Is the Hubbard model appropriate for cuprate superconductors?

Modelling correlated electron systems in presence of non-local interactions and doping

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Kurzgefasst

- Investigating the Hubbard model's phase diagramunder the influence of non-local Coulomb interaction
- Advancing a previously developed variational approach to the doped case
- Investigating the filling and temperature dependence of screening effects

The Coulomb interaction between electrons is by definition long ranged. However, the collective electronic degrees of freedom in solids (especially metals) can lead to an efficient screening of the Coulomb interaction. There by, in many materials it is a good approximation to only consider Coulomb interaction between electrons residing on the same lattice site. The model behind this approximation, the Hubbard model, is one of the central models to understand various aspects of materials with strong electronic correlations. It incorporates the competition between kinetic and interaction energy in the most basic way and exhibits phenomena such as magnetism and metal-insulator transitions accompanied with and without magnetic transitions and is considered a fundamental building block to understand layered high-temperature superconductors.

The fundamental approximation, that the Coulomb interaction is local, however, likely breaks down for two-dimensional materials and surfaces, due to the reduced screening volume, and for insulators, due to the reduced possibility of the immobile electrons to perform screening. The corresponding model to incorporate these non-local contributions of the Coulomb interaction into the Hubbard model is called the extended Hubbard model. Since this model bridges the gap between the Hubbard model, with only local interactions, and real materials, it is crucial to understand how the properties of the rather well understood Hubbard model relate to those of the less understood extended Hubbard model.

In order to relate extended Hubbard models with non-local interactions to effective models with local interactions only, we make use of a variational approach which has been developed in our group. Within this method, we could show in Ref. [1] that non-local interactions induce a discontinuous metal-insulator transition, which is an exciting finding regarding both the fundamental understanding ofthe metal-insulator transition in real materials and possible applications. Recently, we advanced this scheme in order to include non-local exchange effects as well [2], and illustrated that our method captures correlations far better than e.g. simple mean-field decouplings. This finding was helpful in understanding the transitions between different, magnetic phases. Here, however, we focus again on the non-local Coulomb repulsion, and how it effectively screens the local interaction. In contrast to our previous works, however, we extend our method to the doped case and apply it to a doped square lattice, which is widely believed to be an appropriate low-energy model for cuprate superconductors. In such cuprates, it is known that the non-local interactions are not negligible [4].

Our variational method relies on approximating the extended Hubbard model with an effectively defined Hubbard model. We find optimal parameters of the effective model by minimizing a free energy functional. This poses a self-consistency problem which we solve by simulating a range of effective Hubbard models. Since the doped case displays a strong sign problem within quantum Monte Carlo algorithms, especially in the most interesting parameter regimes, we solve the effective models within the Dynamical Cluster Approximation (DCA), an extension to Dynamical Mean Field Theory (DMFT) which includes spatial correlations explicitly. To this end, we are collaborating with the *Gull*-group at the University of Michigan, which provided their DCA code and respective Monte Carlo solver [3] for this task. Since the multiple, effective Hubbard models are independent on each other, the parallelization is trivial.

Our main goal is to understand how the known results for half filling change when doping the system. Test calculations on small clusters reveal that the screening of the local interaction by the nonlocal ones heavily depend on the system's filling (see Fig.(1) for an exactly solved four site cluster), which is especially important when constructing appropriate low-energy models for cuprate superconductors.

WWW

http://www.itp.uni-bremen.de/ag-wehling/

Weitere Informationen

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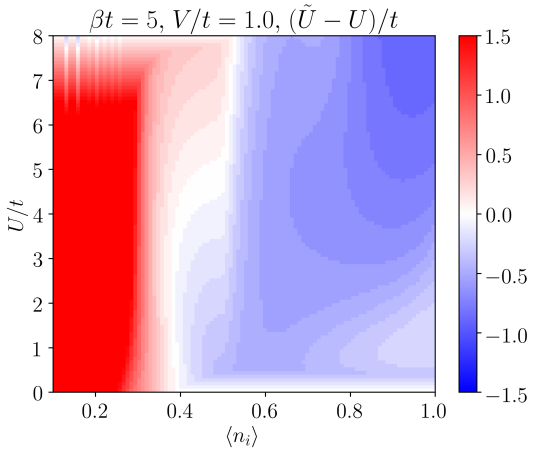

Abbildung 1: *Difference between effective and local interaction, depending on the local interaction and the filling, caused by a fixed non-local Coulomb repulsion in a four site model at a fixed temperature which is solved via Exact Diagonalization. While the nonlocal interaction effectively reduces the local one, it increases it in the case of an almost empty system. Both strength and sign of the screening depend heavily on the filling.*

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Projektpartner

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