Spatial coherence in correlated superconductors

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

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In Short

- Study of spatial coherence in unconventional, electron correlated superconductivity
- Discussion of fundamental length scales in sucperconductors
- Characterization of C_{60}-based materials and high-temperature cuprate systems
- Analysis of (magneto)transport properties in the strange metal phase of cuprates

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 organic conductors to potentially more recent findings in magic angle twisted bilayer graphene and infinite-layer nickelate. The physics in these systems is governed by spatiotemporal fluctuations linked to the coherence of the macroscopic condensate.

Central to its characterization is the knowledge of the coherence length ξ, as it specifies the relevant length scales for fluctuations pertinent to, e.g., the formation of vortex lattices or magneto-thermal transport. Physically, it describes the length scale on which the superconducting state can tolerate phase twists without a collapse of the condensate. Together with the London penetration depth λ, it is one of the fundamental length scales that determine the properties of superconductor like, e.g., the classification into type I and type II superconductors with vortex lattices. Hence, its knowledge is important for tayloring superconducting devices for applications in novel nanostructures, measuring devices or quantum computing.

While the description of the coherence length is well established in weak-coupling Bardeen-Cooper-Schrieffer (BCS) theory and Eliashberg theory, it is a generally unknown quantity in strongly correlated superconductors. In this project, we establish a link to directly calculate the coherence length for superconductors with strong electron correlations from microscopic theories and first principles. As a test case, we embeded this new approach in dynamical mean-field theory (DMFT), a strong coupling approach to describe many-body physics of strongly correlated and localized electrons, and applied it to the material family of alkali doped fullerides (A_3C_{60}).

In these materials, Buckminsterfullerene C_{60} molecules ("Bucky balls"), which are carbon atoms arranged in a soccer-ball-like shape, are put in a crystaline environment. Upon doping with Alkali atoms (A=K,Cs,Rb) these materials become an isotropic s-wave superconductor with critical temperatures T_c in the range of 20-30 K [1]. Recently, the A_3C_{60} materials moved into the spotlight because the phenomenon of light-induced superconductivity was discovered [2,3].

To calculate the coherence length ξ, we use the physical idea of position-dependent phase spirals where we allow the order parameter of the superconducting state to have a spatially varying phase $e^{i\mathbf{q}\mathbf{r}}$ with wave momentum $\mathbf{q}$ and position $\mathbf{r}$. Due to this phase, the Cooper pairs that form the superconducting condensate gain a finite center of mass momentum equal to $\mathbf{q}$ that increases the kinetic energy and hence reduces the binding energy. It can be imprinted on the order paramater by an external pairing field that carries the same phase.

We illustrate this idea in Figure 1. The left panel shows the order parameter $|\Psi|$, which characterizes the phase, as a function of temperature T and momenta q. Upon increasing q, the order parameter is reduced and hence superconducting order is suppressed. The length scale $1/q^\star$, on which the order vanishes, is the associated length scale given ξ. The results of extracting ξ from the spatially varying order parameter is shown in he right panel of Figure 1. It diverges towards T_c and reaches a finite value ξ_0

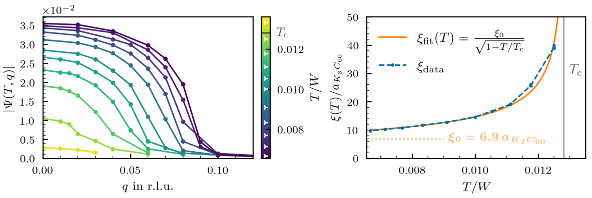

Figure 1: *Left panel: Superconducting order parameter $|\Psi|$ as a function of phase spiral momentum $q = |\mathbf{q}|$ in reciprocal lattice units (r.l.u.) and temperatures T in units of bandwidth $W = 0.5$ eV for fixed interaction $U = 0.7$ eV, $J = -20$ meV. Right panel: Coherence length ξ in units of lattice constant $a_{K_3C_{60}}$ as a function of temperature with Ginzburg-Landau fit.*

at zero temperature which can be fit by a Ginzburg-Landau description.

