Fixed Point of the Finite System DMRG

Hiroshi Takasaki, Toshiya Hikihara,¹ and Tomotoshi Nishino²
Department of Physics, Graduate School of Science and Technology,
Kobe University, Rokkodai 657-8501

¹Division of Information and Media Science, Graduate School of Science and Technology,
Kobe University, Rokkodai 657-8501
²Department of Physics, Faculty of Science, Kobe University, Rokkodai 657-8501

Abstract

The density matrix renormalization group (DMRG) is a numerical method that optimizes a variational state expressed by a tensor product. We show that the ground state is not fully optimized as far as we use the standard finite system algorithm, that uses the block structure \(B \bullet B\). This is because the tensors are not improved directly. We overcome this problem by using the simpler block structure \(B \bullet B\) for the final several sweeps in the finite iteration process. It is possible to increase the numerical precision of the finite system algorithm without increasing the computational effort.
Establishment of the density matrix renormalization group (DMRG) by White [1] is one of the major progresses in computational condensed matter physics. DMRG enables us to calculate ground states of relatively large scale one-dimensional (1D) quantum systems. [2, 3, 4, 5, 6]. Two-dimensional (2D) classical systems, [7, 8, 9, 10] and 1D quantum system at finite temperature [11, 12, 13, 14] have also been investigated.

Östlund and Rommer [15] examined the thermodynamic limit \((N \rightarrow \infty)\) of the infinite system algorithm, and they pointed out that the block state \(\mathbf{B}\) corresponds to a product of position independent tensor. It should be noted that their result does not show that the infinite system algorithm creates a translationally invariant — position independent — variational state for the whole system \(\mathbf{B} \bullet \mathbf{B}\), where “•” denotes a bare spin variable between the left and the right blocks. Actually, the variational state has a slight position dependence. For example, the bond energy \((\bullet \bullet)\) at the center of the antiferromagnetic \(S = 1/2\) Heisenberg chain, which is calculated by the infinite system algorithm, is lower than the exact ground state energy per site. [16] Such a position dependence in the variational state spoils the numerical efficiency of the infinite system algorithm. [17] As we show in the following, the finite system algorithm does not fully improve the variational state in the same reason. The purpose of this letter is to remove the source of such a numerical error, and to increase the numerical precision in DMRG.

Let us briefly review the construction of the variational state, which is used in the standard finite system algorithm. We consider the IRF model [18] as a reference system, and they pointed out that the block state \(\mathbf{B}\) approximates the eigenvector of the transfer matrix using a variational state block spin variables. (Fig.1a) The tensors \(A_{\xi_i}^{s_i}\) and \(B_{\xi_i}^{s_i}\) are dependent on their positions \(i\) and \(j\), and each of them satisfies the orthogonal relation

\[
\sum_{\xi_i} A_{\xi_i}^{s_i} A_{\xi_i}^{s_i'} = \delta_{s_i, s_i'}
\]

\[
\sum_{\xi_i} B_{\xi_i}^{s_j} B_{\xi_i}^{s_j'} = \delta_{s_j, s_j'}
\]

where we have written \(s_1\) and \(s_N\) as \(\xi_1\) and \(\xi_N\), respectively. Normally, they impose the normalization [19]

\[
\sum_{\xi_{M-1}\xi_{M+1}\xi_{M+2}} (\tilde{V}_{\xi_{M-1}\xi_{M+1}}^{s_{M-1} s_{M+1}})^2 = 1.
\]

The standard finite system algorithm improves the variational state (Eq.2) so that (Fig.1b)

\[
\chi^{(M)} = \sum_{\text{all indices}} V_{s_i\ldots s_N}^{(M)} T_{s_i\ldots s_N}^{(M)} V_{s_i\ldots s_N}^{(M)}
\]
is maximized via the tuning of $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+2}^{sM+1}}$, under the constraint Eq.4. The best $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+2}^{sM+1}}$ is determined by the diagonalization of the renormalized transfer matrix

$$T_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1} \xi_{M+2}^{sM+2}} = \tilde{L}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}} W_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1} \xi_{M+2}^{sM+2}} \tilde{R}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}}$$

