Master Thesis: Quantum Kondo-Lattice Model on the triangular lattice

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1 Background

In strongly correlated electron systems, various degrees of freedom interact with each other. As the full interacting many-body problem would be prohibitively hard to treat, one often looks at model Hamiltonians. Moreover, such a model can greatly help in identifying the relevant physical mechanisms in various situations. One often studied model is the Kondo-lattice model: It describes itinerant electrons that interact with localized spins. The corresponding Hamiltonian can be written as

$$H = -\sum_{i,j,s} \left(t_{i,j} c^{\dagger}_{i,s} c_{j,s} + H.c. \right) \pm J \sum_{i} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{s}}_i \qquad (1)$$

where $c_{i,s}$ ($c^{\dagger}_{i,s}$) is the annihilation (creation) operator for an electron with spin $s = \uparrow, \downarrow$ at site i. Hopping $t_{i,j}$ can in principle be arbitrary, but will usually be chosen to be translationally invariant and restricted to short distances. Operator vector $\hat{\mathbf{s}}_i$ denotes the spin of an itinerant electron at site i, its components are thus given by $\hat{s}^{\alpha}_i = \frac{1}{2} \sum_{s,s'} c^{\dagger}_{i,s} \sigma^{\alpha}_{s,s'} c_{i,s'}$, with Pauli matrices $\sigma^{\alpha} = \sigma^{x/y/z}$. The localized spin is denoted by by $\hat{\mathbf{S}}_i$, its length does not have to be restricted to $1/2$. Coupling J between localized and itinerant spins can be ferro- or antiferromagnetic (AFM).

Ferromagnetic $J < 0$ arises through Hund's rule coupling, such a case has been extensively studied in the context of manganites. In that case, the localized moment is given by 3 electrons, i.e., has a length $\frac{3}{2}$. It turned out that this situation can be well captured by neglecting quantum fluctuations of the localized spins; studying classical spins interacting with non-interacting electrons is computationally much simpler. As a consequence, the resulting classical model has been studied on a large variety of lattices. Even in this classical approximation, the stage set by localized spins and electrons turned out to host interesting physics like, e.g., a quantum anomalous Hall state on the frustrated triangular [1] and checkerboard [2] lattices, a mechanism likely relevant to UCu_5 [3].

Antiferromagnetic $J > 0$ can arise through a mechanism that is somewhat similar to super-exchange: the Anderson impurity model of interacting localized levels hybridized with non-interacting itinerant ones yields this physics. While the sign of J does not matter for classical spins, a *quantum* localized spin $\frac{1}{2}$ is a different matter: For AFM $J > 0$, but not for $J < 0$, the localized moment can be screened by an itinerant electron. In this AFM regime, behavior of a single (or few) localized spins have been discussed very extensively ("Kondo" impurities), as has the effective interaction between impurity spins ("RKKY"). One striking aspect that has been established is the crossing over from a 'small' Fermi surface in the regime where the localized quantum spins are largely independent from the itinerant electrons to a 'large' Fermi surface for the case with strong coupling: the system then looks in some sense as if the localized spins were part of the itinerant-electron pool. Moreover, ordered states can exist, as they do for $J < 0$. Since systems with quantum spins are less accessible to simulation than those with classical spins, numerical studies are rarer.

2 Goals and Methods

In this Master's thesis, the Kondo-lattice model with quantum localized spins on the triangular lattice is to be investigated. The method to be used is the variational cluster approach (VCA), because it combines a full inclusion of local quantum fluctuations and correlations with access to long-range order. The VCA has been applied to the same model on the *square* lattice, where AFM order and superconductivity have been discussed [4].

In the triangular-lattice model with classical spins, quite different magnetic patters were found, e.g. a non-coplanar anomalous quantum Hall state [1]. For the triangular-lattice *Hubbard* model, which may also give some indication of potential phases, the same magnetic order and triplet superconductivity were reported.

Questions to be discussed here include the stability of non-coplanar magnetic order and triplet superconductivity. Moreover, the impact of quantum fluctuations can be studied: Since quantum localized spins can be expected to induce quantum fluctuations in the non-coplanar phase seen for classical spins, the question arises whether the magnetic order can survive stronger quantum fluctuations. Possibly, an 'intermediate' scenario is realistic, namely that chiral order remains and long-range AFM order vanishes, as has recently reported for a spin model [5].

2.2 Work program

The goal is to investigate the triangular Kondo-lattice model with quantum localized spins and antiferromagnetic spin-electron coupling using the variational cluster approach (VCA).

- Learn to use existing VCA code.
- Write input files for the Kondo-lattice model.
- Check stability of non-coplanar AFM.
- Compare to superconductivity.
- Investigate spectral density, Fermi surface ...
- Possibly implement some tricks useful for this model into the code.
- Possibly compare to *ferromagnetic* coupling between localized and itinerant spins.

3 Bibliography

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