Material realistic approach to superconductivity

Cluster dynamical mean-field approach to correlated electron superconductivity in real materials

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In Short

- Study of unconventional superconductivity with material realistic models
- Material description by downfoling methods
- Investigation of influences like structural distortion

Many complex phenomena and competing phases appear in materials with strong electron correlations, like Mott-insulating behavior, charge density waves, or magnetic order. In addition, unconventional superconductivity emerges in many strongly correlated materials, a state of matter with zero electrical resistance and perfect diamagnetic properties.

Over time, many materials have been found that show this complex state of matter. Examples range from heavy fermion compounds, cuprates, and iron-based superconductors to potentially more recent findings in magic angle twisted bilayer graphene and infinite-layer nickelate. An ab initio based or realistic material specific description of superconductivity presents an outstanding problem in condensed matter physics.

An adequate description of real material systems is difficult due to material complexity and low energy correlations. The former describes the interplay of many internal degrees of freedom and the coverage of multiple energy scales for which a comprehensive description is demanding. To analyze the latter, different low energy models have been formulated for which a variety of computational methods has been introduced.

In the context of cuprate-based high-temperature superconductors, the Hubbard model on the square lattice serves as a standard model. Different approaches for studying superconducting properties of the system range from weak-coupling, perturbative methods to strong-coupling expansions. Approaches potentially covering strong to intermediate coupling include cluster extensions of Dynamical Mean-Field Theory (DMFT). These have been able to compute spectral functions and phase diagrams.

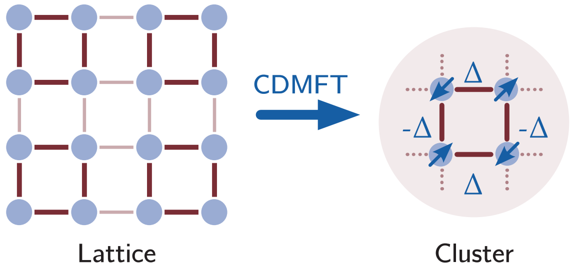

Figure 1: *Schematic mapping of a lattice model onto a cluster-impurity with d-wave superconductiving gap Δ.*

One recently put forward approach, which combines the physics of strong short-ranged correlations with longer-ranged fluctuations, is the combination of Cellular DMFT (CDMFT) with approaches to the Josephson lattice model [1]. In our project we attempt to advance on this and extend the analysis to material realistic descriptions.

We aim to study different cuprate material systems in order to gain a better understanding of the underlying mechanisms leading to the formation of unconventional superconductivity. To this end, we consider existing material descriptions [2] as well as plan to derive material realistic input based on downfolding methods [3]. Our goal is to get a better understanding of the superconducting phase and investigate the influence of structural distortions on the Josephson lattice coupling as experimentally realized [4].

WWW

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

More Information

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Project Partners

Prof. A. I. Lichtenstein (University of Hamburg)

Funding

DFG Research Training Group Quantum Mechanical Materials Modeling (QM^3) (Project P3).