Heavy-Fermion Superconductivity and Localized-Itinerant Crossover in the Kondo Lattice

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Abstract
Superconductivity in the two-dimensional Kondo lattice model is derived by means of the dual-fermion approach. This framework takes full account of local correlations based on the dynamical mean-field theory and further includes influence of critical antiferromagnetic fluctuations. It is found that pairing with $d_{x^2-y^2}$ symmetry similar to the Hubbard model appears only in the weak-coupling regime. As the coupling is increased, we observe transition to $p$-wave spin-singlet superconductivity. The emergence of the unconventional $p$-wave pairing is ascribed to formation of large Fermi surface, which embodies itinerancy of $f$-electrons.

Keywords: Kondo lattice, dual-fermion approach, dynamical mean-field theory, odd-frequency pairing

1 Introduction

Some heavy-fermion materials exhibit superconductivity when an antiferromagnetic transition is suppressed by external and/or chemical pressure. The superconducting phase typically lies around the magnetic critical point, indicating unconventional pairing induced by low-energy magnetic excitations. It reminds us of the cuprate superconductors where pairing with $d_{x^2-y^2}$ symmetry emerges near antiferromagnetic phase of $\mathbf{q} = (\pi, \pi) \equiv \mathbf{Q}$. On this analogy, we may naively expect a possibility of $d$-wave pairing in heavy-fermion materials as well. A question remains, however, whether the antiferromagnetic fluctuations of $\mathbf{q} = \mathbf{Q}$ indeed leads to the $d$-wave pairing in heavy-fermion systems, because the microscopic interactions causing magnetism are different between $d$- and $f$-electron systems.

In this paper, we address unconventional superconductivities in $f$-electron systems, considering a simple model which shows antiferromagnetic instability of $\mathbf{q} = \mathbf{Q}$ as well as heavy-fermion states. The simplest model for this purpose is the Kondo lattice model (KLM) given by the Hamiltonian

$$\mathcal{H}_{\text{KLM}} = \sum_{\mathbf{k} \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J \sum_{\mathbf{i}} \mathbf{s}_{\mathbf{i}} \cdot \mathbf{s}_{\mathbf{i}}. \quad (1)$$

where $\epsilon_{\mathbf{k}} = -2(\cos k_x + \cos k_y)$ and $\mathbf{s}_{\mathbf{i}} = (1/2) \sum_{\sigma\sigma'} c_{\mathbf{i}\sigma}^\dagger \mathbf{\sigma}_{\sigma\sigma'} c_{\mathbf{i}\sigma'}$. The KLM describes a quantum phase transition between antiferromagnetic phase in the weak-coupling side and Kondo...
paramagnetic phase in the strong-coupling side. The boundary \( J_c \) is estimated to be \( J_c \approx 1.45 \) at half-filling [1]. We expect an unconventional superconductivity caused by the critical antiferromagnetic fluctuations around half-filling. A number of numerical investigations have been devoted to clarify rich phenomena emerging in the two-dimensional KLM [2–7].

We also consider the Hubbard model with the same energy dispersion

\[
\mathcal{H}_{\text{Hubbard}} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.
\]

(2)

By a comparative study between the Hubbard model and the KLM, we shall clarify consequences of different types of interactions, \( U \) and \( J \), on superconducting properties.

2 Dual Fermion Approach

Theoretical descriptions of heavy-fermion superconductivity requires simultaneous treatment of the Kondo physics and formation of unconventional pairing. The former is related to spin fluctuations in time domain (local correlations) and the latter to spin fluctuations in spatial domain (spatial fluctuations). Methodological development is a long-standing issue for addressing heavy-fermion superconductivity from microscopic models.

In this situation, there are several attempts [8–14] which take account of long-range fluctuations on the top of the dynamical mean-field theory (DMFT) [15]. We apply the dual-fermion approach to perform “quasiparticle expansion” around the heavy-fermion state described by the DMFT [10,16,17]. In particular, we evaluate diagrams similar to the fluctuation exchange (FLEX) approximation to incorporate influences of antiferromagnetic fluctuations on heavy quasiparticles [18–20]. This framework thus yields combined description of heavy-fermion states in the DMFT and unconventional superconductivity in the FLEX approximation.

The computational procedure is briefly summarized as follows [16,20]. We first solve an effective impurity Kondo model to evaluate the singlet-particle Green’s function \( g_\omega \) and the vertex part \( \gamma_{\omega\omega'\nu} \). Here, we use the continuous-time quantum Monte Carlo method [21] applied to the Kondo impurity model (CT-J algorithm) [22] in the case of \( \mathcal{H}_{\text{KLM}} \) and that applied to the Anderson impurity model (CT-HYB algorithm) [23] in the case of \( \mathcal{H}_{\text{Hubbard}} \). We next solve the dual-lattice problem defined with \( g_\omega \) and \( \gamma_{\omega\omega'\nu} \). In this step, the FLEX-like equations are solved with numerical iterations [18,20]. The results obtained here renew the effective impurity model. The above two-step calculations are repeated until convergence is reached.

