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
- Characterization of anomalous normal state transport properties in the strange metal phase

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. 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) (see Fig. 1) with approaches to the Josephson lattice model [1].

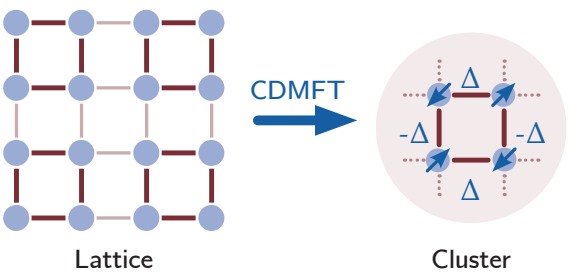

Figure 1: *Schematic mapping of a lattice model onto a cluster-impurity with d-wave superconducting gap Δ.*

In our project we attempt to advance on this and extend the analysis to material realistic descriptions based on ab initio calculations. We aim to study different cuprate material systems in order to gain a better understanding of their phase diagram [4], specifically the 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 [5].

As a part of this project, we worked on normal state properties of cuprate materials in a collaboration with the experimental group of Prof. Dr. N. Hussey. A longstanding problem is the description of the anomalous T-linear resistivity measured in the so-called strange metal phase of cuprates. It is different to the conventional T^2-behavior of a metal as described in Fermi liquid theory and observed for very large hole doping beyond the strange metal phase. Recent measurements [6,7] indicate the possibility that the transition between these regions can be explained by two charge sectors, one with coherent quasiparticles and the other with incoherent non-quasiparticle charge carriers. This raises the question from which carriers superconductivity arises and how it fits to the description of the microscopic mechanism forming this state.

We aim to answer this problem by studying the applicability of a Fermi liquid description and by quantifying which carriers contribute to transport. For this, we investigate the corresponding electron filling or hole doping regions using a complementary approach by employing the strong-coupling CDMFT method and the weak-coupling Fluctuation Exchange ('FLEX') approximation [8,9]. We obtained

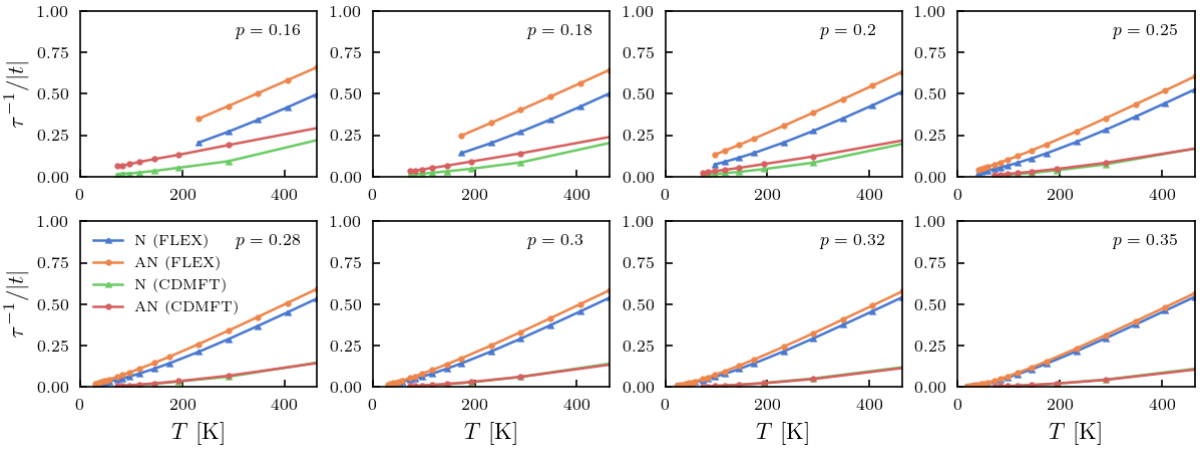

Figure 2: *Temperature dependence of scattering rates (inverse lifetimes) τ^{-1} in units of the nearest-neighbor hopping t from nodal (N) and antinodal (AN) momentum regions for hole dopings p in the optimally ($p \sim 0.18$) to overdoped region ($p \gtrsim 0.2$). Calculations were performed using the FLEX and CDMFT method.*

first results by analyzing the temperature dependence of inverse lifetimes or scatterings rates τ^{-1} of carriers from two different momentum-regions with respect to the hole doping p which we we show in Fig. 2. The two momentum regions, the nodal (N) and antinodal (AN) direction, are termed after the nodes in the momentum structure of the d-wave superconducting gap and play an important role in the discussion of, e.g., the pseudo-gap phase.

We observe several quantitative aspects also seen in experiment. For large dopings ($p \gtrsim 0.25$), we observe a T^2-behavior of the scattering rates, which are proportional to the resistivity. Decreasing the doping two changes occur: First, a dichotomy of carriers from the N and AN regions starts to develop, i.e., scattering rates start to differ. Second, the scattering rates change to a T-linear power law, with the AN region showing stronger linearity than the N region. In future work, we aim to understand how the nodal-antinodal dichotomy affects transport properties and to compare with experimental data.

More Information

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Project Partners

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