Product Wave Function Renormalization Group: construction from the matrix product point of view

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We present a construction of a matrix product state (MPS) that approximates the largest-eigenvalue eigenvector of a transfer matrix $T$, for the purpose of rapidly performing the infinite system density matrix renormalization group (DMRG) method applied to two-dimensional classical lattice models. We use the fact that the largest-eigenvalue eigenvector of $T$ can be approximated by a state vector created from the upper or lower half of a finite size cluster. Decomposition of the obtained state vector into the MPS gives a way of extending the MPS, at the system size increment process in the infinite system DMRG algorithm. As a result, we successfully give the physical interpretation of the product wave function renormalization group (PWFRG) method, and obtain its appropriate initial condition.

§1. Introduction

Calculation of the maximum eigenvalue of a transfer matrix is one of the most fundamental task in statistical mechanics of lattice models. In two dimensional (2D) classical systems, the density matrix renormalization group (DMRG) method is a powerful tool for this purpose, where the maximum eigenvalue is variationally evaluated by implicit use of the matrix product state (MPS). In actual applications of the DMRG method to classical systems, most of the computational time is consumed for the determination of the largest-eigenvalue eigenvector of the renormalized transfer matrix. The matrix product structure of the variational state helpfully tells us how to save the computational time. For instance, in the finite system DMRG algorithm, a good trial vector for the diagonalization of the renormalized transfer matrix can be constructed from the MPS. For the infinite system DMRG algorithm, however, such preparation of the trial vector is rather difficult, since we have to extrapolate the MPS — increase the number of matrices — toward a larger system size.

The solution of this problem is partially achieved by the product wave function renormalization group (PWFRG) method, which increases the number of matrices in the MPS on the basis of the relation between block-spin transformations. The numerical efficiency of the PWFRG method has been demonstrated for classical systems as well as quantum ones. In spite of the efficiency of the PWFRG method, we have two problems to be solved from theoretical view point. One is in the physical interpretation of the extrapolation of the MPS, in particular, when the system size is small. This is because the extension process has been justified only in the thermodynamic limit. Another is in the preparation of initial matrices, which is necessary to start the recursive computation of the PWFRG method. So far these matrices are set empirically, which may not guarantee the numerical stability.

To find the solution of the above problems of the PWFRG method, it is instructive to recall the physical substance of the Baxter’s corner transfer matrix (CTM) method or its variant, the corner transfer matrix renormalization group (CTMRG) method. These CTM type methods calculate the partition function of the finite size cluster recursively, where the number of iterations corresponds to the linear dimension of the system. A preferable point on the methods is that the initial condition is well-defined as CTMs with appropriate boundary spin configurations. In this paper, we import such well-controllable aspects of the CTM-type methods into the extension process of the MPS.

In the next section we consider a way of the extension of the finite size clusters, which can be regarded as a variant of the CTMRG method. In §3 we analyze the MPS structure of the approximate largest-eigenvalue eigenvectors generated by the recursive extension process obtained in §2. We successfully give the physical interpretation of of the PWFRG method, and reconstruct its numerical algorithm, which includes the appropriate initial condition. In the last section, we conclude the obtained results.

§2. Recursive Construction of State Vectors

As an example of 2D statistical models, let us consider the interaction-round-a-face (IRF) model, which contains the Ising model as its special case. The IRF model is defined by the local Boltzmann Weight $W(s' s | s)$ assigned for each face of the square lattice, where $s$,
\(s', \sigma\) and \(\sigma'\) represent \(q\)-state spin variables on lattice points. (See Fig.1.) For simplicity, we consider 2-state Ising spins \((q = 2)\) and assume the symmetry \(W(s'\sigma'|s\sigma) = W(\sigma'\sigma|s\sigma)\) and \(W(s'\sigma'|s\sigma) = W(s\sigma|s'\sigma')\) throughout this article.\(^{26}\) Let us consider the finite size cluster of width \(2N\) shown in Fig.1.\(^{27}\) The partition function of the cluster is given by the spin configuration sum of the product of all the Boltzmann weights in the cluster

\[
Z_N = \sum \prod W, \quad (2.1)
\]

where we have omitted spin variables for simplicity. Throughout this section we assume the free boundary condition.

