Superconductivity in the Kondo lattice: a mean-field approach

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We calculate the superconducting critical temperature \(T_c\) and the Kondo temperature \(T_K\) of the Kondo lattice, decoupling the Kondo exchange interaction in the unrestricted Hartree-Fock (HF) Bardeen-Cooper-Schrieffer (BCS) approximation. We obtain that both \(T_K\) and \(T_c\) have an exponential dependence in the Kondo coupling \(J_K\). For optimum doping and realistic parameters, both temperatures fall in the experimentally observed range.

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I. INTRODUCTION

One of the main characteristics of heavy-fermion systems is the competition between Kondo effect and magnetic long-range order, both stemming from the local antiferromagnetic (Kondo) coupling between localized moments and conduction-electron spins. The non-magnetic compounds, like CeAl\(_3\), present a low-temperature state resembling a Fermi liquid with enhanced carrier mass, the so called heavy-fermion regime. In addition to that, superconductivity is observed below \(T_c \sim 1\)K in some systems, the best known being CeCu\(_2\)Si\(_2\), UBe\(_{13}\), and UPt\(_3\). Although the nature of superconductivity in these systems is still unclear, it has been suggested that the Kondo interaction itself might provide a pairing mechanism. Indeed, there is experimental evidence that heavy electrons are involved in the superconducting state, as a high value is observed for the specific-heat jump at the superconducting transition.

Lately, the competition between Kondo effect and magnetism has been studied in a mean-field approximation based on a simple decoupling of the Kondo exchange term, but superconductivity has not been studied within a similar approach. If fluctuations are not included, this mean-field approximation is equivalent to considering only part of the terms of an unrestricted Hartree-Fock (HF) decoupling of the exchange interaction. In this work, we include all relevant terms in this HF decoupling. Among them, a singlet pairing coupling appears, which we treat in the Bardeen-Cooper-Schrieffer (BCS) approximation, leading to superconductivity in the model. Although there are experimental grounds to the notion that superconductivity in heavy-fermion systems presents non-trivial symmetry properties, and can even coexist with magnetic ordering, it is instructive to explore, in a simple theoretical approach, the existence of a superconducting solution in which the pairing mechanism is the same local Kondo interaction that is also responsible for magnetic ordering and compensation of local moments.

II. MODEL AND MEAN-FIELD APPROACH

We consider the standard Kondo-lattice model used to describe heavy-fermion systems, writing the Hamiltonian in the form

\[
H = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + J_K \sum_i S_i \cdot s_i, \quad (1)
\]

where \(c_{i\sigma}^\dagger\) creates a conduction electron with spin \(\sigma\) at site \(i\), and \(S_i\) (\(s_i\)) is the localized (conduction) spin operator at site \(i\).

The HF-BCS approximation has been described before and has been used, for example, to study d-wave superconductivity in a generalized Hubbard model with results which are in qualitative agreement with exact diagonalization of finite systems. We use a fermionic representation of the localized spins, assigning them to \(f\) electrons, whose occupation number is restricted to one per site. Then, neglecting expectation values which do not conserve spin (e.g., triplet pairing), the unrestricted HF decoupling of the interaction term reads

\[
S_i \cdot s_i = \frac{1}{4} \left( f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow} \right) \left( c_{i\uparrow} c_{i\uparrow} - c_{i\downarrow} c_{i\downarrow} \right) + \frac{1}{2} \left( f_{i\uparrow}^\dagger f_{i\downarrow} + c_{i\uparrow} c_{i\downarrow} \right) + \sum_{\sigma} \left[ \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma}^\dagger \rangle + \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma}^\dagger c_{i\sigma}^\dagger \rangle \right]
\]

\[
\approx \left( S_i^\uparrow S_i^\uparrow - S_i^\downarrow S_i^\downarrow \right) + \frac{1}{4} \sum_{\sigma} \left[ \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma}^\dagger \rangle + \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle - 2 \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma}^\dagger c_{i\sigma}^\dagger \rangle + \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle \right)
\]

\[
+ 2 \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle + 2 \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle - 2 \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle
\]

\[
+ 2 \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle + 2 \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle - 2 \langle f_{i\sigma} c_{i\sigma} \rangle \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle
\]

\[
+ \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle - \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle \langle f_{i\sigma} c_{i\sigma} \rangle \text{,} \quad (2)
\]
where $\sigma = -\sigma$. The constraint of one localized ($f$) particle per site is taken only on average, i.e.,

$$\frac{1}{N} \sum_{i} \langle f_{i\sigma}^\dagger f_{i\sigma} \rangle = 1,$$

where $N$ being the number of sites, and is imposed by adding to the Hamiltonian the term

$$H_c = E_f \sum_{i} f_{i\sigma}^\dagger f_{i\sigma},$$

where $E_f$ is a Lagrange multiplier. This procedure reduces the Hamiltonian to an effective one-body problem.

