i \omega_m) \quad (3)
\]

\[
P_{StCs} = T \sum_{nm} f_- (i \omega_n) \chi_+ (i \omega_n, i \omega_m) f_- (i \omega_m)
\]

\[
P_{SsCt} = T \sum_{nm} f_+ (i \omega_n) \chi_- (i \omega_n, i \omega_m) f_+ (i \omega_m)
\]

Here \(f_{\pm}(i \omega_n)\) are odd functions of Matsubara frequency used to project out the odd-frequency pairing, and, for example, \(P_{SsCs}(T)\) is the spin-singlet channel-singlet pair-field susceptibility.

To determine the form of \(f_{\pm}(i \omega_n)\), we employ the pairing matrix formalism of Owen and Scalapino [18]. Here we represent each of \(\chi_{\pm}\) in a two-particle Dyson equation and extract the irreducible vertex functions \(\Gamma_{\pm}\). The pairing matrices are then

\[
M_{\pm}(i \omega_n, i \omega_m) = \sqrt{\chi_{\pm}^0 (i \omega_n)} \Gamma_{\pm} (i \omega_n, i \omega_m) \sqrt{\chi_{\pm}^0 (i \omega_m)}
\]

where \(\chi_{\pm}^0 (i \omega_n)\) are the particle-particle diagrams in Fig. 1 without vertex corrections. \(f_{\pm}(i \omega_n)\) is the eigenvector corresponding to the dominant eigenvalue of \(M_{\pm}\) (that with the largest absolute value).

**Results.** In this model antiferromagnetism is driven by both RKKY interactions and a novel type of superexchange. The latter arises from hopping between adjacent spin 1/2 screening clouds, whose overall spin is determined by the conduction electrons; the Pauli principle forbids hopping unless neighboring spins in the same channel are antiparallel. As a result, for large \(J\), the superexchange goes as \(\sim (t^*)^2/J\). For conduction band fillings close to \(N = 1\) both the RKKY (evaluated at nearest neighbor sites) and the superexchange favor antiferromagnetism (the RKKY exchange remains antiferromagnetic until \(N \lesssim 0.5\)), and an antiferromagnetic transition results, as shown in Fig. 2. Due to screening of the local moments by the conduction spin, the transition is very weak, as measured by the full susceptibility. Specifically, \(\chi_{AF}\) is not significantly enhanced over the bulk susceptibility \(\chi_F\) until \(T \gtrsim T_N\). However, the \(f\)-electron contribution to the susceptibility shows a protracted scaling region. Here screening effects non-linear feedback that reduces the susceptibility exponent \(\gamma\) from the mean field value \(\gamma = 1\). \(\gamma\) increases with doping \((N < 1)\), and the transition becomes incommensurate as \(T_N \rightarrow 0\).

To explore superconductivity, it is necessary to find the frequency form factors \(f_{\pm}\), which, as discussed above, are the eigenvectors corresponding to the dominant eigenvalues of the pairing matrices \(M_{\pm}\). As the temperature is lowered, the dominant eigenvalue first becomes large (divergent) and negative, and then abruptly switches to a large and positive value at the transition. This happens first in \(M_-\), and the corresponding eigenvector of \(M_-\) is plotted in the inset to Fig. 3. It can be fit quite accurately to the form \(T/2\omega_n\) as shown by the solid line, which corresponds to the form factor of Ref. [8]. Thus, we
use \( f_-(i\omega_n) = T/2\omega_n \) to project out the odd-frequency pair-field susceptibilities shown in Figs. 3 and 4. (Other form factors \( f(i\omega_n) = \text{tanh}(T_0/\omega_n) \) and \( \text{sign}(\omega_n) \) were tried and produce qualitatively similar results.)

The first transition is found in the spin-singlet channel-singlet pairing combination, as shown in Fig. 3. (Note that this pair state is of necessity even in parity, so that the odd-frequency condition is required to satisfy the Pauli principle, in contrast with the spin-parity selection rules in the single channel case [3].) To interpret this result, remember that the inverse pair field susceptibility may be \( \propto S_{sCs}^2 \) at low temperatures; detailed exploration within the highly exotic [4].

The excitation spectrum of such a transition may well be \( S_{sCs}^2 \) at low temperatures; detailed exploration within the highly exotic [4]. We also find that, \( T^* \approx 0 \) pairs are forbidden a systematic study for these values of \( \bar{\omega}_s \). (Other form factors \( f(i\omega_n) = \text{tanh}(T_0/\omega_n) \) and \( \text{sign}(\omega_n) \) were tried and produce qualitatively similar results.)

Second, \( T \approx 0.5T_0 \) is also the temperature at which the slope of the real part of the self energy becomes one [2], so that the quasiparticle renormalization factor diverges. This result suggests that when the system cannot form a Fermi liquid due to a large residual scattering rate (which also yields a large residual entropy), it forms a superconducting state to quench the entropy. The antiferromagnetic transition temperature, on the other hand, depends upon both \( J \) (through the intersite exchange) and upon \( T_0 \) (through moment screening and superexchange). As noted above, we cannot determine whether these states coexist without a detailed exploration within the ordered phases. At half filling, where the antiferromagnetism produces an insulating phase, clearly the superconductivity will be suppressed for \( J \leq 0.75 \).