![Diagram of spins](image)

Fig. 1. The arrangement of spins of the local Boltzmann weight \(W(s'\sigma'|s\sigma)\) (in the left) and the finite size cluster of width \(2N\) considered in the partition function \(Z_N\) in Eq.(2.1) (in the right). We show the case \(N = 4\), equivalently, \(2N = 8\).

We divide the system into the upper and lower halves. Figure 2(a) shows the lower half of the system, where we label the spins on the cut as \(s_1 \ldots s_N \sigma_N \ldots \sigma_1\) from the left to right. Considering the product of local Boltzmann weights in the lower half, and taking the configuration sum of spins except for \(s_1 \ldots s_N \sigma_N \ldots \sigma_1\), we obtain a \(2^N\)-dimensional vector \(|\Psi_N\rangle\) whose elements are \(\Psi_N[s_1 \ldots s_N \sigma_N \ldots \sigma_1]\). In the same manner we obtain the \(2^N\)-dimensional vector \(|\Psi_N\rangle\) that corresponds to the upper half of the original cluster. Let us call these vectors state vectors in the following. By definitions of \(\langle \Psi_N|\) and \(|\Psi_N\rangle\), the partition function in Eq.(2.1) is expressed by the inner product

\[
Z_N = \langle \Psi_N|\Psi_N\rangle. \quad (2.2)
\]

Let us introduce the row-to-row transfer matrix

\[
T_N[s'_1 \ldots s'_N \sigma'_N \ldots \sigma'_1|s_1 \ldots s_N \sigma_N \ldots \sigma_1] = W(s'_1 s'_2|s_1 s_2)W(s'_2 s'_3|s_2 s_3) \cdots W(\sigma'_2 \sigma'_1|\sigma_2 \sigma_1). \quad (2.3)
\]

For simplicity, we introduce ‘dot product notation’ with which we abbreviate eq.(2.3) as \(T_N = W \cdot W \cdots W\).

The state vector \(|\Psi_N\rangle\) can be used as a good variational vector for \(T_N\), when the system is off critical and \(N\) is sufficiently larger than the correlation length.\(^{23}\) This is because the variational ratio

\[
g = \frac{\langle \Psi_N|T_N|\Psi_N\rangle}{\langle \Psi_N|\Psi_N\rangle} = \frac{\langle \Psi_N|T_N|\Psi_N\rangle}{Z_N} \quad (2.4)
\]

well approximates the largest-eigenvalue of \(T_N\) in the sense that, as \(N\) increases, \(f = -(k \ln g) / 2N\) where \(k\) is the Boltzmann constant approaches to the free energy per site in the thermodynamic limit.

![Graphical representations](image)

Fig. 2. Graphical representations: (a) The state vector \(|\Psi_N\rangle\) when \(N = 4\). (b) The reduced density matrix \(\rho_N^R\). Black dots denote spin variables that are summed.

We occasionally interpret \(|\Psi_N\rangle\) as a \(2^N \times 2^N\) matrix \(\Psi_N\), whose elements \(\Psi_N(s_1 \ldots s_N \sigma_N \ldots \sigma_1)\) are equal to \(\Psi_N[s_1 \ldots s_N \sigma_N \ldots \sigma_1]\). (We have put the vertical line \(|\) between the first matrix index \(s_1 \ldots s_N\) and the second one \(\sigma_N \ldots \sigma_1\), respectively, which corresponds to the left and the right half-row spins. We reverse the spin order \(s_N \ldots s_1\) for the later convenience.) This notation is useful when we consider the reduced density matrix \(\rho_N^R = \text{Tr}_L (|\Psi_N\rangle\langle \Psi_N|)\), where \(\text{Tr}_L\) represents the spin contraction for all the \(s_i\) in the left side. Figure 2(b) shows the graphical representation of \(\rho_N^R\).\(^{2,23,24}\) Using the matrix notation \(\Psi_N\), we can simply write \(\rho_N^R\) as the matrix product \(\Psi_N^\dagger \Psi_N\), since the elements of \(\rho_N^R\) are explicitly given by

\[
\rho_N^R(\sigma'_N \ldots \sigma'_1|\sigma_N \ldots \sigma_1) = \sum_{s_N \ldots s_1} \Psi_N(s_1 \ldots s_N \sigma_N \ldots \sigma_1) \langle \Psi_N(s_1 \ldots s_N \sigma_N \ldots \sigma_1)| \langle \Psi_N(s_1 \ldots s_N \sigma_N \ldots \sigma_1)\rangle. \quad (2.5)
\]

