Interaction-round-a-face density-matrix renormalization-group method

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Abstract

We demonstrate the numerical superiority of the interaction-round-a-face (IRF) density-matrix renormalization-group (DMRG) method applied to SU(2) invariant quantum spin chains over the conventional DMRG. The ground state energy densities and the gap energies of both $S = 1$ and $S = 2$ spin chains can be calculated using the IRF-DMRG without extensive computations. We have also studied the effect of tuning boundary interaction $J_{\text{end}}$ at both ends of the chain from the IRF viewpoint. It is clearly observed that the magnon distribution is uniform when the best $J_{\text{end}}$ is chosen.

Key words: DMRG, face model, Haldane gap, quantum spin chain

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1 introduction

Quantum spin chains are one of the most extensively studied systems by way of numerical calculations. In this article we consider isotropic spin-$S$ antiferromagnetic Heisenberg (AFH) spin chain, whose Hamiltonian is represented as

$$H = J \sum_{i=1}^{N-1} S_i \cdot S_{i+1},$$ (1)

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where $J$ is a positive coupling constant and $\mathbf{S}_i$ denotes spin operator at $i$-th site. After Haldane conjectured the existence of finite excitation gap for integer spin chains and the absence for half-integer ones [3], many efforts have been performed to confirm this conjecture. We focus on numerical analysis of the AFH model in the following.

A simple but concrete way to obtain the gap energy of the spin-$S$ AFH chain in the thermodynamic limit is to numerically calculate the excitation energies for finite size systems, and to perform the finite size scaling. Conventionally Lanczos method is applied to the Hamiltonian (Eq. (1)) expressed as a large sparse matrix in order to obtain lower lying states and their energies. The major shortcoming of this way is that the Lanczos diagonalization requires huge numerical resources. This is because the matrix dimension of the $N$-site system is of the order of $(2S + 1)^N$, that rapidly increases with both $N$ and $S$. The largest system size $N$ which is manageable with current computer is around 36 (for $S = 1/2$) even now.

The Density-matrix renormalization-group (DMRG) invented by White [1,2] is a novel and powerful computational method, which overcomes the limitation of the manageable system size in the Lanczos diagonalization. It enables us to obtain physical observables such as ground state energy, correlation functions, etc., of large scale systems very accurately without performing extensive computations. It is not overwhelming to say that the DMRG is one of the standard tools to study low dimensional quantum systems. DMRG is a real-space renormalization method, which divides the whole system into the left and the right blocks, and reduces the degree of freedom of each block using the eigenvalues of the reduced density matrix (DM) as probabilistic measures to choose the relevant block-spin states. The number of the block spin state kept under the RG transformation is conventionally represented by the letter $m$. It is important to choose sufficiently large $m$ in order to keep numerical precision. The computational cost in DMRG is, roughly speaking, proportional to $m^3$, which is not heavily dependent on size $N$.

When applying DMRG to the spin-$S$ AFH chain specified by Eq. (1), the block spin states have total spin $L$ up to $nS$, where $n$ is a non-negative integer and depends on the number of spins in the block, we have to keep sufficient numbers of the block-spin state up to a certain total-spin $L$. This is problematic for large $S$ chains, because the system has spin rotational symmetry; the eigenvalues of the DM are $(2L + 1)$-fold degenerated, since a block spin state with spin $L$ belongs to $2L + 1$ spin multiplet. Consequently the necessary block spin states ($= m$) increases rapidly with $S$.

The problem of $(2L + 1)$-fold degeneracy can be overcome by integrating out the $SU(2)$ symmetry of the spin chain, and by representing the AFH Hamiltonian using the total spin basis. As a result, the AFH system can be rep-
resented as a quantum limit of the interaction round a face (IRF) model [7]. Sierra and Nishino [4] have modified DMRG algorithm for the $S = 1/2$ and 1 AFH models in the IRF representation (rep), where their numerical procedure is called ‘IRF-DMRG’. Wada [6] has further developed IRF-DMRG for the cases $S = 1$ and $S = 2$. It is easily understood that the computational cost of IRF-DMRG is much lower than that of the conventional DMRG, since the dimension of the associated Hamiltonian matrix in IRF rep is much smaller than that in conventional (= vertex) rep.

2 IRF-DMRG applied to $S = 1$ and 2 AFH systems

Now we demonstrate the numerical efficiency of IRF-DMRG when it is applied to AFH model for higher spin ($S \geq 1$) chains. In order to treat large $S$ systems, Wada [6] has developed a way of obtaining the IRF expression for the Heisenberg interaction for $S \geq 1$. In the IRF formulation, the spin excited states can be targeted by putting an additional auxiliary (or ghost) spin to the spin chain; more details are shown in Ref. [6].

