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Number of Repetitious States in One Dimensional Hubbard Model: a Density Matrix Renormalization Group Perspective

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In this work we investigate some aspects of density matrix renormalization group (DMRG) method. We intuitively show why DMRG works better for open boundary conditions and why the number of sweeps in a periodic system is greater than an open one. We also describe reduction of the Hilbert space dimension using symmetries. Finally, we show that eliminating the repetitious states may help as much as symmetries to reduce the Hilbert space and thus increase the DMRG speed.

Keywords: Density matrix renormalization group, Repetitious states, Reduction of the Hilbert space dimension.

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1. INTRODUCTION

Density Matrix Renormalization Group Method (DMRG) is one of powerful methods to investigate the one dimensional system (nanowires). By increase the dimension to two and three, DMRG accuracy decreases considerably but still is the most powerful existing method. There are different type of DMRG and among its different types, the Lanczos-DMRG which was introduced by Hallberg, uses the Lanczos method in DMRG to calculate the dynamical properties of lattice quantum many body systems [1]. Then it was used in other branches of physics such as calculation of the dynamical correlation functions [2]. Different types of DMRG are generally time-consuming but a fast version (has been called Dynamical-DMRG (DDMRG)) presented by jeckelmann et al [3-4]. It is very similar to correction vector-DMRG which was proposed by Ramasesha et al. to calculate some types of dynamical correlation functions [5]. Despite the fact that researchers are working on DMRG to extend it to reach more precision in their calculations [6], some authors complain that DMRG does not satisfy them. When Kampf et al. applied the DMRG to one-dimensional ionic Hubbard model, They showd that the accuracy of the currently available DMRG data is not enough to provide a stringent argument in their studies and with the available chain length and DMRG accuracy limitations it was not possible to precisely identify and locate the second transition point in their system [7]. In two dimensions, the accuracy in k-DMRG and r-DMRG decreases with the system size. The accuracy becomes rapidly worse with increasing interaction and is not significantly better at half filling [8]. In the meantime, boundary condition had a very important role in the works uses from the DMRG method and people consistently try to modify the boundary scheme to extract more precise results [9]. Sometimes, the boundary conditions influence the spectrum of the reduced density matrix (RDM) and generally DMRG performs substantially worse for systems with periodic rather than open boundary conditions [3-4]. In addition, periodic boundary conditions are normally highly preferable to the open ones, as surface effects are eliminated and finite size extrapolation gives better results for smaller system sizes. Legeza et al. found that because of the increase in the entanglement of their periodic states the number of states kept tends to be the square of that required for open boundary conditions [10, 15]. To keep the accuracy of the results, people need much more basis states in each block of the DMRG method. The reduction of the accuracy comes from the boundary condition and when the interactions across the boundaries are weak, the accuracy of the DMRG calculation will be improved [11].

In this work, it is shown why DMRG with doubling the block size is less satisfactory than DMRG with adding a single site at a time. It is quantitatively shown that when we add a single site to the chain in each step, some repetitious states appear that lead to some decrease in the speed of DMRG method. Getting rid of these repetitious states may help us to find more flexible DMRG variants. We have also investigated the reduction of the Hilbert space dimension by using of symmetries. In our previous work we have used some these aspects [12].

2. THEORY

There are different types of DMRG computer implementation. Doubling the block sizes in each iteration or adding single site to the left and right block is two approaches among them. Doubling the block size in DMRG leads to rough results. An obvious test is that, when we are generating the desired states of a 8-sites chain from tensor product of the possible states of a 4-sites chain in quarter-filling in DMRG method, for simplicity all spins up,

$$\begin{matrix} \uparrow\uparrow 00 \\ \uparrow 0 \uparrow 0 \end{matrix} \qquad \text{(II-1)}$$

the state $\uparrow 0 \uparrow\uparrow 0 \uparrow 00$ can not be obtained from the all

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possible tensor product of the (II-1) configurations unless we use the tensor product of $0\uparrow 0\uparrow$ and $\uparrow 0\uparrow 0$ and a translation. Possible states of a 4-sites chain in quarter-filling in DMRG method, is written as (II-1) equations because the following states have the same probability as above ones.

$$\begin{array}{l} 00\uparrow\uparrow \\ 0\uparrow\uparrow 0 \\ 0\uparrow 0\uparrow \end{array} \qquad \text{(II-2)}$$

When we use the periodic boundary condition $\uparrow 0\uparrow\uparrow 0\uparrow 00$ may be identical with $0\uparrow 0\uparrow\uparrow 0\uparrow 0$ that is generated from (II-2), the translation may is not necessary but these tasks in DMRG lead to lose of speed (because we have to retain the repetitious states II-2 that we discuss below) and when we use the open boundary condition this state can not be generated (using doubling the block size method and II-1) and we are not able to consider its probability and finally DMRG loses its accuracy.