In our study, we scanned different system parameters to understand the influence of strongly-correlated Mott-insulating states on the spatial coherence of the superconducting condensate. We found that near the Mott states the coherence length is strongly supressed to a few lattice constants and that the transition can be surprisingly well described using Eliashberg theory. This indicates that the knowledge or rather reproducibility of the critical temperature in theory alone might not be sufficient to understand the physics to superconductivity, but additional properties like the coherence length need to be analyzed for a full picture. Our current work entices a more detailed analysis of these findings to also put them into the context of a BCS-BEC (Bose-Einstein condensation) crossover.

A second focus of our work is the study of cuprate-based high-temperature superconductors [4]. A long-standing 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 [5,6] 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 question by studying the applicability of a Fermi liquid description and by quantifying which carriers contribute to transport. To this end, we investigate the Hubbard model on the square lattice which serves as a standard model for the description of cuprate materials. Different

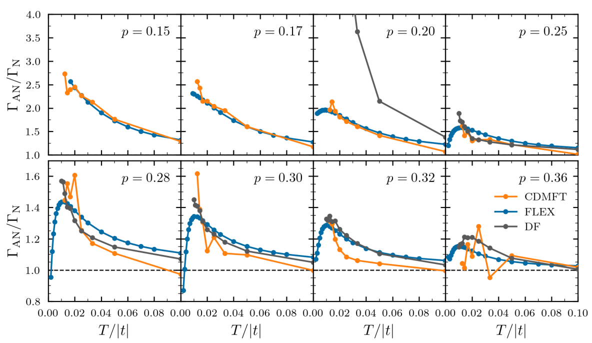

Figure 2: *Temperature dependence of the ratio of nodal (N) and antinodal (AN) scattering rates Γ for dopings in the optimally ($p \sim 0.18$) to overdoped region ($p \gtrsim 0.2$) calculated using different many-body techniques ("FLEX", "CDMFT", "DF").,*

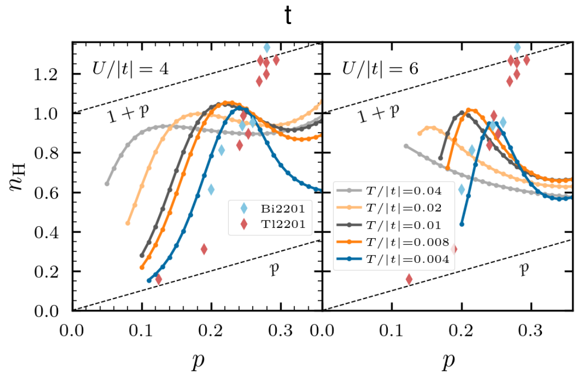

Figure 3: *Hall carrier density n_H as a function of hole doping p as calculated from FLEX using a modified Boltzmann theory. Left and right panel show two different interactions U and line represent temperatures T. Experimental data is marked by diamonds.*

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 extensions of DMFT. We apply a complementary approach of employing the strong-coupling Cluster DMFT (CDMFT) method [7], the weak-coupling Fluctuation Exchange (FLEX) [8], and Dual Fermion (DF) theory [9] which combines ideas from both sides.

Some results of our study are given in Figure 2, where we show the T-dependence of scattering rates Γ of carriers from two different momentum-regions with respect to the hole doping p. 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 indicated by the experiments. 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 of particles in the AN change to a T-linear power law.

We also studied (magneto)transport properties, particularly to understand the Hall carrier density n_H measurements. We found very unexpected results. The standard approach using the Kubo formalism, a fully quantum mechanical linear-response theory, fails to reproduce the experimental data. On the other hand, by applying the semiclassical Boltzmann theory with a modification of the quantum particle distribution yields results in much better agreement with experiments. We show preliminary results in Figure 3 from FLEX calculations which also show the drop of n_H towards low hole dopings p. We are working to understand this a priori unexpected results from a fundamental theoretical perspective at the moment.

In future work, we plan to extend our idea of phase spirals for calculating the coherence length to well established models of the cuprate systems [10]. For this, we will adjust the formalism to the anisotropic d-wave pairing and finite clusters. We will compare this we the put forward idea, which combines the physics of CDMFT with approaches to the Josephson lattice model [7] from which related but different phase stiffness can be extracted.

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https://www.physik.uni-hamburg.de/en/th1/ag-wehling.html

More Information

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Project Partners

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