In the following we consider only the non-magnetic homogeneous solution with singlet superconductivity. The order parameters are $\lambda = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$, characterizing the singlet Kondo state, and $\eta = \langle f_{i\uparrow}^\dagger f_{i\downarrow} \rangle$, which is the usual superconducting order parameter. Both can be made real through a gauge transformation.

In absence of superconductivity ($\eta = 0$), the problem is easily solved. The electronic structure of $H + H_c$ is composed of two hybrid bands with energies

$$E^{a(b)}_K = \frac{\epsilon_K + E_f}{2} - (+) \sqrt{\left(\frac{\epsilon_K - E_f}{2}\right)^2 + V^2},$$

where $\epsilon_K$ is the dispersion relation of the unperturbed conduction band, and

$$V = \frac{3}{4} J_K \lambda.$$

Both, $E_f$ and $\lambda$ must be determined selfconsistently. The latter shows the usual behavior of a mean-field order parameter as a function of temperature, going to zero at a critical temperature which we identify as the (mean-field) Kondo temperature $T_K$. In the limit $\lambda \to 0^+$, the self consistent conditions lead to a simple equation for $T_K$:

$$1 = \frac{3}{8N} J_K \sum_{K} \frac{\tanh(\frac{\epsilon_{K} - \mu}{2T_K})}{\epsilon_{K} - \mu}.\quad (7)$$

The chemical potential $\mu$ in this limit is determined by the number of conduction electrons of the unperturbed band,

$$n_c = \sum_{\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = 2 \int \rho_0(\epsilon) f(\epsilon) d\epsilon,\quad (8)$$

with $f(\epsilon)$ standing for the Fermi function, and $\rho_0(\epsilon)$ being the unperturbed density of states (DOS) per spin. In the following we take, for simplicity, a parabolic DOS, $\rho_0(\epsilon) = \frac{3(1 - \epsilon^2)}{4}$, choosing the half band width of the unperturbed band as the unit of energy.

Since $H$ is electron-hole symmetric, we can assume, without loss of generality, $n_c \leq 1$, so that the Fermi level falls in the lower hybrid band. The pairing terms in $H$ can be written in terms of the hybrid operators describing the quasi-particles in the lower band, and we can safely neglect the upper one, as the superconducting critical temperature $T_c$ turns out to be much lower than $T_K$. After some algebra, we arrive at the following four equations, which determine $E_f$, $\lambda$, $\mu$, and the superconducting critical temperature $T_c$:

$$n_f = 2 \sum_{\sigma} \langle f_{i\sigma}^\dagger f_{i\sigma} \rangle = \frac{2}{N} \sum_K \left[Y^2_K f(E^a_K) + X^2_K f(E^K_b)\right],$$

$$\lambda = \frac{V}{2N} \sum_K \frac{1}{r_K} [f(E^a_K) - f(E^K_b)],$$

$$n_f + n_c = \frac{2}{N} \sum_K [f(E^a_K) + f(E^K_b)],$$

$$1 = \frac{3J_K V^2}{16N} \sum_K \frac{1}{r_K^2 (E^a_K - \mu)} \tanh \left(\frac{E^a_K - \mu}{T_c}\right),\quad (9)$$

where $X^2_K = 1/2 + (E_f - \epsilon_K)^2/(4r_K)$, $Y^2_K = 1 - X^2_K$, and $r_K = [(E_f - \epsilon_K)^2/4 + V^2]^{1/2}$.

