Master Thesis: Kugel-Khomskii Model with spin-orbit coupling

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1 Background

In strongly correlated electron systems, various degrees of freedom interact with each other. Charge and spin are probably the best known examples, but the orbital of an electron can also be relevant, if several bands contribute to the states near the Fermi level. In the case of a Mott insulator, strong Coulomb interactions suppress charge fluctuations, so that spin and orbital remain as the dominant degrees of freedom.

The iconic model for such a scenario is the Kugel-Khomskii Hamiltonian that can then be derived in perturbation theory [1]. In various generalizations, it is relevant to arbitrary fillings and orbital degeneracies, let us here focus on one electron (or one hole) in the three-fold t_{2g} manifold. The Hamiltonian involves spin and orbital densities, operators S describing spins and matrices T referring to the orbital degree of freedom. A typical term (here projecting onto a spin triplet) might for sites i and j look like this:

$$\left(\vec{S}_i\vec{S}_j + \frac{3}{4}\right)\left(T_i^\dagger T_j^\dagger + T_i\,T_j\right) \tag{1}$$

as well as other combinations of operators. Virtual processes can thus (i) induce spin flips and/or exchange of orbital flavors on neighboring sites and (ii) lower the energy of various ordered phases. Such a KK model has, e.g., been discussed for the triangular and honeycomb lattices and been shown to support a variety of unconventional phases like dimer solids, orbital liquids or, possibly, a fermionic analogue to a supersolid, an orbital 'pinball liquid' [2–4].

In recent years, one hole [5, 6] in the t_{2g} shell has been a focus of intense interest in the case of strongly spin-orbit coupled iridates. [1] If spin-orbit coupling can be assumed to be large, the hole occupies one of two states forming a Kramers doublet corresponding approximately to *total* angular momentum $j = 1/2$. In a honeycomb geometry, this system might then, for the right parameters, host a Kitaev spin liquid. In that case, the superexchange Hamiltonian becomes considerably less complex, as only this $j = 1/2$ degree of freedom is kept, so that it looks like a rather anisotropic spin Hamiltonian without an orbital degree of freedom.

Very recently, the KK model supplemented by moderate spin-orbit coupling has been proposed in this context [9]. In the limit of vanishing $\lambda = 0$, the model corresponds to the t_{2g} KK model mentioned above, in the $\lambda \to \infty$ limit, it should transform into $j = 1/2$ model. This first study has, however, left out some material features like direct d-d overlap and crystal field splitting that may me relevant and has also not fully studied the potential ordered states and the phase diagram. In particular, analytic considerations are missing.

2 Goals and Methods

In this Master's thesis, The KK model for one hole (or electron) should be studied on the honeycomb model when going from $\lambda = 0$ to $\lambda \to \infty$, varying Hund's rule coupling as

[1] To a lesser extend, one electron has also been studied [7, 8]. This case has quite different physics, but similar questions arise as here.

well as the ratio of oxygen-mediated and direct hopping. To this effect, the Hamiltonian of Refs. [2–4] has to be extended with spin-orbit coupling, similar to Ref. [9]. The resulting model should then be analyzed in a similar manner as Refs. [2–4] have done for the triangular lattice.

Possibly, other geometries could also be considered, e.g., generalizations of honeycomb systems, other edge-sharing geometries, or even square lattices, where the superexchange looks quite different.

2.2 Work program

The goal is to investigate the honeycomb Kugel-Khomskii model with spin-orbit coupling, using analytic (classical energy comparison for ordered phases, some quantum corrections like linear spin-/orbital-wave theory, quantum-mechanical approximation of dimer phases) as well as probably numerical approaches (exact diagonalization).

- Understand and rederive model
- Check its limit for $\lambda \to \infty$
- Focus on $\lambda = 0$ by expanding first results reported in Ref. [2]:
  - Switch on Hund's-rule coupling
  - Consider ordered phases
- Introduce finite λ:
  - Compare energies of phases found to relevant to limiting cases
  - For ordered states: analyze spin/orbital waves in linear spin-(orbital-)wave theory
  - Compare to Ref. [9] where appropriate.
  - Are there liquid states in addition to the Kitaev liquid?
- Numerics
  - Implement Hamiltonian for small cluster
  - Check analytic results, or extend where inconclusive

3 Bibliography

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