When we use adding a single site in each iteration, we should also note that the repetitious configurations may lead to some decrease in the speed of DMRG method. For a periodic chain an obvious example of repetitious configurations appears when we reach 8 sites chain by adding sites to an initial 4 site chain in quarter filling. $(\uparrow 0\uparrow 0)\oplus(\uparrow\uparrow 00)$ and $(\uparrow\uparrow 00)\oplus(\uparrow 0\uparrow 0)$ lead to the same configurations. These two configurations even for an open boundary condition have the same probabilities since in the first case atoms are aligned leftward and in the next case they are aligned rightward. Note that rotating left ward has not any advantage to the rightward rotation. Another intuitive example is presented in the Table I and a quantitative diagram is presented in the Fig. 1.

Table 1 – Schematic presentation of the configurations obtained from adding a single site in a RG procedure in a bosonic Hubbard chain in half filling. '1' is a symbol of site with an electron and '0' represent an empty site. L is the chain length, N is number of repeated configurations at half filling for a Hubbard ring, M is the number of all possible configurations at quarter filling, O is the number of configurations at half filling and P is number of configurations after reduction of the Hilbert space dimension using symmetries

	$L=4$ $N=0$, $M=2$, $O=2$ $P=2$	$L=6$ $N=0$, $M=8$, $O=4$ $P=3$	$L=8$ $N=2$, $M=32$, $O=12$ $P=8$	$L=10$ $N=15$, $M=128$, $O=41$ $P=16$
1	1100	1 1 0 0 1 0	1 1 0 0 1 1 0 0	1 1 0 0 1 1 1 0 0 0
2	1010	1 1 0 0 0 1	1 1 0 0 1 0 1 0	1 1 0 0 1 1 0 1 0 0
3		1 0 1 0 1 0	1 1 0 0 1 0 0 1	1 1 0 0 1 0 1 0 1 0
4		1 0 1 0 0 1	1 1 0 0 0 1 1 0	1 1 0 0 1 0 1 0 0 1
5			1 1 0 0 0 1 0 1	1 1 0 0 1 0 1 1 0 0
6			1 1 0 0 0 0 1 1	1 1 0 0 0 1 0 1 1 0
7			1 0 1 0 1 1 0 0	1 1 0 0 0 1 0 1 0 1
8			1 0 1 0 1 0 1 0	1 1 0 0 1 0 0 0 1 1
9			1 0 1 0 1 0 0 1	1 1 0 0 0 1 1 1 0 0
10			1 0 1 0 0 1 1 0	1 1 0 0 0 1 1 0 0 1
11			1 0 1 0 0 1 0 1	1 1 0 0 1 0 0 1 1 0
12			1 0 1 0 0 0 1 1	1 1 0 0 1 0 0 1 0 1
13				1 1 0 0 0 1 0 0 1 1
14				1 1 0 0 0 0 0 1 1 1
15				1 1 0 0 0 0 1 0 1 1
16				1 1 0 0 0 0 0 1 1 1 0
17				1 1 0 0 0 0 1 1 0 1
18				1 0 1 0 1 1 1 0 0 0
19				1 0 1 0 1 1 0 1 0 0
20				1 0 1 0 1 0 0 1 1 0
21				1 0 1 0 1 0 1 1 0 0
22				1 0 1 0 1 0 1 0 1 0
23				1 0 1 0 1 0 1 0 0 1
24				1 0 1 0 1 1 0 0 1 0
25				1 0 1 0 1 1 0 0 0 1
26				1 0 1 0 1 0 1 1 0 0
27				1 0 1 0 1 0 0 1 1 0
28				1 0 1 0 1 0 1 0 1 0
29				1 0 1 0 1 0 1 0 0 1
30				1 0 1 0 1 0 0 1 0 1
31				1 0 1 0 1 0 0 0 1 1
32				1 0 1 0 0 1 1 1 0 0
33				1 0 1 0 0 1 1 0 1 0
34				1 0 1 0 0 1 1 0 0 1
35				1 0 1 0 0 1 0 1 1 0
36				1 0 1 0 0 1 0 1 0 1
37				1 0 1 0 0 1 0 0 1 1
38				1 0 1 0 0 0 0 1 1 1
39				1 0 1 0 0 0 1 0 1 1
40				1 0 1 0 0 0 1 1 1 0
41				1 0 1 0 0 0 1 1 0 1