Similarly we obtain the reduced density matrix for the left side \(\rho_N^L = \text{Tr}_R (|\Psi_N\rangle\langle \Psi_N|) = \Psi_N \Psi_N^\dagger\). It should be noted that all the elements of \(\Psi_N\), \(\rho_N^R\) and \(\rho_N^L\) are real and non negative. The partition function in Eq.(2.2) is expressed as

\[
Z_N = \text{Tr} \rho_N^L = \text{Tr} \rho_N^R = \text{Tr} \Psi_N^\dagger \Psi_N. \quad (2.6)
\]

In the following we consider a recursive construction of \(\Psi_N\), starting from \(N = 1\) up to a certain system size. Let us first take the configuration sum for 2 spins on the local Boltzmann weight

\[
\Psi_1(s'_1|\sigma'_1) = \sum_{s_1, \sigma_1} W(s'_1 \sigma'_1|s_1 \sigma_1) \quad (2.7)
\]

to obtain a state vector \(|\Psi_1\rangle\) of the smallest width. (See Fig.2(a) and imagine the case \(N = 1\).) In order to extend the system size and construct \(|\Psi_N\rangle\), consider the row-to-row transfer matrix \(T_2 \equiv W \cdot W \cdot W\), whose elements are expressed as

\[
T_2[s'_1 s'_2 \sigma'_1|s_1 s_2 \sigma_2] = W(s'_1 s'_2|s_1 s_2)W(s'_2 \sigma'_2|s_2 \sigma_2)W(\sigma'_2 \sigma'_1|\sigma_2 \sigma_1). \quad (2.8)
\]
Consider the case $m$. It should be noted that the variables contained in $\Psi$ are given by
\[
\begin{align*}
T^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1) &= W(\sigma'_2\sigma'_1|\sigma_2\sigma_1) \\
T^L_2(s'_2s'_1|s_2s_1) &= W(s'_2s'_1|s_1s_2),
\end{align*}
\]
where the order of spin indices in $T^R_2$ is reversed for convenience, so that $T^L_2 = T^R_2$ holds when $W$ is symmetric. To obtain $|\Psi_2\rangle$, we “join” $T_2^L \equiv T_2^R \cdot W \cdot T_2^R$ to $|\Psi_1\rangle$ as follows. First we contract a spin in the half-row transfer matrices as
\[
\begin{align*}
P^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1) &= \sum_{s_1} T^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1) \\
P^L_2(s'_2s'_1|s_2s_1) &= \sum_{s_1} T^L_2(s'_2s'_1|s_1s_2).
\end{align*}
\]

For the later use we define a $2^2 \times 2^2$ matrix $P_2 \equiv P^L_2 \cdot W \cdot P^R_2$ shown in Fig.3(b), whose elements are given by
\[
P^L_2(s'_2s'_1|s_2s_2)W(s'_2s'_2|s_2s_2)P^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1).
\]

Then we can obtain $|\Psi_2\rangle$ by applying $P_2$ to $|\Psi_1\rangle$ as shown in Fig.3(c), where the matrix elements of $\Psi_2$ is explicitly given by
\[
\Psi_2(s'_2s'_1|\sigma'_2\sigma'_1) = \sum_{s_2} P^L_2(s'_2s'_1|s_2) \times W(s'_2s'_2|s_2s_2)P^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1)\Psi_1(s_2|\sigma_2).
\]

It should be noted that the variables contained in $\Psi_1$ are $s_2$ and $\sigma_2$ only. In short, we write Eq.(2.12) as $|\Psi_2\rangle = P^L_2 \cdot W \cdot P^R_2 |\Psi_1\rangle$.

In the same manner we obtain $|\Psi_3\rangle$ by applying $P_3 \equiv P^L_3 \cdot W \cdot P^R_3$ to $|\Psi_2\rangle$, where the matrix elements of $P^L_3$ are given by
\[
P^L_3(\sigma'_3\sigma'_2|\sigma_3\sigma_2) = W(\sigma'_3\sigma'_2|\sigma_3\sigma_2)P^R_2(\sigma'_2\sigma'_1|\sigma_2\sigma_1).
\]

Hereafter we do not refer to the calculations of $T^L_N, P^L_N$, and $\rho^R_N$ for book keeping purpose.