(6)

and by identifying its eigenvector $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1} \xi_{M+2}^{sM+2}}$ with the tensor $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}}$. The factor $\tilde{L}_{\xi_{M-1}^{sM}}$ and $\tilde{R}_{\xi_{M+1}^{sM+2}}$ represent the renormalized half-row transfer matrix for the left and the right half of the system, respectively. (Fig.1c) A pair of tensors $A_{sM, sM+1}^{sM, sM+1}$ and $B_{sM+1, sM+1}^{sM+1, sM+1}$ are then improved indirectly by rewriting the improved tensor $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}}$ using the singular value decomposition (SVD)

$$\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}} = \sum_{\xi_M} A_{\xi_{M-1}^{sM} \xi_M}^{sM} \Omega_{\xi_M \xi_{M+1}}^{sM} B_{\xi_{M+1}^{sM+1} \xi_{M+2}^{sM+2}}$$

(7)

and by restricting the degree of freedom of $\xi_M$ and $\xi_{M+1}$ down to $m$. The matrix $\Omega_{\xi_M \xi_{M+1}}$ is a $2m$-dimensional diagonal matrix

$$\Omega = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_{2m} \end{pmatrix},$$

(8)

where the diagonal elements are in the decreasing order $|\omega_1| \geq |\omega_2| \geq \cdots |\omega_{2m}|$. The matrix $\Omega$ satisfies the normalization $\text{Tr} \Omega^2 = \sum_{\xi} \omega_\xi^2 = 1$. The finite system algorithm improves other tensors in Eq.2 by shifting the position of $\tilde{V}$ by use of the wave function renormalization.

In the above standard improvement process for the variational state $V_{s_1, s_N}^{(M)}$, the tensors $A_{\xi_M-1, \xi_M}^{sM, sM+1}$ and $B_{\xi_M+1, \xi_M+2}^{sM+1, sM+1}$ are improved indirectly, only through the tuning for $\tilde{V}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1}}$. As a result, $A_{\xi_M-1, \xi_M}^{sM, sM+1}$ and $B_{\xi_M+1, \xi_M+2}^{sM+1, sM+1}$ are determined under the condition where $2m$ degrees of freedom is allowed for both $\xi_M$ and $\xi_{M+1}$, although only $m$ states are allowed for other block spin variables $\xi_2 \cdots \xi_{M-1}$ and $\xi_{M+2} \cdots \xi_N$. It is apparent that additional $m$ numbers of freedom is allowed at the position where $\tilde{V}$ is. (This excess freedom is common to both the finite and the infinite system algorithms.) Thus the variational state $V_{s_1, s_N}^{(M)}$ is dependent on $M$, even after many sweeps of the finite system process. Figure 2 shows $\ln (\lambda^{(M)})$ of the square lattice Ising model of the width $N = 200$ with free boundary condition, where we define the local Boltzmann weight as

$$W_{s_i, s_{i+1}}^{s_i', s_{i+1}'} = \exp \left\{ \frac{K}{2} \left( s_i s_{i+1} + s_i s_{i+1} + s_i s_{i+1} + s_i s_{i+1} s_{i+1} - 4 \right) \right\}$$

(9)

for the Ising spins $s = \pm 1$. We keep $(m =) 8$ states for the block spins. We have chosen the critical temperature $K = J/k_B T_c$. Since $2m$ degrees of freedom is allowed for both $\xi_M$ and $\xi_{M+1}$, the eigenvalue $\lambda^{(M)}$ of the renormalized transfer matrix $\tilde{T}_{\xi_{M-1}^{sM} \xi_{M+1}^{sM+1} \xi_{M+2}^{sM+2}}$ is dependent on $M$; $\lambda^{(M)}$ takes its maximum when $M = N/2$.
model using the formulation

$$\langle s_M \rangle = \sum_{s_1 \ldots s_N} V^{(M)}_{s_1 \ldots s_N} s_M V^{(M)}_{s_1 \ldots s_N}$$

(10)

$$= \sum_{\xi_{M-1} s_M \xi_{M+1} \xi_{M+2}} \tilde{\xi}_{M-1} s_M \xi_{M+1} \xi_{M+2}$$

and therefore $\langle s_M \rangle$ and $\langle s_{M'} \rangle$ for $M \neq M'$ are calculated for different variational states $V^{(M)}_{s_1 \ldots s_N}$ and $V^{(M')}_{s_1 \ldots s_N}$, respectively. The way to avoid such an ambiguity is simply to obtain a variational state that is independent on $M$.

