Dynamical Mean Field Study of the Kondo Lattice Model with Frustration

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Abstract. We analyze the antiferromagnetic Kondo lattice model for the two-dimensional square lattice including frustration. The Kondo lattice model is especially interesting in the context of heavy fermion physics, as it possibly exhibits a quantum phase transition between an antiferromagnetically ordered state and a paramagnetic heavy Fermion state. The latter can, depending on the electronic properties be either a metallic state with dynamically generated flat bands at the Fermi energy, or an insulator, the so-called Kondo insulator. We analyze the effects of next nearest neighbor (NNN) hopping upon the properties of the Kondo lattice model, especially focusing on the paramagnetic and antiferromagnetic properties around half filling. To this end we use the dynamical mean field theory (DMFT) with the Numerical Renormalization Group (NRG) as an impurity solver. Whereas the paramagnetic results remain qualitatively unchanged when introducing the NNN hopping, the Néel state at half filling is replaced by a spin-density wave. Also the transition between the magnetic ordered state and the Kondo insulator depends on the NNN hopping. An interesting effect of the NNN hopping is the stabilization of Néel states away from half filling.

1. Introduction
Heavy fermion materials have been in the focus of intense research for over 30 years [1]. Their name originates from the fact that density of states (DOS) at the Fermi energy of approximately 100 or 1000 times higher than in ordinary metals has been measured. Besides this very large DOS, a common feature of these materials is a continuous transition between an antiferromagnetic and a paramagnetic phase at $T = 0$ driven by an external control parameter like pressure or magnetic field. The transition point at $T = 0$ is usually referred to as Quantum Critical Point (QCP) [2, 3], as quantum fluctuations dominate the behavior of the system at this point. Near this QCP new physics like unconventional superconductivity or non-Fermi-liquid behavior has been found.

Heavy fermion materials usually include rare earth ions, whose partially filled f-shells form a lattice of local moments. These local moments are coupled to the s- or p-bands of the material. A single localized moment coupled to a bath of non-interacting electrons is usually called an impurity model. These models have become famous for the Kondo effect [4, 5]. Thus, it is not surprising that Kondo physics plays an important role for describing heavy fermion compounds. The other major ingredient is the RKKY interaction [6, 7, 8] between the local moments favoring a magnetic phase. The quantum criticality comes as a consequence of the competition of these two mechanisms.
In the limit of strong local Coulomb interactions within the f-shells, this situation can be modeled by a lattice of spins $S_i = 1/2$, which are antiferromagnetically coupled to non-interacting electrons on a lattice. This Hamiltonian is the Kondo lattice Hamiltonian [9, 10, 11], reading

$$H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + J \sum_i \vec{S}_i \cdot (c_{i,\sigma_1} \vec{\tau}_{\sigma_1,\sigma_2} c_{i,\sigma_2}),$$

for which $c_{i,\sigma}^\dagger$ creates an electron with spin $\sigma$ on site $i$, and $t_{i,j}$ is the hopping amplitude for the electrons from site $i$ to $j$. These electrons are coupled via a spin-spin interaction to the localized spins $\vec{S}_i$ of the rare earth ions with strength $J$, for which $\vec{\tau}_{\sigma_1,\sigma_2}$ denotes the Pauli spin matrices.

In this article we assume an antiferromagnetic coupling being relevant for heavy fermion physics.

The phase diagram for the half filled Kondo lattice including only nearest neighbor (NN) hopping can be summarized as follows [10, 11, 12, 13, 14, 15]: For ferromagnetic or small antiferromagnetic coupling $J$, the ground state is an antiferromagnetic Néel state. For increasing antiferromagnetic coupling the ground state eventually changes into a paramagnetic insulating state, the Kondo insulator.