Our results offer a number of routes to be explored for explaining the complex superconducting phase diagrams of UPt\(_3\) and U\(_{1-\frac{1}{2}}\)Th\(_{2}\)Be\(_{13}\): 1) Competition between phases with a multi-point irreducible star. As mentioned above, for \( \bar{\omega}_s < 0 \) in finite dimensionality, \( \bar{q} \neq 0 \) pairs are favored. In this simple case of a bipartite lattice, the zone corner has a one-point irreducible star. For lattices with frustration, such as hexagonal UPt\(_3\) and face-centered cubic UBe\(_{13}\), it is possible to produce multi-point irreducible stars for staggered order parameters which can then have multiple phases [3]. 2) Competition between Different \( \bar{q} \) values. As mentioned above, \( T^* \), the lower bound for the first order superconducting transition temperature is independent of \( \bar{q} \) in our calculations. Thus multiple phases may thus correspond to superconducting transitions with different \( \bar{q} \) values. 3) Possible Instability of Spin Triplet/Channel Triplet Pairing. At yet lower temperatures than those identified in Fig. 4, we observe a sign change in the pair field susceptibility associated with spin triplet-channel triplet odd-frequency pairing. Hence it is possible that the competition between this triplet-triplet and the singlet-singlet odd frequency pairing may explain the complex phase diagrams.

In closing, we note that this superconducting transition can agree with experiment only if it is weakly first order; this is plausible given the rapid change in free energy curvature at the order parameter origin. Detailed investigations in the ordered phase will resolve this issue and whether any of the above scenarios can describe the complex phase diagrams of UPt\(_3\) and U\(_{1-\frac{1}{2}}\)Th\(_{2}\)Be\(_{13}\).

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\[
\chi_{11}(i\omega_n,i\omega_m) = \begin{cases} 1 & \text{if } n = m \text{ and } \omega_n \neq \omega_m \\ 2 & \text{otherwise} \end{cases}
\]

\[
\chi_{12}(i\omega_n,i\omega_m) = \begin{cases} 1 & \text{if } n = m \text{ and } \omega_n \neq \omega_m \\ 2 & \text{otherwise} \end{cases}
\]

FIG. 1. Particle-particle interchannel opposite spin diagrams which contribute to the pair-field susceptibility. Here 1 and 2 label the channel and \( \uparrow \) and \( \downarrow \) the spin.

\[
\frac{1}{\chi(T-T_N)^{1/2}} \quad \chi(T-T_N)^{1/2}
\]

FIG. 2. Full antiferromagnetic \( \chi_{AF} \) and ferromagnetic \( \chi_F \) susceptibilities of the two-channel Kondo lattice with \( J = 0.75 \) and \( N = 1.0 \). \( \chi_{AF} \) shows very little enhancement until \( T \approx T_N \). As shown in the inset, the Kondo spin contribution to the susceptibility \( \chi_{AF}(T) \) displays a protracted scaling region. The solid line is a fit of \( 1/\chi_{AF}(T) \) to the form \( a(T-T_N)^\gamma \). The large difference between \( \chi_{AF} \) and \( \chi_{AF}(T) \) as well as the reduced exponent \( \gamma < 1 \) indicate the importance of screening of the local spin in this transition.
FIG. 3. Odd-frequency (spin-singlet, channel-singlet) pair-field susceptibility at both the zone center and corner. At low temperatures $T = T^* \leq T_c$, $P_{S_aC_s}(T)$ becomes negative, indicating a thermodynamic instability to the formation of a pairing state. The lack of a divergence of $P_{S_aC_s}(T)$ rules out a continuous transition, hence the system must undergo a discontinuous transition. In the inset, the dominant eigenvector of the pairing matrix $M_-$ is plotted versus Matsubara frequency. It can be fit to the form $T/(2\omega_n)$ (solid line), which corresponds to the frequency variation of the gap function found in Ref.4.

FIG. 4. Phase diagrams of the two-channel Kondo lattice for various values of $J$. The solid lines are fits to the data. For each value of $J$ shown the antiferromagnetic transition occurs first (at a higher temperature) at half filling $N = 1$ (albeit very weakly when $J = 0.75$). $T_N$ falls quickly with doping $N < 1$, with the transition becoming incommensurate near $T_N \to 0$. Away from half filling, superconductivity occurs first above a temperature $T^* \geq T_c$ is roughly equal to $CT_0$, ($C = 0.43, 0.51,$ and 0.58, for $J = 0.5, 0.625, 0.75$ respectively) consistent with the local nature of the transition. $T^*$ should be regarded as a lower bound on the superconducting transition temperature $T_c$ (see text).