Advantage and Limitation of Density Matrix Renormalization Group Method

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Density matrix renormalization group method introduced recently by White proves to be highly successful for interacting one and quasi-one dimensional systems. We compare this new method with the conventional numerical renormalization group. We discuss the common goal and different strategies used in both methods. The limitations of the new method as well as the ways to overcome them are explored.

KEY WORDS: density matrix and numerical renormalization group methods; Hubbard model.

As discussed by Dagotto and Moreo in this conference, it is now possible using numerical method to obtain spectral information directly from strongly correlated Hamiltonian and to make meaningful comparisons with photoemission experiments on high $T_c$ superconductors[1]. In order to make further progress especially in understanding the transport properties and the relation between superconductivity and strong electron-electron correlations in the high $T_c$ copper oxide materials, we need to go to lower energy. Access to lower energy reliably is also needed in investigating the possible non-fermi liquid behavior in two dimensional Hubbard model. Since the lowest energy of an extended state is proportional to $1/L$ where $L$ is the linear system dimension, We need larger system sizes.

With the numerical method presently available it is difficult extending the calculations to larger system sizes. The so called 'minus sign' problem prevents quantum Monte Carlo from reaching low temperatures. In the other often-used method, i.e. exact diagonalization, the dimension of the Hilbert space grows exponentially with the number of electrons. It is quite impossible to do calculation on larger clusters.

In a seminal work, White[2] has developed the density matrix renormalization group (DMRG) technique. In this method, the ground state wave function is expanded in terms of a small number of states which is only a tiny fraction of the dimensions of the Hilbert space. The ground state wave function and energy are calculated approximately. For one dimensional spin-$\frac{1}{2}$ Heisenberg model, one easily gets an energy within $10^{-6}$ of the exact answer. Furthermore, the ground state energies obtained are variational upper bounds. The DMRG method has been applied successfully to many one dimensional systems[4-11].

Our purpose in this talk is to discuss the advantage and limitation of the DMRG method. We will compare the DMRG with Wilson’s numerical renormalization group technique (NRG)[12,13] in order to elucidate what make them work as well as identify the common features and the differences between the two methods. We believe it is possible to develop better Hilbert space pruning technique[14].

We begin with a general discussion of renormalization group technique as applied to calculating low energy spectrum of a many-body hamiltonian. The main problem is how to truncate the Hilbert space without effecting much its low energy spectrum. To illustrate that this is quite possible, let us discuss an example. Let the hamiltonian $H$ be a $m_H \times m_H$ matrix where $m_H$ is the dimensions of many-particle Hilbert space. Let $T$ be a $m_H \times m_H$ unitary matrix so that the columns of $T$ form an orthonormal basis set of the many-particle Hilbert space. Then transformation $H' = T^\dagger H T$ does not change the eigenvalue of the hamiltonian $H$. Suppose $T$ can be so chosen

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that the matrix elements of $H'$ are only non-zero on and close to the diagonal. Let us further assume that the diagonal elements are arranged in increasing order: $H'_{11} < H'_{22} < \ldots < H'_{m_H m_H}$. Matrix $H'$ describes a one dimensional system of a particle hopping among quantum states each of which has an on-site energy $H'_i$. The off-diagonal elements $H'_{ij}$ represent hopping between the states. Since $H'_{ij}$ are only non-zero close to the diagonal, the hopping is short ranged. We know for this particle-moving-against-hill problem, the wave functions of the ground state and the low energy excitations are exponentially small in the classically forbidden region at large $H'_i$. It is clearly safe in this case to discard the states with $H'_{ii}$ much larger than the energy of interests.

NRG and DMRG represent two different strategies in choosing the transformation matrix $T$. In the NRG method, $T$ is chosen to make diagonal energy separation $H_{ij} - H'_{ij}$ large and the eigenstates of block hamiltonian is usually used. As we will discuss further later, it only works when there is a cascade of energy scales associate with the degrees of freedom being truncated. On the other hand, in the DMRG method, the transformation matrix $T$ is chosen to make $H'_{ij}$ 'localized', i.e., $H'_{ij}$ is big only for a few pairs of $ij$. States kept in the DMRG method are the eigenstates of density matrix. In order to construct the density matrix one needs a good guess of the ground state wave function.

The strategy used in Wilson’s NRG is divide and conquer. For this method to work, the problem must have interacting energy ranging from large to small[13]. In Wilson’s NRG calculation of Kondo problem, all the interacting electrons have the same diagonal energy. The energy splitting is determined by the interaction between particles. In the initial step of renormalization group calculation, the hamiltonian of the most strongly interacting particles is diagonalized. Only the lowest few energy eigenstates are kept and then mixed with the next strongest interaction in the problem. Since the interaction in the initial step is strongest, the energy level splitting caused by them is larger the that caused by the second strongest interaction. It is therefore safe to discard the high energy states in the initial step. This procedure is repeated going to lower energy scale.

Essentially, the NRG method maps the original problem of diagonalizing a $m_H \times m_H$ hamiltonian, where $m_H$ is exponential in $N$, the number of particles, to $N$ steps each of which is a problem of fixed size which depends on number of states kept. In order for this method to work, the hamiltonian must exhibit a cascade of energy scales from large to small. The difficulty in applying the NRG to interacting hamiltonians relevant to high $T_c$ superconductors is that in the lattice models there is no energy scale apparent, at least in the real space.

The DMRG method employs a somewhat different strategy that does not require a cascade of energy scales. The DMRG method attempts to use a small number of states to accurately expand the ground state. One divides the lattice under study into two parts, i.e. the system and the rest of the world (environment), and asks if one is allowed to use only $m$ states each for the system and the environment, which $m$ states should one choose? The answer depends on which wave function one wants to accurately represent and is formulated in a pioneering work[2] by White as follows: starting from a good guess of the ground state wave function of the whole lattice, construct the density matrix of the system from the wave function by summing over the Hilbert space of the environment and pick the $m$ largest weight eigenvectors of the density matrix. This is different from the NRG method where, instead, the $m$ lowest energy eigenvectors of the system are chosen. Since the ground state wave function of the whole system is generally not known before hand, one tries to improve the initial approximation by an iterative procedure which is discussed in detail by White[2]. Thus, the DMRG method systematically improves the approximation to the ground state wave function and the procedure usually converge after a few iterations through the lattice. In addition to the ground state, this procedure also works for low-lying excited states.

As we have mentioned before, the DMRG does not rely on the presence of scales in the diagonal energy. Instead, it attempts to preserve the inter-block off-diagonal matrix elements well. How and when this works can be analyzed by an argument similar to the scaling argument in the localization problem[15]. If two blocks, system and environment, are coupled by an interaction of strength $t$, we know from the perturbation theory that in describing the ground state of the superblock the energy levels of the two blocks within $\delta E \approx t$ of the block ground state will be mixed. Since the number of states within energy $\delta E$ of the ground state energy increases exponentially with $\delta E$, the number of states needed to expand the ground state of the superblock grows exponentially with the inter-block interaction. Keeping a constant