Recently, it was proposed that frustration will play an important role in explaining heavy fermion materials [16, 17]. It was asked how frustration influences the quantum phase transition. In this article we want to explore this question and analyze, if and how the Kondo insulator and the transition between the antiferromagnetic phase and the paramagnetic phase is changed, when a NNN hopping is included into the system. This additional hopping will impose frustration onto the antiferromagnetic state, but also influences the paramagnetic state. To determine the phase diagram we use the dynamical mean field theory (DMFT) [18, 19]. DMFT relates the lattice model to an impurity model, which has to be solved self-consistently. Thus DMFT neglects spatial fluctuations, which are of course important to the actual quantum critical point. Nevertheless, DMFT has proved to provide a thermodynamically consistent phase diagram being able to describe paramagnetic as well as antiferromagnetic phases and their properties. For solving the impurity model we employ the numerical renormalization group (NRG) [4, 20].

This article is organized as follows: In the next section we will introduce the lattice for which we have performed the calculations and show some results for non-interacting fermions. The next two sections deal with the paramagnetic and antiferromagnetic properties of the Kondo lattice model, which are followed by a conclusion to this article.

### 2. Two-dimensional frustrated square lattice

We have performed our calculations for a two-dimensional square lattice with NN and NNN hopping, see Fig. 1. Besides the usual NN hopping $H_1$, we introduced a special kind of NNN hopping $H_2$ consisting of two terms: a diagonal hopping $t_2$ and a NNN hopping along the axis with $t_2/2$. This allows us to perform the Hilbert transformation analytically, which increases the accuracy during the DMFT self-consistency. Using this kind of hopping, the NNN hopping $H_2$ can be related to the NN hopping $H_1$, as $H_2 = H_1^2 - 4$. Therefore, the Hilbert transformation and the local DOS of the whole hopping Hamiltonian can be deduced from the original NN hopping Hamiltonian. The dimensionality does not play a big role in our calculations as we use DMFT, i.e. only the local DOS enters the calculation. Nevertheless, from previous studies we have the experience that the detailed structure of the longer-range hopping does not play a significant role for the qualitative structures. The most important aspect is the generation of an asymmetry in the DOS [21]. Thus, our at first glance rather strange choice is mainly due to numerical reasons, but we do not expect strong qualitative changes when using a more physical DOS. Antiferromagnetic solutions within DMFT are obtained by breaking the spin-symmetry in the very first iteration and then using an AB-sublattice version of the Hilbert transformation, which for the frustrated lattice includes additional entries imposing frustration upon the antiferromagnetic Néel state.
Figure 1. Left: Allowed hopping processes for the used two-dimensional lattice. Right: Energy landscape for different \( k \)-vectors for the frustrated case \( t_1 = -1 \) and \( t_2 = 1 \). Especially observe the local maximum at \((k_x, k_y) = (0, 0)\) which is completely absent in the unfrustrated case.

Figure 2. DOS for different strengths of NNN hopping \( t_2 \).

The right panel in Fig. 1 shows the energy landscape for non-interacting fermions for \( t_1 = -1 \) and \( t_2 = 1 \). Note that the sign of \( t_1 \) does not affect the DOS, thus has no effect on the DMFT results. Especially interesting is \((k_x, k_y) = (0, 0)\), where for \( t_2 = 0 \) a local minimum can be found. For increasing \( t_2 \) this completely changes and a local maximum is formed. This local maximum will especially change the physics for fillings \( n < 1 \). Finally, the local DOS for 3 different systems is shown in Fig. 2. The formation of the local maximum results in a divergence of the DOS at the lower band edge. The bandwidth \( W \) of the system is taken as energy unit.

3. Paramagnetic Phase

Let us briefly look at the paramagnetic results not allowing for antiferromagnetic ordering. Figure 3 summarizes the results for \( J = 1/4W \). Qualitatively, the NNN hopping does not change the low temperature physics. Changing \( t_2 \), the \( k \)-dependent band-structure changes (see upper panels in Fig. 3), but the region around the Fermi energy shows the same effects: Exactly for half filling a gap at the Fermi energy is formed (bottom left panel), and there is a very narrow band near the Fermi energy for \((k_x, k_y) \approx (\pi, \pi)\) \cite{23, 22, 24}. Finally this narrow band can be hole doped, thus crossing the Fermi-energy.
Figure 3. Frequency and $k$-dependent DOS: The upper panels show half filled solutions for $t_2/t_1 = 0.3$ (left panel) and $t_2/t_1 = 1$ (right panel) for $J = 1/4W$. The color encodes the weight. The lower panels show magnifications around the Fermi energy, $\omega = 0$, for $t_2/t_1 = 1$ and $J = 1/4W$. The bottom left panel shows the half filled solution, the bottom right panel shows a slightly hole doped solution (electron filling $n = 0.95$). The green line corresponds to $\omega = 0$.