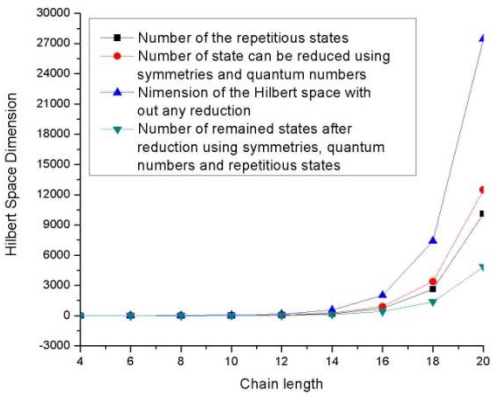

Fig. 1 – Hilbert space dimension of a Heisenberg spin chain and the amount of reduction due to Symmetries and repetitious states

States mentioned in the table is ones remained after reduction by translational symmetry. In this case we have not the spin inversion symmetry. A rapid increase in the number of repetitious configurations is clear from the Table 1. As we have mentioned in the previous section, one has to do greater number of sweeps for fermionic systems to reach satisfactory accuracy than spin system. Here we can construct fermionic system using two bosonic one.

Let the total number of electrons in the fermionic system be even. At first to generate the desired states of a one-dimensional fermionic system in a given filling, we can construct two set of configurations. The first set contains the probable Configurations with one half of the entire electrons with spin up and the other set is include the same configurations but with spin down. By selecting a configuration from each mentioned set and defining the following summations,

$$\begin{aligned} &\uparrow \oplus \downarrow = \updownarrow \\ &\uparrow \oplus 0 = \uparrow \\ &\downarrow \oplus 0 = \downarrow \\ &\uparrow \oplus \uparrow = 0 \\ &\downarrow \oplus \downarrow = 0 \end{aligned} \qquad \text{(II-3)}$$

we construct the states of the fermionic system. For a 4-site chain the two mentioned sets are,

$$\begin{aligned} &\uparrow\uparrow 00 \\ &\uparrow 0 \uparrow 0 \end{aligned} \qquad \text{(II-4)}$$

And

$$\begin{aligned} &\downarrow\downarrow 00 \\ &\downarrow 0 \downarrow 0 \end{aligned} \qquad \text{(II-5)}$$

All possible states of the 4-sites chain at half filling can be calculated using the Eqs. (II-4 and II-5). For example $\uparrow\uparrow 00 + \downarrow 0 \downarrow 0 = \updownarrow\uparrow\downarrow 0$ is a possible state for a 4-sites chain at half-filling.

If we do not discard the repetitious configurations in DMRG method and generate the states of the fermionic system, it is easy to see that this number of repetitious configurations grows more rapidly. This extremely more repetitious configuration enforces one to do more sweeps for fermionic systems to get a satisfactory accuracy. Note the in this picture we break a fermionic 4-stite chain into two chains that all electrons has the same spin.

When we are to generate the most appropriate state of an eight sites Hubbard chain another difficulty may be seen. To generate the most probable states of a linear chain in routine DMRG method, we have to store the most probable state of a seven sites Hubbard chain with 6, 7 and 8 electrons since adding $\updownarrow$, $\uparrow$ or $\downarrow$ and an empty site to them, respectively, may lead to a probable state for the 8 site Hubbard chain and this number of state increases logarithmically by growing the number of atoms in the chain. Usually people do not do this work and retain only $S_z = 0$ in each iteration.

The repetitious states in DMRG generate more difficulties because lead to a greater superblock dimension. Number of repetitious states of the superblock is presented in the Fig. 2.

