Correlated Materials
Models & Methods

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Abstract

This thesis encompass a series of studies on methods and models for electron systems with local interactions, relevant for correlated materials. The first study focus on the canonical model for local correlation, the Hubbard model. Using dynamical mean field theory, the critical properties of the finite temperature end point of the metal insulator transition are determined. The issue of computing real frequency spectral functions is also addressed through the development of the novel method, distributional exact diagonalization.

Next topic is the multiband Gutzwiller variational method, for which an efficient solver is presented, applicable to realistic d-electron models when accounting for lattice symmetries. The solver is applied to the iron based superconductors FeSe and FeTe, where the Hund's coupling is found to drive orbital differentiation in the correlated parent state.

A central issue is how to model the local Coulomb interaction. Imposing rotational invariance on the complete set of d-states results in the Slater-Condon interaction, to be compared with the simpler Kanamori interaction, that is shown to be a Laporte-Platt degenerate point of the former. The derivation of a minimalistic form for the Kanamori interaction in terms of density-density, total spin, and total quasi-spin operators enables an exact parametrization of the Slater-Condon interaction in terms of the Kanamori parameters.

The additional interactions contained in the Slater-Condon form are identified as higher order multipole scattering, and the parametrization enables a direct study of the effect of these interaction processes. The multipole scattering is found to drive charge disproportionation and valence-skipping for a subset of multipole active d-band fillings, and raises the question whether such multipole effects are manifested in real materials.

Keywords: correlated electrons, Hubbard model, multiband Hubbard model, dynamical mean field theory, exact diagonalization, Landau theory, Mott metal-insulator transition, Gutzwiller method, many-body point group symmetry, iron chalcogenides, Kanamori interaction, Slater-Condon interaction.