Master Project

Quantum criticality in the 2D Hubbard model: a study via plaquette-DMFT+NRG

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Quantum criticality in metals has attracted great interest in condensed matter physics during the last three decades. While mostly studied in the context of heavy-fermion materials [1–3], the existence of a quantum critical point (QCP) has also been conjectured in cuprate superconductors [4, 5], backed by several experimental hints [6–8].

Numerous experimental studies, carried out on a variety of different systems, established several features common to these QCPs. A prominent one is a reconstruction of the Fermi surface (FS) when crossing the QCP at $T = 0$, leading to a violation of Luttinger's theorem [9, 10] on one side of the QCP. This FS reconstruction leads to a sharp crossover in the Hall coefficient at low temperatures, which has been observed both in heavy-fermion systems [11] and cuprate superconductors [7]. Further, a non-Fermi-liquid (NFL) "strange metal" phase is observed when varying temperature in the vicinity of the QCP. It features a linear in temperature resistivity [8, 12] which is to date unexplained.

A widely-used theoretical approach for tackling strongly correlated matter is dynamical mean-field theory (DMFT) [13–15]. It treats the interplay between a given lattice site (the "impurity") and the rest of the lattice (the "bath") as a quantum impurity model with a self-consistently determined hybridization function. This approach neglects non-local correlations. However, there are growing indications that these are crucial for driving these systems towards a QCP. To incorporate short ranged non-local correlations, quantum cluster methods [16] like the Cellular DMFT (CDMFT) and the Dynamical Cluster Approximation (DCA) have been developed. These use a cluster of sites, rather than a single site, as elementary unit (or impurity), to be embedded in a self-consistently determined environment.

DMFT methods crucially depend on a reliable numerical method to solve quantum impurity problems. In order to study quantum critical behavior, the impurity solver should be able to access low temperatures and resolve very low energy scales. Both requirements are met by the Numerical Renormalization Group (NRG) [17–19], a tensor-network method which yields spectral data directly on the real-frequency axis. The NRG code developed in our group has been applied in numerous DMFT studies over the last years with great success. Moreover, recent work on quantum criticality in heavy-fermion systems using CDMFT [20] showed that our NRG code can provide insights far beyond the capability of Quantum Monte Carlo [21] or exact diagonalization [22, 23] methods.

The goal of this Master's project is to study quantum criticality in the t-t'-U 2D Hubbard model with nearest- and next-nearest-neighbor hopping. This model is believed to capture key ingredients needed to understand high-temperature superconductivity in the cuprates [24]. We will use plaquette-DMFT+NRG, choosing the elementary unit to be a 4-site plaquette [25] – the minimal reference system that contains the spatial structure needed to support d-wave superconducting fluctuations [24]. Additionally, the plaquette has an important degenerate point at hole doping of $\delta = 0.25$. This degeneracy has been argued to lead to quantum critical behavior for the self-consistent solution of the 2D Hubbard model near that filling. Plaquette-DMFT+NRG will be used to study this quantum critical behavior, exploiting the ability of NRG to reveal low-energy and low-temperature properties with unprecedented resolution.

Project roadmap

- **Background:** Familiarize yourself with the basic ideas underlying DMFT [13, 16], NRG [17–19], CDMFT+NRG [20], quantum criticality in metals [1–3] and cuprates [4–8], and plaquette physics in cuprates [24, 25].
- **Set up numerical code:** Building on an existing DMFT+NRG package developed in our group, set up a plaquette-DMFT+NRG code for the t-t'-U 2D Hubbard model. As a first step, study the plaquette-impurity model without self-consistency in the vicinity of the degeneracy point at $\delta = 0.25$. Then implement self-consistency and study its consequences (in the normal phase, i.e. without breaking symmetries).
- **Study phase diagram near $\delta = 0.25$:** Scan the parameter space near this degeneracy point and study various observables (local spectral functions, spin, charge and pairing susceptibilities, optical conductivity) to set up a phase diagram of temperature versus doping. Identify the location of the putative QPC and study signatures of FS reconstruction in its vicinity.

Further details: The project involves mainly numerical work, but requires a solid grasp of many-body physics and condensed-matter field theory. Prerequisites: Courses on Theoretical Condensed-Matter Physics, Condensed-Matter Field Theory, Tensor Networks, as well as coding skills (MATLAB).

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