Since such recursive extensions of $|\Psi_N\rangle$ cause the exponential blow-up of the vector (or matrix) dimensions, we have to introduce the density matrix renormalization to reduce the dimensions below a certain number $m^1,^2$

The value of $m$ is normally chosen to be $10 \sim 1000$. (In the following explanation we assume $m \geq 8$.) Let us consider the case $N = 2$ as an example. We diagonalize the reduced density matrix
\[
\rho^R_3(\sigma'_3\sigma'_2|\sigma_3\sigma_2) = \sum_{s_2} \tilde{\Psi}_3(s_3s_2|\sigma'_3\sigma'_2)\tilde{\Psi}_3(s_3s_2|\sigma_3\sigma_2) = \sum_{\xi_3} U_3(\sigma'_3\xi_2|\xi_3)\lambda_3(\xi_3)U_3(\sigma_3\xi_2|\xi_3)
\]
in order to obtain the block spin transformation $U_3$ that maps $\sigma_3\xi_2$ to the 8-state block spin $\xi_3$. This time we perform the extension from $\tilde{P}^R_3$ to $\tilde{P}^R_4$ operating $U_4$ from

\[
\tilde{P}^R_3(\sigma'_3\xi_2|\sigma_3\sigma_2) = \sum_{\sigma'_2} U_2(\sigma'_2|\xi_3)\lambda_2(\xi_3)U_2(\sigma_2|\xi_3).
\]
the left and $\hat{U}_2$ from the right

$$\hat{P}_4^R (\sigma'_4 \xi_3 | \sigma_4 \eta_3) = \sum_{\sigma'_3 \xi_2} U_3 (\sigma'_3 \xi_2 | \xi_3) W (\sigma_4' \sigma'_3 | \sigma_4 \sigma_3)$$

$$\times \hat{P}_3^R (\sigma'_3 \xi_2 | \sigma_3 \sigma_2) U_2 (\sigma_3 \sigma_2 | \eta_3) \quad (2.18)$$
as shown in Fig.5(b), or in short $\hat{P}_4^R = \hat{U}_4^R (W \cdot \hat{P}_3^R) \hat{U}_2$.
(Note that the matrix $U_2$ in the right hand side contains $\sigma_3$ and $\sigma_2$, not $\sigma_4$ and $\sigma_1$.) Up to this stage, we keep all the block spin states since we have assumed $m \geq 8$.

Fig. 5. Graphical representations: (a) Extension from $|\Psi_i\rangle$ to $|\tilde{\Psi}_{i+1}\rangle = \hat{P}_i^L \cdot W \cdot \hat{P}_i^R$ in Eq.(2.16). (b) Extension from $\hat{P}_i^R$ to $\hat{P}_i^R \equiv \hat{U}_i^R (W \cdot \hat{P}_i^R) \hat{U}_{i-1}$ in Eq.(2.18).

Now we can generalize the extension process up to arbitrary system size. If we have $|\tilde{\Psi}_i\rangle$ up to a certain size $i \geq 2$, we can construct the extended one

$$|\tilde{\Psi}_{i+1}\rangle = \hat{P}_{i+1}^L \cdot W \cdot \hat{P}_{i+1}^R |\tilde{\Psi}_i\rangle \quad (2.19)$$

with

$$\hat{P}_{i+1}^R \equiv \hat{U}_{i+1}^R (W \cdot \hat{P}_{i+1}^R) \hat{U}_{i}$$

where the block spin transformations $\hat{U}_i$ and $\hat{U}_{i-1}$ have been obtained by the diagonalizations of $\hat{P}_i^R$ and $\hat{P}_{i-1}^R$, respectively. The matrix elements of Eq.(2.19) and (2.20) are explicitly given by

$$\tilde{\Psi}_{i+1} (s'_{i+1} \xi_1 | s_{i+1} \xi_1) =$$

$$\sum_{s_{i+1} \xi_1} \hat{P}_{i+1}^L (s'_{i+1} \xi_1 | s_{i+1} \xi_1) W (s'_{i+1} \xi_1 | s_{i+1} \xi_1)$$

$$\times \hat{P}_{i+1}^R (s'_{i+1} \xi_1 | s_{i+1} \xi_1) \tilde{\Psi}_i (s_{i+1} \xi_1 | s_{i+1} \xi_1) \quad (2.21)$$

and

$$\hat{P}_{i+1}^R (s'_{i+1} \xi_1 | s_{i+1} \xi_1) = \sum_{\sigma_{i+1} \xi_1} U_i (s'_{i+1} \xi_1 | s_{i+1} \xi_1)$$

$$\times W (s'_{i+1} \xi_1 | s_{i+1} \xi_1) \hat{P}_i^R (s'_{i+1} \xi_1 | s_{i+1} \xi_1) U_{i-1} (s_{i+1} \xi_1 | s_{i+1} \xi_1) \quad (2.22)$$