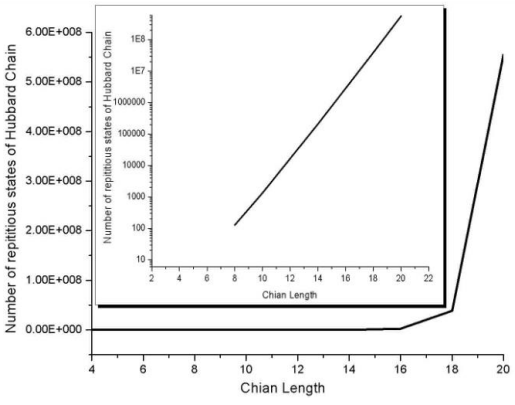

Fig. 2 – Number of repetitious states of a fermionic Hubbard Chain

Calculating the amount of reduction of the Hilbert space is not so straightforward since even two symmetric states of the left and right block may lead to an asymmetric state of the superblock.

When we generate the desired states of a fermionic system by using equations (II-4) and (II-5), each repetitious state from each set leads to a repetitious state of the fermionic system. Thus to evaluate the above information for fermionic NRG system when you use these equations to generate the desired states of a fermionic chain from spin chain, we note that eliminating the repetitious states of spin chain before generating the desired states of the fermionic chain may lead to loss some non-repetitious states of the fermionic chain. For example $\uparrow\updownarrow\downarrow 0$ can not be generated from equations (II-4) and (II-5), because the translation has eliminated $0\downarrow\downarrow 0$. Using rotation of $\downarrow\downarrow 00$ on $\uparrow\uparrow 00$ we are able to generate this state, but it leads to more repetitious states. According to the mentioned facts, counting the number of repetitious state of a fermionc chain is a little more difficult than the spin system. Here we evaluate a minimum number of repetitious states may appear in the calculations. If we do not rotate the states of the group with spin up on the group with spin down, we loss some non-repetitious states, if we ignore them (an approximation) the number of repetitious states of the fermionic chain is equal to the number of repetitious states of the superblock in DMRG method. Thus we can use the Fig.1 for the fermionic system. For a linear chain with L sites like Hubbard that each site can have four different states (empty, one spin up electron and a doubly occupies site), the number of repetitious states grows more rapid than a Heisenberg like system that each site of it can have two different states(spin up and down).

Entanglement of the states is also an important factor that should be considered. When the entanglement increases and therefore the wave function related to each atom overlap with that of the neighbor ones, roughly speaking, they are able to see each other. In this situation, to get the accurate eigen-states of the system, they should be anti-symmetrized [13]. This means we have to include the anti-symmetrization in DMRG. Ref [10, 15] is an obvious example of this situation where by increase in entanglement of their periodic states, Legeza et al. had to do more sweeps to reach the desired accuracy. Paying attention to the necessity of the anti-symmetrization of the obtained eigen-states and ignoring it when its usage is not so important lead to some increase in the speed of the DMRG method.

In the last step we try to reduce the Hilbert space dimension by means of symmetries and appropriate quantum numbers. Symmetries we propose to reduce the dimension of the Hilbert space for a Hubbard ring is the spin inversion symmetry, L time's rotation which L is the ring (or chain) length and mirror reflection with respect to a diameter of the ring(center of the chain). Reduction of the Hilbert space dimension using symmetries like has also done previously. For an example that has used constrains such as $S_z = 0$, spin inversion, 40 translations, 4 rotations on a $S = 1/2$ Heisenberg model on a tilted square lattice with $\sqrt{40} \times \sqrt{40}$ sites you may see the Ref [14].

3. CONCLUSION

In this work some aspects of DMRG is investigated. Influence of the boundary condition on this method is described. Within a sample ring, reduction of the Hilbert space dimensions using symmetries is specified. We present some repetitious states appear in the all RG methods that lead to reduction of the speed and accuracy of the method. In this paper we do not present a new DMRG type that resolves the difficulty of the repetitious states but we have shown that importance of the repetitious states is as much as using the symmetries. The reason why DMRG works better for fermionic system that bosonic one is somewhat investigated. The main goal of the paper is to find the difficulties of the DMRG thus at first we try to find the authors complain that DMRG do not satisfy them. Then we took a glance on the problem under investigation to find the difficulties. We find that when the system size increases the number of repetitious states also increase rapidly and in the periodic boundary condition this is worse. More information is presented in the text.

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