Density Matrix Renormalization Group Method
for the Random Quantum One-Dimensional Systems
- Application to the Random Spin-1/2 Antiferromagnetic Heisenberg Chain -

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Abstract

The density matrix renormalization group method is generalized to one dimensional random systems. Using this method, the energy gap distribution of the spin-1/2 random antiferromagnetic Heisenberg chain is calculated. The results are consistent with the predictions of the renormalization group theory demonstrating the effectiveness of the present method in random systems. The possible application of the present method to other random systems is discussed.

Keywords: density matrix renormalization group, random antiferromagnetic Heisenberg chain, renormalization group theory

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I. INTRODUCTION

Low dimensional quantum spin systems have been studied intensively in this decade particularly stimulated by its relevance to high $T_c$ superconductivity. Compared to the regular systems, however, the random quantum spin systems are less studied, while their classical counterparts are also intensively studied in the context of spin glass problem.

One of the pioneering works on the quantum random antiferromagnet was done by Blatt and Lee [1] who proposed the random singlet phase. This model was further studied by means of the renormalization group method by DasGupta and Ma [2], Hirsch and José [3] and Fisher [4] for the one-dimensional case. This method was recently applied to the random chain with ferromagnetic and antiferromagnetic interaction by Westerberg et al. [5,6,7] and to the one-dimensional random transverse Ising model by Fisher. [8]

On the other hand, Young and Rieger [9] recently analyzed the one-dimensional random transverse Ising model numerically up to the chain length $N = 128$ taking advantage of the fact that this model is mapped onto the random free spinless fermion model. Their results are in good agreement with the renormalization group theory. [8] However, the numerical study of the ground state of the strongly interacting random systems still remains rather limited. The conventional numerical approach such as exact diagonalization by Lanzcos algorithm requires considerable computational time and memory even for a single system if the system size is large. Such calculation becomes even harder for the random systems for which the average over many large samples must be taken.

The density matrix renormalization group (DMRG) method initiated by White [10,11] is a promising candidate to overcome this difficulty. The major advantage of this method is that it enables one to calculate the low lying states of very large one-dimensional systems quite accurately with relatively small computational time and memory. However, this method is originally developed for the regular uniform systems taking advantage of the uniformness of the system. It is the purpose of the present work to introduce the algorithm to apply this method to random chains. As an example of the application of the present method, we also
calculate the energy gap distribution of the random spin-1/2 antiferromagnetic Heisenberg chain which shows good agreement with the renormalization group theory. [2,3,4]

II. DMRG METHOD FOR THE RANDOM CHAIN

The usual procedure of the infinite size algorithm of the DMRG calculation for the uniform system is as follows,

1. Prepare the left and right blocks $L_{N/2}$ and $R_{N/2}$ where $N/2$ is the number of sites in each block. To start with, choose $N = 4$. In what follows, $N$ is always assumed to be even.

2. Construct the Hamiltonian of the superblock $T_N$ connecting the right end of $L_{N/2}$ and the left end of $R_{N/2}$. Diagonalize it to obtain its low lying states (called target states).

3. Construct the density matrices $\rho_L$ ($\rho_R$) for $L_{N/2}$ ($R_{N/2}$) by tracing out the states of $R_{N/2}$ ($L_{N/2}$) from the target states.

4. Diagonalize the density matrices $\rho_L$ and $\rho_R$ and choose $m$ important eigenstates of $L_{N/2}$ and $R_{N/2}$.

5. Add a unit cell at the right end of $L_{N/2}$ and the left end of $R_{N/2}$ to construct $L_{N/2+1}$ and $R_{N/2+1}$ keeping only $m$ states chosen in the preceding step.

6. Setting $N + 2 \to N$, go to step 2 and repeat.

This procedure is schematically shown in Fig. [4].

White [10,11] has shown that this method allows to calculate the low energy states of very large systems quite accurately, if we pick up appropriate number of states in both left and right blocks.

The essential point which requires the uniformity of the system is the assumption that the important states in $L_{N/2}$ and $R_{N/2}$ are also important in $L_{N/2+1}$ and $R_{N/2+1}$. This is
garanteed because the environment of the boundary spins hardly changes by the addition of the extra spins between $L_{N/2}$ and $R_{N/2}$ as far as the system is uniform.

