Abstract

Superconductivity and Orbital Selectivity in a three-orbital Hubbard model for the iron-based superconductors

Variational Monte Carlo analysis

Vito Marino

The Hubbard model is crucial in condensed matter physics, particularly for studying high-temperature superconductors like cuprates and iron-based superconductors (IBS), where strong Coulomb interactions are the driving force behind superconductivity, unlike traditional BCS superconductors. These materials exhibit superconductivity within two-dimensional layers and depend on d orbitals influenced by the lattice structure. Using the three-orbital Hubbard-Kanamori model appropriate for describing the feature of a generic iron-based superconductor (IBS), we explore the role of orbital selectivity, where Hund's coupling promotes a behavior called orbital-selective Mott phase (OSMP) with differing correlations among orbitals and its interplay with superconductivity.

Through Variational Monte Carlo (VMC) simulations, we analyze the ground state of the model, using a BCS-like variational wave function with Jastrow factors to capture correlations. The VMC is a non-perturbative method that can directly address superconductivity on a two-dimensional lattice. We construct a phase diagram by varying Coulomb repulsion and total electron density, observing orbital selective phase (OSP) and nematicity across densities from the parent compound ($n_e = 4$) to half-filling ($n_e = 3$). The superconductive order appears only in orbitals away from half-filling. Adding antiferromagnetic order alters the phase diagram, exhibiting a positive interplay with OSP while suppressing superconductivity. This thesis aims to deepen the understanding of superconductivity in multi-orbital systems like IBS.