The key point in Eqs.(2.20) and (2.22) is that the label of $\hat{U}_i$ is larger than that of $\hat{U}_{i-1}$ by one, which enables us to “extrapolate” the state vector in Eqs.(2.19) and (2.21).

As is performed in the DMRG method, we keep at most $m$ numbers of relevant states for the block spin variables, and neglect the rest of irrelevant ones in Eq.(2.20). We can thus calculate the approximate partition function $\tilde{Z}_i = \langle \tilde{\Psi}_i | \tilde{\Psi}_i \rangle$ recursively up to arbitrary system size $i = N$. In addition to $\tilde{Z}_N$, we can obtain the nearest neighbor spin correlation function

$$\langle s_N \sigma_N \rangle = \langle \tilde{\Psi}_N | s_N \sigma_N | \tilde{\Psi}_N \rangle$$

(2.23)
at the center of the system.

Fig. 6. Nearest neighbor spin correlation function $\langle s_N \sigma_N \rangle$ in Eq.(2.23) of the Ising model at criticality.

Let us observe the numerical efficiency of the explained recursive algorithm in the application to the Ising model. Figure 6 shows the calculated $\langle s_N \sigma_N \rangle$ at criticality where the correlation length is infinite. The calculated data deviates from the scaling line when the system size exceeds the artificial cut-off length introduced by the restriction of the degrees of freedom down to $m$. The observed cut-off effect is similar to that of the CTMRG method. This is because the system-size extension process defined by Eq.(2.19) and (2.20) is quite similar to the extension of the corner transfer matrix in the CTMRG method.

§3. Product Wave Function Renormalization Group

It is worth looking at the structure of $\hat{P}_i^R \equiv \hat{P}_i^R \cdot W \cdot \hat{P}_i^R$ from the view point of the MPS. Tracing back the recursive construction in Eqs.(2.10), (2.15), (2.18), and (2.20), we can represent $\hat{P}_i^R (\sigma'_i \xi_{i-1} | \sigma_i \eta_{i-1})$ for $i \geq 6$ as

$$\hat{P}_i^R \equiv \hat{U}_{i-1}^R (W \cdot \hat{P}_{i-1}^R) \hat{U}_{i-2}$$

$$= \hat{U}_{i-1}^R (W \cdot \hat{U}_{i-2}^R (W \cdot \hat{P}_{i-2}^R) \hat{U}_{i-3}^R) \hat{U}_{i-2} \quad (3.1)$$

$$= \hat{U}_{i-1}^R (W \cdot \hat{U}_{i-2}^R (W \cdot \cdots (W \cdot \hat{P}_{i-2}^R) \cdots \hat{U}_{i-3}^R) \cdots \hat{U}_{i-2} \quad (3.2)$$

Introducing the $2^i$ by $2^{i-1}$ matrix $P_R (\sigma'_i \cdots \sigma_1 | \sigma_1 \cdots \sigma_2)$, which is defined by $P_R \equiv W \cdot \hat{P}_i^R \equiv \hat{U}_{i-1}^R (W \cdot \hat{P}_{i-1}^R) \hat{U}_{i-2}$, we rewrite Eq.(3.1) as the simpler form

$$\hat{P}_i^R \equiv \hat{U}_1 \hat{U}_2 \hat{U}_3 \hat{U}_4 \hat{U}_5 \hat{U}_6 \hat{U}_7 \hat{U}_8$$