This means that we have to pick up the states in $L_{N/2}$ and $R_{N/2}$ which satisfies the boundary condition that *it is connected with the neighbouring block* in general. However, in the random system, all bonds are inequivalent. Therefore if we add spins between the two blocks, the boundary condition for the block changes and the important states in $L_{N/2}$ and $R_{N/2}$ are no more important in $L_{N/2+1}$ and $R_{N/2+1}$. This is the difficulty in extending the DMRG method to the random systems.

To circumvent this difficulty, we prepare all the blocks from the beginning so that they provide the proper environment for each other in each step and let them grow in parallel keeping the boundary conditions for each block almost unchanged during the course of the calculation.

The calculation proceeds as follows:

1. Prepare a large enough even membered sample $[1 : N]$ which consists of the sites $i = 1, \ldots, N$. Here, $[i : j]$ denote the superblock consisting of the $i, i + 1, \ldots, j$-th sites.

2. Cut out all four-site superblocks $[2i - 1 : 2i + 2]$ ($i = 1, N/2 - 1$) and diagonalize their Hamiltonian to get their target states.

3. By the procedures 3 to 4 for the regular system, find the important states of the blocks $[2i - 1 : 2i]$ and $(2i + 1 : 2i + 2]$ for all $i$. Here the ends connected with the neighbouring blocks are denoted by ( and ), while [ and ] denote the open ends.

4. Add $2i + 1$-th spin to the right end of $[2i - 1 : 2i]$ and $2i + 2$-th spin to the left end of $(2i + 3 : 2i + 4]$. Diagonalize the Hamiltonian of the superblock $[2i - 1 : 2i + 4]$ constructed from the important states of $[2i - 1 : 2i]$ and $(2i + 3 : 2i + 4]$ in addition to all the states of the $2i + 1$-th and $2i + 2$-th spins. By the procedure 3 to 4 for the regular system, find the important states of the blocks $[2i - 1 : 2i + 1]$ and $(2i + 2 : 2i + 4]$ for all $i$. 
5. Repeat until the superblock $[1, N]$ is diagonalized.

This is schematically shown in Fig. 2 for $N = 10$. It should be emphasized the above procedure must be performed in parallel for all $i$ on each step. Therefore we obtain the low lying states of even membered subsystems which are superblocks in each step as by-product. If we pick up only independent subsystems, the data for many small systems are obtained during the course of the calculation of a large single system.

This algorithm corresponds to the 'infinite size method' in the regular case. Therefore the eigenstates obtained in each step are only approximate. To improve the accuracy, we can also include the finite size iteration whose algorithm is an obvious extension of the regular case.

III. APPLICATION TO THE RANDOM SPIN-1/2 ANTIFERROMAGNETIC CHAIN

As an example, we have applied this method to the random spin-1/2 Heisenberg chain whose Hamiltonian is given by,

$$
\mathcal{H} = \sum_{i=1}^{N} 2J_i S_i S_{i+1}, \quad |S_i| = 1/2,
$$

(1)

where $J_i$ takes the random positive values. Here we assume the distribution

$$
J_i = \begin{cases} 
J & \text{with probability } p, \\
J' & \text{with probability } 1 - p.
\end{cases}
\quad (2)
$$

The number of prepared samples with $N = 48$ ranged from 866 to 920. We have studied the cases $p = 0.3, 0.5$ and 0.7 with $J = 1$ and $J' = 0.5$. For all these samples, the DMRG procedure is carried out. During the growth of the system, we have obtained the energy gap for smaller systems with $N < 48$. The number $m$ of the states kept in each step is 60. We have also checked the accuracy taking $m = 80$ and 100 for several samples. For all checked samples, we find $m = 60$ is sufficient without finite size iterations.
According to the renormalization group theory, \[2,3,4\] the logarithm of the characteristic energy \(\Omega\) of the \(N\)-membered system scales with \(\sqrt{N}\). Roughly speaking, this energy scale can be interpreted as a random \textit{product} of the energy scales of the subsystems. Therefore \(\ln \Omega\) is a good statistical variable rather than \(\Omega\) itself. In addition, the renormalization group theory predicts that not only the root mean square deviation of \(\ln \Omega\) but also their overall distribution function is scaled by \(\sqrt{N}\).

As a characteristic energy of each cluster, we have calculated the lowest energy gap \(\Delta\). Figure 3 shows the system size dependence of the average \(<\ln \Delta>\) and root mean square deviation \(\sigma \equiv \sqrt{<\left(\ln \Delta - <\ln \Delta>\right)^2>}\).