Before showing the calculated results we stress that all the numerical data are obtained using personal computer with the moderate power (SPECfp95 $\sim 25$). This is because the Hilbert space dimension in the IRF rep is much smaller than that in the conventional $S^z$ basis rep. For example, in the case of spin-2 spin chain, to keep $m_{\text{IRF}} \sim 90$ states in the IRF rep is equivalent to keep $m_{\text{sz}} \sim 450$ in the conventional rep. We keep 100 states at most, in the IRF rep. The ground state energy density $e_0$ and the estimated gap energy $\Delta$ for $S = 1$ are $e_0 = -1.401484039J$ and $\Delta = 0.4104J$, and those for $S = 2$ are $e_0 = -4.76124816J$ and $\Delta = 0.088J$ [6].

Having described the computational benefits of IRF formulation, now let us observe the boundary effect from the IRF viewpoint. Since DMRG (including the IRF-DMRG) chiefly treats systems with open boundary, it is important to decrease the boundary effect and obtain the properties of bulk state.

In order to estimate the spin excitation gap of AFH in the thermodynamic limit, White et al. [5] minimized the boundary effect by tuning the coupling constants $J_{\text{end}}$ at both ends of the spin chain. They found that for $S = 1$ chain the best $J_{\text{end}}$ is 0.5088 for the first excited state, and is 0.7 for the ground state. Let us review how fast the boundary effect decreases with the system size when $J_{\text{end}} = 0.5088$. Figure 1 shows the gap energies $\Delta$ as a function of the system size $N$. After rapid increase with $N$, the gap energy $\Delta(N)$ becomes almost independent of $N$ when it is larger than 20. It should be noted that it is possible to estimate $\Delta = 0.4015J$ from the data $N \leq 20$. In contrast, when $J_{\text{end}}$ deviates from the best value, $\Delta(N)$ shows very slow increases with $N$. 


this makes the finite size scaling very difficult.

What happens when \( J_{\text{end}} = 0.5088 \) for the first excited state? It is believed that the magnon (or the domain wall excitation) has zero momentum \( (k = \pi \text{ in their definition}) \) and it distributes quite uniformly \([5]\). The situation is quite similar to the case of a particle in tight binding model with shallow negative potential at the system boundary. The IRF rep detects the magnon distribution more clearly, since it is possible to obtain the partial spin average

\[
\langle S_{1i} \rangle \equiv \left\langle \sum_{j=1}^{i} S_j \right\rangle.
\]

(2)

The derivative of \( \langle S_{1i} \rangle \) with respect to the lattice coordinate \( i \) is proportional to the density of the quasi particle (= magnon). To speak precisely, it is possible to obtain \( \langle S_{1i} \rangle \) from the numerical data of the conventional DMRG, but careful treatment of numerical data is required; the IRF-DMRG provides \( \langle S_{1i} \rangle \) more directly. Figure 2 shows \( \langle S_{1i} \rangle \) for three different \( J_{\text{end}} \) s. As is seen the partial spin average is quite linear in \( i \) at the best boundary condition (BC) of \( J_{\text{end}} = 0.5088 \). The partial spin average shall be a good reference data when searching the similar BC for the higher spin chains. More detailed analysis will be published elsewhere.

In conclusion we have demonstrated the numerical advantage of IRF formulation through the study of the AFH model, particularly for higher spin chains. The ground state energy densities \( e_0 \) and gap energies \( \Delta \) are obtained with moderate computational cost. The results are \( e_0 = -1.401484039J, \Delta = 0.4104J \) for \( S = 1 \), and \( e_0 = -4.76124816J, \Delta = 0.088J \) for \( S = 2 \). The estimated spin gap is much more accurate than those obtained so far, under the condition \( m \leq 100 \). In addition, we have discussed how the minimization of the boundary effect is observed from the IRF view point. We have seen that at the best boundary condition at which \( J_{\text{end}} \) minimizes the boundary effect, the partial spin average \( \langle S_{1i} \rangle \equiv \left\langle \sum_{j=1}^{i} S_j \right\rangle \) of the first excited state is almost linear in \( i \). To find out such smooth BCs for higher spin cases is our future subject.

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Fig. 1. The gap energies $\Delta$ as a function of the chain length $N$ for spin-1 AFH spin chain. The number of states $m$ being kept during IRF-DMRG iterations are only 32. The $J_{\text{end}}$ denotes the coupling constants at both ends of the chain. All coupling constants $J$ except $J_{\text{end}}$ set to unity. When $J_{\text{end}}$ sets to 0.5088, $\Delta(N)$ is almost independent of $N$.

Fig. 2. The partial spin average $\langle S_{1i} \rangle$ distribution for the first excited state of the spin-1 AFH chain. When $J_{\text{end}} = 0.5088$, at which the boundary effect is minimized, $\langle S_{1i} \rangle$ becomes linear in site index $i$. 