where $\hat{U}_1 \cdots \hat{U}_3 \hat{U}_4 \hat{U}_5 \hat{U}_6$ represents the successive block spin transformations by $U_j (\sigma'_j \xi_j | \xi_j)$, $U_k (\sigma'_k \xi_k | \xi_k)$, and $U_{i-1} (\sigma'_{i-1} \xi_{i-2} | \xi_{i-1})$. In the same manner $\hat{U}_2 \hat{U}_3 \hat{U}_4 \hat{U}_5$ represents the successive block spin transformations by $U_2 (\sigma_3 \eta_3 | \eta_3)$, $U_3 (\sigma_4 \eta_4 | \eta_4)$, and $U_{i-2} (\sigma_{i-2} \eta_{i-2} | \eta_{i-2})$, where one should pay attention to the indices of spin variables. The structure of $\hat{P}_i^R$ is similar to that of the
renormalized half-row transfer matrix

\[ \tilde{T}_i^R = U_{i-1}^\dagger (W \cdot \tilde{T}_{i-1}^R) \tilde{U}_{i-1} \]

\[ = U_{i-1}^\dagger (W \cdot U_{i-2} \cdot \cdots \cdot (W \cdot T_2) \cdots U_{i-2}) \tilde{U}_{i-1} \]

\[ = U_{i-1}^\dagger \cdot \cdots \cdot U_3^\dagger U_2^\dagger (W \cdot W \cdot T_2) \tilde{U}_2 \tilde{U}_3 \cdots \tilde{U}_{i-1} \]

\[ = U_{i-1}^\dagger \cdot \cdots \cdot U_3^\dagger U_2^\dagger \tilde{T}_i^R \tilde{U}_2 \tilde{U}_3 \cdots \tilde{U}_{i-1}, \quad (3.3) \]

which has been used in the DMRG method. (We have introduced \( T_i^R = W \cdot T_{i-1}^R = (W \cdot T_i^R)^{-1} \).

In Eq.(3.3) the successive block spin transformations \( U_{i-1}^\dagger \cdot \cdots \cdot U_3^\dagger U_2^\dagger \) are the conjugate of \( \tilde{U}_{i-1} \cdots \tilde{U}_3 \tilde{U}_2 \), and are performed by the matrices \( U_2(\sigma_2 \sigma_1 | \xi_2), U_3(\sigma_3 \xi_2 | \xi_3), \ldots \) and \( U_{i-1}(\sigma_{i-2} | \xi_{i-2}) \). Comparing Equations (3.2) and (3.3), let us consider the relation between the renormalization process explained in the previous section and that in the conventional DMRG method.

Since the structure of \( \tilde{T}_i^R \) in Eq.(3.3) is similar to that of \( \tilde{P}_i^R \) in Eq.(3.2), we try to handle \( \tilde{P}_i^R \) and \( \tilde{T}_i^R \) in a unified manner. Let us introduce a new matrix \( V_i \), whose elements are given by

\[ V_i(\sigma_2 \sigma_1 | \sigma_2') = \delta(\sigma_2 | \sigma_2'), \quad (3.4) \]

which is independent of \( \sigma_1 \), and the right hand side is the Kronecker delta. The matrix \( V_i \) has a function of taking configuration sum for \( \sigma_i \) as Eq.(2.10), when it is operated to the half-row transfer matrices. For example, we obtain

\[ P_i^R(\sigma_i | \sigma_1) = \delta(\sigma_i | \sigma_2'), \quad (3.5) \]

which we compactly write as \( P_i^R = T_i^R \tilde{V}_i \). Then we can rewrite \( \tilde{P}_i^R \) in Eq.(3.2) as

\[ \tilde{P}_i^R = U_{i-1}^\dagger \cdots \cdot U_3^\dagger U_2^\dagger \tilde{T}_i^R \tilde{V}_i \tilde{U}_2 \tilde{U}_3 \cdots \tilde{U}_{i-2}. \quad (3.6) \]

Note that \( V_i \) in Eq.(3.4) represents the free boundary condition of the system under consideration. For the system with fixed boundary condition \( \sigma_1 = 1 \), the r.h.s of Eq.(3.4) should be replaced by \( \delta(\sigma_2 | \sigma_2') \delta(\sigma_1 | 1) \).

