Superconductivity in the Kondo lattice model

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Abstract. We study the Kondo lattice model with additional attractive interaction between the conduction electrons within the dynamical mean-field theory using the numerical renormalization group to solve the effective quantum impurity problem. In addition to normal-state and magnetic phases we also allow for the occurrence of a superconducting phase. In the normal phase we observe a very sensitive dependence of the low-energy scale on the conduction-electron interaction. We discuss the dependence of the superconducting transition on the interplay between attractive interaction and Kondo exchange.

1. Introduction

Heavy Fermion (HF) compounds with elements from the lanthanide or actinide series share some rather general features in the Fermi liquid phase, namely a strong enhancement of the effective carrier mass and a similarly enhanced Pauli susceptibility with a Wilson ratio typically of the order, but larger than one [1, 2]. In addition to this well-understood Fermi liquid phase [2–5, 16], HF systems also exhibit a variety of phase transitions, among them magnetic and superconducting phases. This aroused the strong interest of both experimentalists and theorists, as $f$-electrons conventionally tend to suppress superconductivity. The discovery of quantum critical phenomena [6–8] eventually showed the intimate link between the latter two. In spite of the rather large collection of experimental results, an accepted theoretical description of superconductivity has not yet been established. Moreover, the role of phonons on the low-energy properties of HF compounds and in particular their relevance for a microscopic theory of superconductivity in HF systems has not yet been addressed in detail [9–11].

We present the first results of a study of the Kondo lattice model with an effective attractive interaction among the conduction electrons. The latter can be thought to be obtained from an optical phonon mode treated in the antiadiabatic limit (a more realistic description employing a true optical phonon in the calculation is the subject of ongoing investigations). Our model is thus

$$H = \sum_{i,j,\sigma} t_{ij,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow} - \frac{J}{2} \sum_{i,\alpha\beta} \vec{S}_i \cdot \vec{\sigma}_{\alpha\beta} c_{i\alpha}^{\dagger} c_{i\beta}$$  \hspace{1cm} (1)

where $c_{i\sigma}^{\dagger}$ annihilates (creates) a conduction electron at lattice site $\vec{R}_i$ with spin $\sigma$, $U$ is the effective interaction between conduction electrons, and $J$ the Kondo exchange. Note that in our notation antiferromagnetic coupling means $J < 0$. Finally, $\vec{\sigma}$ denotes the vector of Pauli spin matrices. We solve the model with dynamical mean-field theory (DMFT) [12] and
Wilson’s numerical renormalization group (NRG) [13]. Calculations were performed for a Bethe lattice with infinite coordination number. In order to study superconductivity we allow for a corresponding symmetry broken phase [14]. Note that we cannot include unconventional order parameters here, as DMFT only allows for \( s \)-wave phases [12].

2. Results

2.1. Paramagnetic phase

![Figure 1.](image)

Figure 1. Left: Density of states for the Kondo model (1) at half filling with \( J = -W/16 \) at \( T = 0 \). Right: Low-energy scale obtained from the width of the gap in the attractive case \( U < 0 \) for \( J = -W/16 \). The inset shows the different gaps for small repulsive and attractive \( U \).

It is necessary to stress that the model (1) does not show the usual symmetry \( U \leftrightarrow -U \) under simultaneous exchange of spin and charge, i.e. its physics cannot be inferred from the corresponding magnetic properties of the model with repulsive interaction. In Fig. 1 we compare the two cases \( U > 0 \) and \( U < 0 \). Superficially, for weak interaction \(|U| < W\), both seem to be rather similar. However, as is evident from the inset to the right part and the behavior for larger interaction the insulator is much stronger for repulsive \( U \). It here originates from the formation of a local spin singlet rather than being of Mott-Hubbard type [15]. For attractive \( U < 0 \), on the other hand, we find that Kondo screening is strongly suppressed and the system eventually recovers Mott-Hubbard physics in the charge sector for large \(|U|\). This difference can be easily understood. For attractive \( U \) the conduction system namely experiences strong correlations in the charge sector, while the Kondo exchange tries to develop such feature in the spin sector. Obviously, when \(|U| > T_K^{(0)}\), where \( T_K^{(0)} \) is the Kondo scale for \( U = 0 \), spin fluctuations will efficiently be suppressed, leading to the observed behaviour. The suppression of the Kondo scale is actually stronger than exponential, as shown in the right part of Fig. 1.