This result is not very surprising. At half filling within the paramagnetic phase the screening of the local spins results in the mentioned gap at the Fermi energy and the narrow band near the Fermi energy. This screening will always take place as long as the non-interacting DOS has weight at the Fermi energy.

4. Antiferromagnetism

The major focus of this paper is however the antiferromagnetic solution, Fig. 4. The left panel shows a schematic phase diagram for different NNN hopping strengths and couplings $J$. For weak NNN hopping the phase diagram looks very similar to the unfrustrated case. For small $J$ an antiferromagnetic Néel state is stabilized which finally vanishes via a second order phase transition and the Kondo insulator is formed. Increasing the NNN hopping, the Néel state is replaced by an incommensurate (IC) state for small $J$. This IC phase is characterized by oscillations during the DMFT iterations and therefore cannot be analyzed in more detail [25]. For strong $J$, near the QCP, the Néel state seems to remain stable for $t_2 < t_1$. However, the QCP moves to smaller values of $J$ for increasing $t_2$. Therefore, one finds the expected line of second order phase transitions between the Néel state and the paramagnetic Kondo insulator. This behavior can be explained by the argument that for strong coupling $J$ and $t_2 < t_1$, the system is finally dominated by the leading mechanism: the NN antiferromagnetic exchange, and for further increasing $J$ the Kondo screening forming the Kondo insulator. Only for $t_2 = t_1$ the Néel state is completely destabilized towards the IC phase. One more thing should be mentioned: surprisingly, at large $t_2/t_1 = 0.8$ the Néel state can be stabilized for smaller values $J$ than for $t_2/t_1 = 0.6$ or $t_2/t_1 = 0.4$. This behavior comes along with the formation of the local maximum.
in the energy landscape mentioned above. Thus, this stabilization of the Néel state quite likely is an artifact of the special kind of NNN hopping consisting of 2 parts used here, but the actual mechanism is still unclear.

The right panel in Fig. 4 shows the local DOS for two NNN hopping strengths and different couplings $J$. This figure depicts nicely how the non-interacting DOS, which still can be clearly seen for $J/W = 0.1$, is completely changed by increasing the coupling. For $J/W = 0.3$, in the paramagnetic Kondo insulating phase, the structures of the non-interacting DOS are not visible anymore.

Another interesting point, already mentioned in a former study [21], is that NNN hopping can stabilize antiferromagnetic Néel states away from half filling. Figure 5 shows for different strengths of NNN hopping and coupling $J$ the occupation number around which a Néel state
can be stabilized. These antiferromagnetic regions are rather small, in the meaning that doping $\Delta n \approx 0.02$ away from the shown occupation will destabilize the Néel state towards an IC phase. This figure shows again that the Néel states for $t_2/t_1 = 0.1$ as well as $t_2/t_1 = 0.8$ are located at half filling. However, as the coupling $J$ has big influence on the occupation number, we cannot predict these values only from the non-interacting Fermi surface.

5. Conclusions
We have analyzed the paramagnetic and antiferromagnetic properties of the Kondo lattice model including NNN hopping. We find that the paramagnetic properties remain qualitatively unchanged when NNN hopping is included. While the $k$-dependent band structure is changed, the behavior around the Fermi energy qualitatively remains. Exactly at half filling we still find a gap with a narrow band very near the Fermi energy.

The situation is different when studying the antiferromagnetic phase. The NNN hopping destabilizes the Néel state at half filling towards an IC state for weak coupling $J$. However, for $t_2 < t_1$ and strong coupling $J$, we still find a second order phase transition between an antiferromagnetic Néel state and a paramagnetic state. The transition point now depends on the strength of the NNN hopping. Although NNN hopping destabilizes the Néel state at half filling, we show that it can stabilize antiferromagnetic Néel states away from half filling.

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