Does the Hubbard model describe real materials?

Modelling strongly correlated electrons in presence of non-local interactions

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Kurzgefasst

- Investigating the Hubbard model's phase diagram under the influence of non-local interaction and exchange.
- Interest on the order of the metal-insulator transition.
- Investigation of ferromagnetic exchange in the Hubbard model.
- Assessment of a novel variational approach.

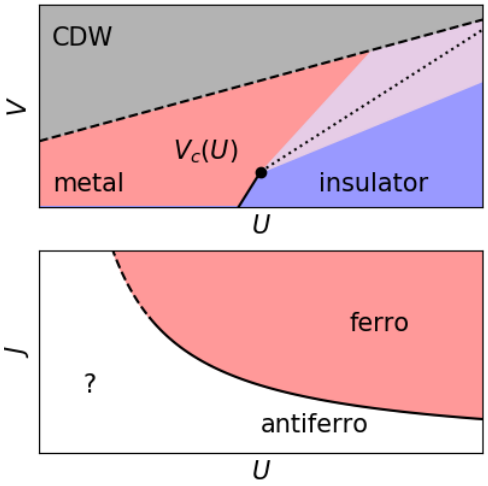

Abbildung 1: *Top: Schematic phase diagram of a lattice model with local interactions U and non-local interactions V: a continuous transition (solid line) from a metal to an insulator turns into a discontinuous transition (dashed line) at $V_c(U)$. Large V induce a charge ordered phase (charge density wave, CDW) where, e.g., only every other site is occupied doubly.*
Bottom: Schematic phase diagram of a lattice model with local interactions U and non-local exchange J: Large J induce a ferromagnetically ordered phase. The phase diagram for large J and small U as well as small J and intermediate U are largely unknown.

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. Thereby, 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.

These non-local interactions are dominated by interactions between charge densities (direct interactions) which favor charge ordering and effectively reduce correlation effects. Typically an order of magnitude smaller are interactions between spin densities (exchange interactions) which lead to ordering of spins. Dependent on the details of the exchange, it favors ferromagnetic or antiferromagnetic ordering.

Figure 1 summarizes the competition between local interactions and both types of non-local interactions (top panel for direct interactions and bottom panel for exchange interactions): The direct non-local interaction disfavors neighboring sites being occupied and thus favors an inhomogeneous occupation of the charge. It thus competes with the local interaction for a lattice with, e.g., every lattice site doubly occupied against an homogeneously singly occupied lattice. Ferromagnetic exchange competes against effective antiferromagnetic exchange induced by local interactions for parallel against antiparallel alignment of spins. In both cases, the non-local interactions favor a symmetry-broken ground state: ferromagnetic exchange promotes breaking of spin-symmetry and direct interaction that of translational symmetry.

While the general role of direct interaction is rather well studied, the role of exchange is largely unknown for models of two-dimensional systems.

The overall goal of this project is first, to understand the influence of non-local exchange and direct interaction in the extended Hubbard model in a novel way and second, to assess the strengths and

weakness of this new method in contrast to established and complementary methods. We focus on the investigation of multiple phase transitions, namely first, the metal-insulator transition under influence of non-local interactions, second, the transition from an anti-ferromagnetic ordering to a ferromagnetic state induced by intrinsic exchange interactions, and third, the breaking of translational symmetry by large non-local interactions from a paramagnetic phase to a charge ordered phase.

We apply new flavors of an established variational method which rely 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. For this solution we use the determinant quantum Monte Carlo method (DQMC) implemented in the QUEST code [2]. The parallelization is embarrassingly simple since the multiple effective Hubbard models are independent of each other.

In the first period of this project we were especially interested in how our novel approach captures the metal-insulator transition under the influence of *V*. Using our established framework we could show in Ref. [1] that non-local interactions induce a discontinuous metal-insulator transition as shown in the top panel of Figure 1, which is an exciting finding regarding both the fundamental understanding of the metal-insulator transition in real materials and possible applications. We could elucidate how this finding translates to novel frameworks of varying the hopping and local interactions simultaneously.

As an example of the effect of different variational degrees of freedom in the case of capturing the effect of non-local interactions, we show the free energy, which has to be minimized, for the case of varying both the interaction U^* and the hopping parameter t^*. In Fig. 2 we show the resulting global minimum marked as black cross. The vertical blue dashed lines are the available variational space for only varying U^* or t^* alone. The respective minima are marked as blue dots.

We can easily assess the quality of the different variational approaches by checking the respective magnitude of the free energy. The variation of the interaction alone leads to a minimal free energy very close to the full variation, whereas the variation of the hopping leads to two local minima, each giving a significantly larger free energy. In this case, the screening induced by non-local interactions is best described by an effectively renormalized local interaction and not a renormalized hopping.

In the next period, we will study a novel variational approach using symmetry broken effective models to tackle the phase diagram of the Hubbard model with non-local exchange.

Ferromagnetic direct exchange favors ferromagnetic ordering, a tendency absent in the effective model used so far. To incorporate ferromagnetic ordering, we extend the effective model by an effective magnetic field which is determined by minimizing the free energy with respect to this field.

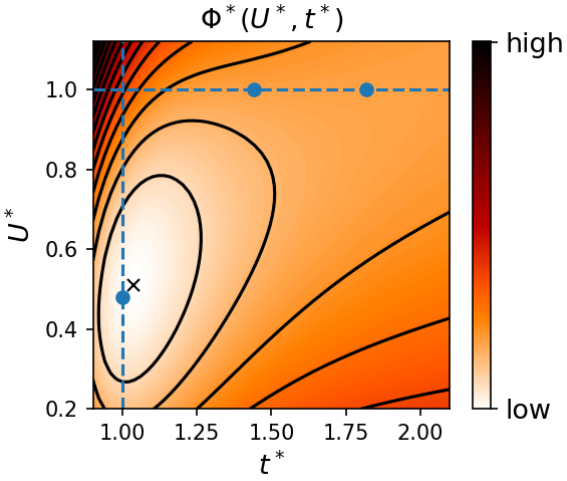

Abbildung 2: *Example of a free energy landscape for the variation of the effective local interaction U* and hopping parameter t* for an exactly solvable finite system defined by local interaction U=1, hopping t = 1, and nonlocal interaction V = 0.4. The minimum of the free energy corresponds to an optimal approximation to the original model with non-local interactions using an effective model without non-local interactions but renormalized local interaction and hopping.*

WWW

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

Weitere Informationen

[1] M. Schüler, E. G. C. P. van Loon, M. I. Katsnelson, and T. O. Wehling. Physical Review B 97 (16), 165135 (2018) https://journals.aps.org/prb/abstract/10.1103/PhysRevB.97.165135.

[2] "QUantum Electron Simulation Toolbox", QUEST 1.3.0, A. Tomas, C-C. Chang, Z-J. Bai, and R. Scalettar, (http://quest.ucdavis.edu/)