From these results we draw two conclusions: 1) phonons are clearly extremely important even to the paramagnetic phase of the Kondo model and thus to properly account for the low-energy scale of HF systems; 2) as the low-energy scale is efficiently reduced by an attractive interaction among the conduction electrons, we expect that \( s \)-wave superconductivity will actually prevail in a large part of the phase diagram, in particular for small Kondo coupling \( J \).
2.2. **Superconducting phase**

In order to allow the system to show superconductivity, we have to reformulate the DMFT equations in Nambu space and extend the NRG accordingly. The latter has been accomplished some time ago already (for a review see [13] and references therein; the actual way to combine DMFT and NRG has been extensively discussed by Bauer [14]).

![Figure 2](image.png)

**Figure 2.** DOS (upper panels) and real part of the anomalous Green’s function (lower panels) for small Kondo exchange $J = -W/25$ for (a) $U = -W/80$, (b) $U = -W/8$ and (c) $U = -W/4$.

For a very small Kondo exchange interaction $J = -W/25$, the ground state of the model is dominated by superconductivity. This becomes apparent from Fig. 2, where the DOS (upper panels) and the real part of the anomalous Green’s function (lower panels) is shown at half filling (full curves) as well as at finite filling $\langle n \rangle \approx 0.75$ (dashed curves). As the low-energy scale of the model with $U = 0$ is always largest at half filling [16], we can expect that this result remains stable for all fillings $\langle n \rangle \leq 1$. Note that in none of the cases one does observe a significant dependence of the gap on the fillings, i.e. local correlations due to Kondo screening are frozen out here since $T_K \ll |U|$. Furthermore, $|U|/W < 1$ and consequently one expects and observes a BCS like gap structure, only weakly smeared out by self-energy broadening.

Increasing $|J|$ has two effects. First, there appears a finite, critical $U_c$ below which no superconducting solution exists. This can be seen in Fig. 3a, where DOS and real part of the anomalous Green’s function are shown for $J = -W/10$ and a small $U = -W/100$. Note that at half filling we find a Kondo insulator, which has a gap in the DOS. From that perspective the result is actually indistinguishable from the superconducting phase. The anomalous part, however, vanishes here, i.e. we have indeed a normal state and thus an insulator. For larger interactions, the superconducting phase reappears. Compared to the case with small $J$, we observe here visible reduction of the gap and also a broadening of the singularities at the gap edges. We attribute this behavior to the correlations induced by the Kondo exchange.

3. **Conclusion**

We have studied the Kondo lattice model with an attractive interaction between the conduction electrons, which may arise in the presence of phonons, notably optical modes like breathing modes. We found a tremendous effect of an attractive interaction on the low-energy scale, drastically reducing it already for comparatively modest $|U|$. This behavior can be understood...
Figure 3. DOS (upper panels) and real part of the anomalous Green’s function (lower panels) for larger Kondo exchange $J = -W/10$ and (a) $U = -W/100$, (b) $U = -W/10$ and (c) $U = -W/5$.

in terms of a competition between a spin Kondo effect and the charge fluctuations introduced by the attractive $U$. As the latter also favour superconductivity we can expect, and indeed do find, that for experimentally relevant values of the Kondo coupling and interaction parameters the model shows an $s$-wave type superconducting ground state. For real systems this underlines the importance of elastic degrees of freedom for a proper description of the physics of HF materials.

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