For the moment let us consider the ideal case \( m = 2^{-1} \), where we keep all the states for every block spin transformations. In such a case the block spin transformation is exact, and the relation

\[ \left[ \begin{array}{c|c|c|c|c|c|} \tilde{U}_2 & \cdots & \tilde{U}_3 & \cdots & \tilde{U}_{i-1} \\ \hline \tilde{U}_2 & \cdots & \tilde{U}_3 & \cdots & \tilde{U}_{i-1} \end{array} \right] \left[ \begin{array}{c|c|c|c|c|c|} U_2 & \cdots & U_3 & \cdots & U_{i-1} \\ \hline U_2 & \cdots & U_3 & \cdots & U_{i-1} \end{array} \right] = I_{i-1} \]

\[ \tilde{P}_i^R = \tilde{T}_i^R \tilde{E}_i^R \quad (3.11) \]

among the matrices \( \tilde{P}_i^R(\sigma_i | \sigma_1) = \tilde{E}_i^R(\sigma_1 | \sigma_1) \), and \( \tilde{E}_i^R(\sigma_i | \sigma_1) \). Introducing the notations \( \tilde{E}_i = \tilde{E}_i^R \cdot \tilde{T}_i \) and \( \tilde{T}_i = \tilde{T}_i^R \cdot W \cdot \tilde{T}_i^R \) we finally reach the relation

\[ \tilde{P}_i = \tilde{E}_i \tilde{T}_i \quad (3.12) \]

for the ideal case where there is no cut-off in the block spin transformation.

In realistic numerical calculation we have to neglect irrelevant states, therefore Eqs.(3.7)-(3.12) do not hold exactly, but still \( \tilde{P}_i^R \) is well approximated by \( \tilde{P}_i \) if sufficiently large numbers of the block spin states are kept. Under this situation let us consider the operation of \( \tilde{P}_i \) to the state vector

\[ | \tilde{\psi}_i \rangle = \tilde{P}_i | \tilde{\psi}_{i-1} \rangle \quad (2.19)' \]

\[ \sim \tilde{T}_i \tilde{E}_i | \tilde{\psi}_{i-1} \rangle = \tilde{T}_i | \tilde{\phi}_i \rangle \quad (3.13) \]

as shown in Fig.7(a), where the whole structure of \( \tilde{T}_i \) is shown in Fig.7(b). We have introduced a new state vector

\[ | \tilde{\phi}_i \rangle = \tilde{E}_i | \tilde{\psi}_{i-1} \rangle = \tilde{E}_i^L \cdot \tilde{E}_i^R | \tilde{\psi}_{i-1} \rangle, \quad (3.14) \]

whose structure is shown in Fig.7(c). If we use the matrix representation for the state vectors \( | \tilde{\Phi}_i \rangle \) and \( | \tilde{\psi}_{i-1} \rangle \), we can rewrite the above equation by the matrix product

\[ | \tilde{\phi}_i \rangle = \left( \tilde{E}_i^L \right) \tilde{\psi}_{i-1} \left( \tilde{E}_i^R \right)^\dagger \quad (3.15) \]

among \( \tilde{E}_i^L(\sigma_i | \sigma_1) \), \( \tilde{\psi}_{i-1}(\sigma_i | \sigma_1) \), and the transpose of \( \tilde{E}_i^R(\sigma_i | \sigma_1) \). The structure of \( \tilde{E}_i = \tilde{E}_i^L \cdot \tilde{E}_i^R \)
As we explain in the following, Eq. (3.10) the new matrix \( \tilde{\Psi} \) is obtained from the definition of \( \tilde{E}^R \) in Eq. (3.9). Substituting \( \tilde{E}^R_3 = U^\dagger_2 I_3 \tilde{V}_1 \) to \( A_3 = \tilde{E}^R_3 U_2 \) we obtain \( A_3 = \left( U^\dagger_2 I_3 \tilde{V}_1 \right) U_2 \), and thus we find the initial condition \( \tilde{A}_2 = V_1 \).

It might be helpful to rewrite Eq. (3.18) by the element:

\[
\tilde{A}_i(\sigma_i \xi_{i-1} | \eta_i) = \sum_{\sigma_{i-1} \xi_{i-2} \eta_{i-1}} U_{i-1}(\sigma_{i-1} \xi_{i-2} | \xi_{i-1}) \times \tilde{A}_{i-1}(\sigma_{i-1} \xi_{i-2} | \eta_{i-1}) U_{i-1}(\sigma_i \eta_{i-1} | \eta_i).
\]

Figure 8 shows the graphical representation of Eqs. (3.18) and (3.20).

