Master Thesis: Non-equilibrium Kondo-lattice model

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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

$$H = -\sum_{i,j,s}\left(t_{i,j}c^{\dagger}_{i,s}c_{j,s} + H.c.\right) + J_{\text{Hund}}\sum_{i}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{s}}_i + \sum_{i,j} J_{i,j}\,\hat{\mathbf{S}}_i\hat{\mathbf{S}}_j \tag{1}$$

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_{Hund} between localized and itinerant spins can be ferro- or antiferromagnetic (AFM). $J_{i,j}$ describes an additional explicit coupling between localized spins, it is usually due to superexchange and antiferromagnetic.

Ferromagnetic $J_{\text{Hund}} < 0$ 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].

Concerning the localized spin system, the basic competing interactions are (i) the direct superexchange $J_{i,j} > 0$ between localized spins, which prefers them to be aligned antiferromagnetically and (ii) the effective interaction mediated via the electrons' kinetic energy, which generally prefers FM alignment. Together, the situation can become quite complex, because the electron system will often select quite complex magnetic patters if their effective electronic Hamiltonian happens to open a band gap at the Fermi level. At least, this is the picture emerging at thermal equilibrium.

A very recent preprint [4], however, called this wisdom into question for non-equilibrium situations: light exciting an FM metal into AFM order has been simulated for cubic lattices from one to three dimensions. It comes rather as a surprise that photo excitations should promote AFM spin alignment. The effect was attributed to the non-equilibrium electron distribution in the excited state.

On the triangular lattice in equilibrium, both the ideal FM and the AFM states are metallic, while the interplay of AFM superexchange and effectively FM kinetic energy supports an anomalous Hall insulator with a non-coplanar spin pattern [1]. It would here be interesting to see whether the photo-excited FM metal is nevertheless likewise driven towards an AFM state. If so, one would be interested to see whether one can again find the non-coplanar state, i.e., a dynamically induced QAH state.

On the honeycomb lattice, in contrast, even the perfect FM state is not a metal, but only half-metallic at half filling, so that electron-driven dynamics might again play out differently. The equilibrium phase diagram of the honeycomb model shows exotic phases with massive ground-state degeneracy or emergent frustration [5], so that a potential dynamic AF interaction might lead to quite different scenarios than for the square lattice.

2 Goals and Methods

In this Master's thesis such non-equilibrium processes should be simulated on the *triangular* and possibly also the *honeycomb* lattices in two dimensions. The first aim is to establish whether effectively AFM interactions also arise in these lattices, whose equilibrium phases are in some respects quite different from those of the square lattice. The second aim is to identify and characterize any non-equilibrium states that may arise and to compare them to spin patterns seen in equilibrium.

2.2 Work program

The goal is to simulate optically induced non-equilibrium physics for the triangular and honeycomb Kondo-lattice model with classical localized spins with the approach of Ref. [4].

- Learn to use existing equilibrium code.
- Learn and implement non-equilibrium method. Reproduce results of Ref. [4].
- Simulate triangular lattice, analyze and interpret results.
- Simulate honeycomb lattice, analyze and interpret results.

3 Bibliography

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