3 Superconductivity

The superconducting transition can be detected by the leading eigenvalue \( \lambda_{\text{SC}} \) of the linearized Bethe-Salpeter equation [20]. The condition \( \lambda_{\text{SC}} = 1 \) corresponds to divergence of the pairing susceptibility, and hence to the second-order phase transition. Figure 1 shows temperature dependence of \( \lambda_{\text{SC}} \) in the spin-singlet channel [(a) and (b) for the KLM and (c) for the Hubbard model]. There are five classes of spatial symmetries, which are classified by the irreducible representations for the point group \( D_4 \). It turns out from Fig. 1(a) that \( \lambda_{\text{SC}} \) for \( B_{1g} \) symmetry exceeds 1. It indicates a transition to superconducting state with \( d_{x^2-y^2} \) symmetry as in the Hubbard model. It is remarkable, however, that the \( E_u \) pairing is almost degenerate with the \( B_{1g} \), in stark contrast to the case with the Hubbard model, where the \( B_{1g} \) pairing exhibits prominent enhancement as shown in Fig. 1(c). For stronger coupling, the \( E_u \) pairing finally
Figure 1: (a),(b) Temperature dependence of $\lambda_{\text{SC}}$ for KLM with $n = 0.84$ and $J = 0.8, 1.0$, respectively. From Ref. [28]. (c) $\lambda_{\text{SC}}$ for the Hubbard model with $U = 8$ and $n = 0.86$. From Ref. [20].

dominates over the $B_{1g}$ pairing [Fig. 1(b)]. We observed the $B_{1g}$ superconductivity in $J \lesssim 0.9$ and the $E_u$ superconductivity in $0.9 \lesssim J \lesssim 1.6$.

Here, a comment concerning the symmetry of the $E_u$ ($p$-wave) spin-singlet pairing is in order. This pairing breaks the time-reversal symmetry to fulfill the Pauli principle [24]. More precisely, the gap function $\phi_{k,\omega}$ changes its sign under inversion of the frequency, $\phi_{k,-\omega} = -\phi_{k,\omega}$, as well as under the momentum inversion, $\phi_{-k,\omega} = -\phi_{k,\omega}$. The odd-frequency $p$-wave pairing was discussed in the context of CeCu$_2$Si$_2$ and CeRhIn$_5$ [25]. There are discussions on thermodynamic stability of the odd-frequency superconducting state [26,27].

4 Origin of the Competing Superconductivities

We discuss the origin of the competing pairing fluctuations found in the KLM. Figure 2 shows the momentum dependence of the gap functions $\phi_{k,\omega_0}$ at the lowest Matsubara frequency $\omega_0 = \pi T$. The $B_{1g}$ and $E_u$ pairings exhibit $d_{x^2-y^2}$-type and $(p_x, p_y)$-type angular dependence, respectively. These functions have common features: Regions with strong intensities
with opposite signs are connected by the nesting vector $Q = (\pi, \pi)$ as indicated in Fig. 2. It implies that both pairing fluctuations are induced by the antiferromagnetic fluctuations.

Which type of pairing is favorable depends on the structure of the Fermi surface (FS). The $d$-wave gap function has intensities around the van Hove point $k_1 = (\pi, 0)$, and is hence realized if the FS passes around $k_1$. This is the case with the Hubbard model near half-filling. On the other hand, if the scattering around $k_2 = (\pi/2, \pi/2)$ plays a dominant role, the $p$-wave may become predominant [25].

Topology of the FS in the KLM varies continuously between a small one in the weak-coupling regime and a large one in the strong-coupling regime depending on $J$ at $T \neq 0$, reflecting localized and itinerant characters of $f$ electrons [29]. We note that the FS can only be either small or large at $T = 0$. To see the continuous evolution of the FS, we define the Fermi momentum $k_F$ at finite $T$ by the condition

$$(\epsilon_k + \text{Re} \Sigma_{\omega=0,k})_{k=k_F} = \mu.$$  

Thus calculated FS is plotted in Fig. 3 for several values of $J$. The FS for $J = 0.8$ is similar to that in the non-interacting limit [Fig. 3(a)]. In this case, scattering around the van Hove point $k_1$ plays a major role and the $d$-wave pairing is favored as in the Hubbard model. For $J = 1.0$, on the other hand, the FS is deformed around $k_1$, keeping the shape around $k_2$ [Fig. 3(b)]. Hence, the $p$-wave fluctuations can dominate over the $d$-wave fluctuations in this parameter regime. For stronger couplings, a large FS is formed [Fig. 3(c)] and the $p$-wave pairing is not enhanced anymore. We conclude from these observations that the deformed FS in the intermediate region is relevant for realization of the $p$-wave pairing.
5 Summary

Using the recently developed dual-fermion approach, we have investigated the superconducting instabilities in the two-dimensional KLM. Unlike the Hubbard model, the $d_{x^2-y^2}$ pairing does not show distinctly strong fluctuations. This behavior in the KLM is due to the change of the FS topology which occurs depending on whether the spins behave as localized spins or itinerant "electrons". As a result of the FS crossover, an odd-frequency superconductivity with the $p$-wave spin-singlet pairing emerges. Our results demonstrate a possible exotic superconductivity in the intermediate regime between small and large FSs.

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References