### III. RESULTS

In Fig. 1 we present $T_K$ and the superconducting critical temperature $T_c$ as a function of conduction-band filling $n_c$ for a typical value of $J_K$. The Kondo temperature $T_K$ increases with $n_c$ and has its maximum at $n_c = 1$ (as explained above, $T_K(n_c) = T_K(2 - n_c)$). Instead, $T_c$ should vanish at $n_c = 1$ because this case corresponds to a Kondo insulator, with the Fermi level falling in a gap whose magnitude is larger than the effective pairing interaction. In other words, while the effective pairing interaction and the density of states increase as $n_c$ tend to one, the effective number of carriers around the Fermi level tends to zero. As a consequence of this competition, $T_c$ shows a maximum around $n_c \sim 0.65-0.7$, whose position is not strongly dependent on the coupling, as shown in Fig. 2. Assuming that the magnitude of the unperturbed half band width is of the order of 1 eV, then, for $J_K \sim 0.3$ eV we obtain $T_c \sim 1$ K at optimum doping (see Fig. 1).

![FIG. 1. Kondo temperature $T_K$ and superconducting critical temperature $T_c$ as a function of doping for $J_K = 0.3$.](image-url)
Figure 3 shows $T_K$ and $T_c$ as functions of $J_K$ for $n_c = 0.7$ (near optimum doping). The dependence of both temperatures with $J_K$ can be fitted very well by exponential functions:

$$T_K = A \exp(-\alpha/J_K),$$
$$T_c = B \exp(-\beta/J_K),$$

as clearly evidenced by the logarithmic plots of Fig. 4. The meaning of the coefficients is not obvious. The parameter values used in Figs. 2 and 3 yield $A = 0.7289$, $\alpha = 1.876$, $B = 0.3250$, and $\beta = 2.425$. For a single Kondo impurity, in the limit of infinite band width, it is known that $T_K^{\text{imp}} = (1/\rho_0) \exp[-1/(\rho_0 J_K)]^{13}$, where $\rho_0$ is the magnitude of the unperturbed density of states, assumed constant. The natural extension to the case of a finite band width would be to write the single-impurity Kondo temperature as the first of equations (10) with $\alpha^{\text{imp}} = 1/\rho_0(\varepsilon_F)$, which would have the value 1.3905 for the example considered. However, in the present case the coefficients are not only affected by the finite band width but also by the mean-field approximation and the fact that we are dealing with a Kondo lattice instead of a single impurity. The dependence of $T_c$ with $J_K$ is even more difficult to predict. From usual BCS theory one might expect an exponential dependence on the product of the interacting density of states and the effective pairing interaction, if the latter is small. This in turn, is proportional to $J_K$ and $\lambda^2$ (see Eq. (3)), with a prefactor that, being generally of the order of magnitude of the band width, should vanish as $n_c \to 1$.

IV. DISCUSSION

We have shown that the Kondo-lattice model, treated within the HF BCS approximation, can lead to a superconducting phase within the Kondo (heavy-fermion) regime, with the Kondo temperature $T_K$ and superconducting critical temperature $T_c$ of the order of magnitude observed in experiments. While both temperatures depend exponentially on the exchange interaction, their doping dependences are different, and $T_c$ vanishes for a half-filled band. If one wants to make quantitative comparisons with experimental results, an appropriate choice of parameters that gives a good agreement for $T_c$ will yield a slightly overestimated $T_K$. This is typical of a mean-field solution, and one expects the true Kondo temperature to be reduced by fluctuation effects. Actually, we would like to remark that $T_K$ signals a second-order phase transition in the mean-field approach, while only broad features characteristic of a crossover behavior are observed in experiments.

It is interesting to notice that other approximations can be obtained if one explicitly uses the constraint $n_f^i n_i^c = n_i^f$ to rewrite parts of the Hamiltonian before performing the HF decoupling. For example $n_f^i n_i^c = n_i^c$ ceases to be an exact equality once the first term is decoupled. The use of different approximations affect the strength of the different decoupled terms, and therefore affect the relative stability of the different phases. However, assuming that magnetic ordering does not occur, the qualitative behavior of $T_K$ and $T_c$ should be the same as in our approach.
We have not analyzed here the stability of our solution with respect to magnetic ordering. However, previous results have shown that within a mean-field approach one needs an explicit intersite exchange in order to obtain magnetic long-range ordering. Even in that case, the non-magnetic solution should be stable for moderate or large Kondo interaction $J_K$. On the other hand, the possibility of obtaining a wave-vector dependent superconducting gap, as suggested by experimental results has more to do with the model itself, as one should consider a non-local Kondo interaction. The present approach can be easily extended to such a case.

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