Now we show that we can further improve the variational state using the block structure $B \bullet B$, and that the improved variational state is not dependent on $M$. The block structure $B \bullet B$ is known from the establishment of DMRG, [12], but the difference between $B \bullet B$ and $B \bullet B$ has not been investigated from the view point of the numerical precision. In this case, the renormalized transfer matrix is constructed as

$$\tilde{T}^{\xi}_{M-1} s_M \xi_{M+1} = L^{\xi}_{M-1} s_M \tilde{R}^{\xi}_{M+1}$$

(11)

where the improvement for the variational state is performed via the diagonalization of this $2m^2$-dimensional matrix. The eigenvector $\tilde{U}_{\xi_{M-1} s_M \xi_{M+1}}$ of the transfer matrix (Eq.11) is $2m^2$-dimensional, and it is possible to rewrite it as [22]

$$\tilde{U}_{\xi_{M-1} s_M \xi_{M+1}} = \sum_{\xi_M} A^{\xi}_{\xi_{M-1} s_M} \Omega'_{\xi_M s_{M+1}}$$

(12)

using the Gramm-Schmidt orthogonalization; $A^{\xi}_{\xi_{M-1} s_M}$ are orthogonal matrices that satisfy Eq.3, and $\Omega'_{\xi_{M-1} s_M}$ and $\Omega'_{\xi_M s_{M+1}}$ are $m$-dimensional diagonal matrices. (Note that in general $\Omega_{\xi_{M-1} s_M}$ is not equal to $\Omega'_{\xi_{M} s_{M+1}}$.) Therefore, to use the block structure $B \bullet B$ in the finite system algorithm is equivalent to write down the variational state using the tensor product (Fig.3)

$$U^{(M)}_{s_1 \ldots s_N} = \sum_{\xi_1 \ldots \xi_{N-1}} A^{s_1}_{\xi_1 \xi_2} \ldots A^{s_{M-1}}_{\xi_{M-1} \xi_M} \Omega'_{\xi_M s_{M+1}}$$

(13)

$$B^{s_{M+1}}_{\xi_{M+1} \xi_{M+2}} \ldots B^{s_{N-1}}_{\xi_{N-1} s_N}$$

and to improve $A^{s}_{\xi_{M-1} \xi_M}$ and $B^{s}_{\xi_{M+1} \xi_{M+2}}$ directly via diagonalization of $\tilde{T}^{\xi}_{M-1} s_M \xi_{M+1}$. All block spins $\xi_2 \ldots \xi_{N-1}$ are at most $m$-state; this is the non-negligible difference between $U^{(M)}_{s_1 \ldots s_N}$ in Eq.13 and $V^{(M)}_{s_1 \ldots s_N}$ in Eq.2.

Since $\xi_2 \ldots \xi_{N-1}$ are less than $m$-state in $U^{(M)}_{s_1 \ldots s_N}$ (Eq.13) we keep all the non-zero eigenvalues of the density matrix during the numerical calculation of the finite system algorithm; we don’t cut off any states. As we repeat the improvement for the tensors $A^{s}_{\xi_{i-1} \xi_i}$ and $B^{s}_{\xi_{j+1} \xi_j}$ for all $i$ and $j$, the variational state $U^{(M)}_{s_1 \ldots s_N}$ gradually approaches to its fixed point $U_{s_1 \ldots s_N}$, which is not dependent on $M$. As a result, unlike $\lambda^{(M)}$ in Eq.5, the expectation value

$$\lambda' = \sum_{\text{all indices}} U^{s_1 \ldots s_N} T^{s_1' \ldots s_N'}_{s_1 \ldots s_N} U^{s_1 \ldots s_N}$$

