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Title of Ph.D. :Exact diagonalization as impurity solver in dynamical mean-field theory: Applications to high-temperature superconductors

ABSTRACT

To accomplish theoretical study of a particular model that describes a given material, the tools required are of utmost importance. Computational methods put a check on approximate methods and provide directions for development of new approaches.

Dynamical mean-field theory(DMFT) has been extensively used to study the strongly correlated quantum many-body systems over the past decade. Exact Diagonalization(ED) is an important technique providing an exact solution of quantum many-body Hamiltonians on finite clusters.

The small coherence length ξ of high-temperature superconductors renders the mean-field treatment to be inaccurate and provides another reason to resort to computation. In recent years, dynamical mean-field theory has been used to study high-temperature superconductors mapping the lattice model onto impurity model that again is to be solved using numerical methods like exact diagonalization.

The primary focus of the work presented in this thesis is to carry out computational studies on exact diagonalization of Hubbard model (especially in context of exact diagonalization being an impurity solver in dynamical mean-field theory) to develop:

• New and efficient schemes and algorithms that are economical in terms of CPU time and memory thereby making feasible large computation on smaller machines.

• Simple combination method based on different diagonalization algorithms that helps to do away with errors inherent in an algorithm and has better convergence properties.

• Efficient algorithms of correlation functions required in the study of high-T_c cuprates.

The work presented in this thesis primarily consists of:

• Developing a new basis scheme for exact diagonalization of Hubbard model that uses the basis states of one-spin configuration ($\uparrow$ or $\downarrow$) at a time.

• Developing a new combination method based on Davidson algorithm and Lanczos algorithm for computation of Green's function at very low temperature required in DMFT self-consistency loop.

• Application of our one-spin configuration scheme for solving the Hamiltonian used to describe high-T_c cuprates and computing various correlation functions.

Organization of thesis

Chapter 1 provides a brief introduction of strongly correlated materials, Hubbard model, dynamical mean-field theory, exact diagonalization and high-temperature superconductors.

Chapter 2 presents our proposed new one-spin configuration basis scheme

for exact diagonalization of Hubbard model. We present the generation of basis states, generation of Hamiltonian matrix including both diagonal and non-diagonal parts and also the storage of non-diagonal part of Hamiltonian matrix required in diagonalization. The scheme is also shown to be inherently parallelizable. The comparision in terms of CPU time of our new one-spin configuration scheme with the conventional two-spin configuration scheme is also reported. The use of our scheme in translationally symmetric systems, computation of finite temperature and zero temperature Green's function, also as impurity solver in dynamical mean-field theory are discussed. The extension of our scheme to other models is also described.

Chapter 3 describes a combination method based on the Davidson algorithm and the Lanczos technique for solving the impurity Hamiltonian obtained in dynamical mean-field theory procedure (computation of continued-fraction expansion of the Green's function required in DMFT self-consistency loop) at a very low temperature. The comparision of our proposed method with the full diagonalization on a single-band Hubbard model is also reported.

Chapter 4 presents algorithms for computation of $s-$wave, extended $s-$wave, $d-$wave order parameters, pairing amplitudes, spin and charge correlation functions of high-temperature cuprate superconductors on one-band extended Hubbard model using our one-spin configuration basis scheme. The efficiency of the algorithms is discussed. Some test results are also shown.

Chapter 5 deals with the extension of classical computation to quantum computation. A new qubit is proposed and a quantum algorithm using the proposed qubit for the procedure of Pauli spin blockade readout is presented.

Chapter 6 summarizes the results presented in the thesis and the conclusions drawn during the course of this study.