They are well fitted by the linear function of \(\sqrt{N}\). In addition, the ratio \(<\ln \Delta> / \sigma\) remained almost equal to 2 irrespective of \(N\) and \(p\) as shown in 4. This suggests that the distribution is scaled by a single variable \(\Gamma \equiv \ln(\Delta/\Delta_0)/\sqrt{N}\) as expected from the renormalization group theory where \(\ln \Delta_0\) is determined by the linear extrapolation of \(<\ln \Delta>\) to \(\sqrt{N} \rightarrow 0\).

Based on this observation, the logarithm of the distribution function \(P(\Gamma)\) is plotted against \(\Gamma^2\) in Fig. 5. It follows the universal curve irrespective of the system size in accordance with the renormalization group prediction. For small \(\Delta\) (large \(\Gamma\)), \(\ln P(\Gamma)\) is linear to \(\Gamma^2\). This is also in agreement with the prediction of the renormalization group theory. It should be remarked that the renormalization group calculation becomes more and more accurate for small energy scale. Thus this agreement confirms that our algorithm of the DMRG for the random system works sufficiently well.

All the data from Fig. 5 to 6 depend weakly on \(p\). It is not clear whether this actually implies the breakdown of universality with respect to \(p\). From Fig. 7, the major difference comes from the samples with very small \(\Delta\) for which the numerical accuracy is relatively poor. In addition, the number of samples having such small gaps is small and statistical error is also expected to be large in this regime.
IV. SUMMARY AND DISCUSSION

The algorithm to apply the DMRG method to the random one-dimensional systems is presented. It is demonstrated that the results of the renormalization group theory for the random spin-1/2 antiferromagnetic Heisenberg chains are reproduced using our method.

As discussed in the introduction, the random quantum spin chain is attracting the renewed interest quite recently. It is predicted that the random Heisenberg chain with ferromagnetic and antiferromagnetic interactions belongs to the universality class different from random spin-1/2 antiferromagnetic Heisenberg chain. \[5\]. The DMRG study of this model is now being carried out.

The present algorithm is also useful to the study of the systems with large unit cell. In the conventional DMRG, two unit cells must be added on each step and therefore the effective Hamiltonian matrix of the superblock becomes huge and hardly tractable. On the contrary, in the present method, we need to add only 2 spins on each steps even if the unit cell is large. Therefore we can keep the size of the Hamiltonian matrix modest. For example, we may apply this method to the trimerized system \[12,13,14\].

Application of the present method is not limited to the quantum spin system. The itinerant electron systems should provide wide possibility of application. For example, the interplay between the Anderson localization and electron correlation or the quantum effect on the randomly pinned charge density wave remain to be investigated even in the one-dimensional systems. \[15\]

Recently, Nishino and Okunishi \[16\] have introduced the product wave function renormalization group method based on the observation of Östlund and Rommer \[17\] that the DMRG wave function is expressed as a product of matrices. This method is much faster than the conventional DMRG method, because it can skip the Lanzcos diagonalization of superblocks. If this method can be incorporated into the present algorithm, the computational efficiency will be much improved. This is left for future study.

The numerical calculation has been performed using the FACOM VPP500 at the Super-
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FIGURES

FIG. 1. The schematic procedure of the DMRG calculation for the uniform systems.

FIG. 2. The schematic procedure of the DMRG calculation for the random systems for $N = 10$.

FIG. 3. The system size dependence of the average $< \ln \Delta >$ and root mean square deviation $\sigma$ for $p = 0.3$ (○; solid line), 0.5 (●; dotted line) and 0.7 (□; broken line) with $J = 1$ and $J' = 0.5$.

FIG. 4. The relation between the average $< \ln \Delta >$ and root mean square deviation $\sigma$ for for $p = 0.3$ (○; solid line), 0.5 (●; dotted line) and 0.7 (□; broken line) with $J = 1$ and $J' = 0.5$.

FIG. 5. The energy gap distribution $P(\Gamma)$ plotted against $\Gamma^2 (\equiv \ln^2 (\Delta E/\Delta_0)/N)$ for (a) $p = 0.3$, (b) $p = 0.5$ and (c) $p = 0.7$ with $J = 1$ and $J' = 0.5$. 
Choose $m$ important states in $L_{N/2}$ and $R_{N/2}$

Repeat

FIG. 1
FIG. 2