(14)
\[ \sum_{\text{all indices}} \tilde{U}_{\xi_{M-1}^M \xi_{M+1}^M} \tilde{T}_{\xi_{M-1}^M \xi_{M+1}^M} \tilde{U}_{\xi_{M-1}^M \xi_{M+1}^M} \]

is not dependent on \( M \). Figure 4 shows \( \ln (\lambda') \) of the Ising model; we use the same system size and parameter as those in Fig.2. As we have expected, \( \lambda' \) calculated from Eq.14 does not show any \( M \) dependence. It should be noted that \( \lambda' \) is always larger than \( \lambda(M) \), which is shown for comparison. Since both \( \lambda(M) \) and \( \lambda' \) are variational lower bound for the partition function per row (= unit transfer), it is apparent that \( \lambda' \) is better than \( \lambda(M) \) in this case.

We have used the block structure \( B \bullet B \) to obtain \( \lambda' \) after we calculated \( \lambda(M) \) using the standard block structure \( B \bullet \bullet B \). \[25\] The additional calculation for \( B \bullet B \) is not time consuming at all, because the matrix dimension of \( \tilde{U}_{\xi_{M-1}^M \xi_{M+1}^M} \) in Eq.11 is smaller than \( \tilde{T}_{\xi_{M-1}^M \xi_{M+1}^M} \) in Eq.6, and the finite system process can be done very rapidly with the use of the wave function renormalization. \[21, 22\] Thus, treating \( B \bullet B \), one can increase the numerical precision in DMRG without increasing computational time so much.

One might insist that the difference between \( \lambda(M) \) in Eq.2 and \( \lambda(M) \) in Eq.13 is negligible if \( m \) is sufficiently large. The statement is correct. We have to keep in mind, however, that occasionally people are suffering from increasing \( m \) in order to keep numerical precision. It is worth improving DMRG \textit{without} increasing \( m \), \[26\] because to keep large \( m \) is difficult for complicated models.

It is straightforward to introduce the \( B \bullet B \) structure to the infinite system algorithm in order to recover the translational invariance of the variational state in the thermodynamic limit. The way is, as we have done for the finite system algorithm, first to employ the block structure \( B \bullet \bullet B \) and to perform the infinite RG processes till the renormalized wave function converges, \[27\] and then to use \( B \bullet B \) to perform additional infinite processes. In this way, the translationally invariant variational state by Östlund-Rommer \[15\] is obtained numerically via DMRG.

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Figure Captions

Fig.1 Graphical representation of (a) the variational state, (Eq.2) (b) the variational eigenvalue of the transfer matrix, (Eq.5) and (c) the renormalized transfer matrix. (Eq.6) Circles and squares denote bare and renormalized spin variables, respectively. We use black marks when the variables are summed up in the corresponding equations.

Fig.2 The logarithm of $\lambda^{(M)}$, which is the eigenvalue of the renormalized transfer matrix

$$\tilde{T}^{s_{M-1} \ldots s_{M+1} \xi_{M+2}}_{s_{M-1} \ldots s_{M} \xi_{M+1}}$$

of the Ising model at the critical temperature when $N = 200$ and $m = 8$. Open boundary condition is chosen.

Fig.3 The graphical representation of the variational state $U^{(M)}_{s_1 \ldots s_N}$ defined in Eq.13. The finite system algorithm for $B \cdot B$ gradually improves the state, and finally $U^{(M)}_{s_1 \ldots s_N}$ lose the $M$ dependence.

Fig.4 The logarithm of $\lambda'$, which is the eigenvalue of $\tilde{T}^{s_{M-1} \ldots s_{M} \xi_{M+1}}_{s_{M-1} \ldots s_{M} \xi_{M+1}}$ for the Ising model at the critical temperature when $N = 200$ and $m = 8$. Unlike $\ln(\lambda^{(M)})$ shown for comparison, $\ln(\lambda')$ shown by circles does not show any $M$ dependence.
\[ \ln \lambda^{(M)} \]

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T. Nishino
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Fig. 3

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