

Can light induce superconductivity?

Quantum Monte Carlo approach to the dynamics of strongly correlated systems

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In Short

- Modeling of materials that exhibit unconventional superconductivity
- Search for new strongly correlated non-equilibrium states
- Development of real-time quantum Monte-Carlo methods

Understanding complex phases and dynamics of strongly correlated electrons in solids poses one of the most challenging problems in the field of condensed matter physics. In this project we will investigate the electronic dynamics of models for materials exhibiting unconventional superconductivity, which is a macroscopic quantum state that conducts without dissipation and whose theoretical description is fundamentally different than in phonon-based BCS-theory. The ultimate goal is the understanding of the superconducting mechanism and how its critical temperature T_c can be tuned up to room temperature. So far, the materials with the highest T_c have been found to be cuprates and iron pnictides. Their T_c 's are much higher than in conventional superconductors, but still far from room temperature making them unsuitable for most technologies.

An actively followed approach to obtain high-temperature superconducting states is an attempt to induce and stabilize them with light. In particular, a large body of experimental work in this field has been performed in Hamburg within a Cluster of Excellence (The Hamburg Centre for Ultrafast Imaging) [1]. The experiments have shown that certain materials can be driven by laser pulses system into new non-equilibrium transient states, which can exhibit superconductivity. We intend to support those experimental results with numerical calculations.

We model the cuprates using the single orbital Hubbard model which is capable of capturing many phenomena found by experiments, such as the Mott transition, antiferromagnetic order, superconductivity and other complex phases. Despite the simple appearance of the model, analytical methods can resolve only very limited regions in the phase diagram and numerical methods are inevitable for further progress. Iron pnictides have been classified as

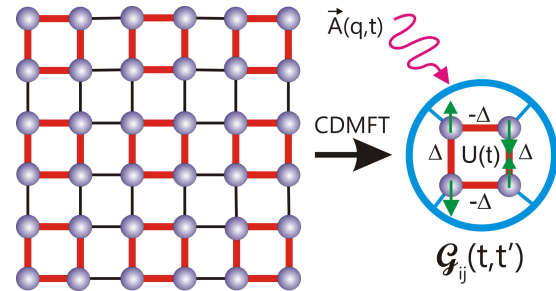


Figure 1: Schematic mapping from the square lattice to a cluster-impurity with dynamic interaction $U(t)$, d -wave superconducting gap Δ and Weiss-field \mathcal{G} . The system is driven out of equilibrium by a laser pulse, that is represented by the vector potential $A(\mathbf{q}, t)$.

Hund's metals and can be modeled in a similar fashion using multi-orbital generalizations of the Hubbard model.

For the solution of Hubbard model we make use of the dynamical mean-field theory (DMFT). The dynamical mean-field treats the local quantum fluctuation exactly which makes it a very successful method for the uncovering of the physics of interacting systems. With extensions of DMFT even certain non-local correlations can be taken into account, which our group accomplished recently thanks to the computing resources provided by HLRN [2–4]. One of the great achievements of DMFT was to provide a comprehensive picture of Mott insulators and Hund's metals at finite temperatures. We have already successfully developed working implementations for the equilibrium DMFT and also cluster-DMFT, that can find superconducting solutions [5]. We also plan to apply an existing non-equilibrium [6] cluster-DMFT implementation (Fig. 1). The success of DMFT is based on the state-of-the-art numerical methods for the solution of the Anderson impurity model. The solution involves the computation of high-dimensional integrals that is a well-suited problem for quantum Monte-Carlo (QMC) methods using Metropolis sampling. For the latter we use a continuous-time formulation without time-discretization errors [7]. Our setup uses the hybridization expansion of the partition function, that is also known as the strong coupling approach. We develop new QMC-based methods for the non-equilibrium case, that e.g. reduce the dynamical sign problem. Furthermore, we implement strong coupling diagrammatic methods, such as non-crossing approximation, to benchmark and complement QMC calculations.

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More Information

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