Using the recursion relation Eq. (3.18) and the approximation from Eq. (2.19)' to Eq. (3.13), let us reformulate the recursive creation of the state vectors proposed in the previous section. Suppose that we have the renormalized transfer matrix \( \tilde{T}_{i-1} \), the state vector \( | \tilde{\Psi}_{i-1} \rangle \) and the matrix \( \tilde{A}_{i-1} \). We obtain \( | \Psi_i \rangle \) as follows.

(a) Perform the diagonalization \( \tilde{\Psi}_{i-1} \rightarrow \tilde{U}_{i-1} \Omega_{i-1} \tilde{U}_{i-1}^\dagger \) in Eq. (3.16) to obtain \( U_{i-1} \) and \( \Omega_{i-1} \).
(b) Obtain \( \tilde{A}_i = \left[ \tilde{U}_{i-1}^\dagger \left( id \cdot \tilde{A}_{i-1} \right) \right] \tilde{U}_{i-1} \) by Eq. (3.18).
(c) Extend the linear dimension of the renormalized transfer matrix by \( \tilde{T}_{i}^R = \tilde{U}_{i-1}^\dagger \left( W \cdot \tilde{T}^R_{i-1} \right) \tilde{U}_{i-1} \) in Eq. (3.3) and the same for \( \tilde{T}^L_i \).
(d) Obtain \( \tilde{\Phi}_i = \tilde{A}_i \Omega_{i-1} \tilde{A}_{i-1}^\dagger \). (Eq. (3.17).)
(e) Multiply \( \tilde{T}_{i} \) to \( | \Phi_i \rangle \). Admitting the approximation from Eq. (2.19)' to Eq. (3.13), substitute the obtained vector \( \tilde{T}_{i} | \Phi_i \rangle \) to \( | \Psi_i \rangle \) and proceed to the next iteration.

With use of this recursive calculation, we obtain the state vectors and the partition functions explained in the previous section. (The obtained data is of use for the finite size scaling at the criticality.)

The recursive calculation starts from the initial condition given by Eq. (3.19). The calculation can be stopped when the observed physical quantities, such as the free energy per site, converge to their values at the large
system size limit. Alternatively, the difference between $\hat{\rho}^R_1/\hat{Z}_1$ and $\hat{\rho}^R_{i+1}/\hat{Z}_{i+1}$ (or in some cases $\hat{\rho}^R_1/\hat{Z}_1$ and $\hat{\rho}^R_{i+2}/\hat{Z}_{i+2}$) can be used for the confirmation of the convergence, since when $i$ is several times larger than the correlation length the recursive procedures (a)-(e) becomes just the repetition of the same calculation. It should be noted that even in the large $i$ limit the condition $\hat{U}_{i+1} = \hat{U}_i$ is not always satisfied, as reported by Okunishi et al.\textsuperscript{20}

The recursive process (a)-(e) is actually a special case of the numerical algorithm of the ‘product wave function renormalization group (PWFRG) method’.\textsuperscript{15} In order to clarify this point let us consider the numerical problem of obtaining the largest-eigenvalue eigenvector of the renormalized transfer matrix $\hat{T}_1$ during the calculation by infinite system DMRG method. Normally one of the power, the Lanczos, the Davidson, or the Arnoldi methods is employed for the diagonalization of $\hat{T}_1$. The computational time required for these diagonalization methods is greatly dependent on the choice of the initial vector, and therefore it is important to create a good initial (or trial) vector for the diagonalization of $\hat{T}_1$. From the arguments in the previous section — see Eqs.(2.19) and (2.20) — it is apparent that $|\tilde{\Psi}_1\rangle = P_1 \tilde{\Psi}_{i-1}\rangle$ in Eq.(2.19) is a candidate of the initial vector. (The choice is not so bad if the correlation length of the system is much shorter than the system size $2i$, as was explained in the paragraph that contains Eq.(2.4), and expected to be of use for modest system size.) Since $P_1$ is further approximated by $\hat{E}_1$ we can say that $\hat{E}_1$ has a function of extending the vector dimension of $|\tilde{\Psi}_{i-1}\rangle$ to create $|\tilde{\Phi}_1\rangle = \hat{E}_1|\tilde{\Psi}_{i-1}\rangle$ in Eq.(3.14), and that $\hat{T}_1$ improves $|\tilde{\Phi}_1\rangle$ to give an approximation for $|\tilde{\Psi}_1\rangle$. We find that $|\tilde{\Phi}_1\rangle$ is also of use as the initial vector, since the diagonalization methods creates $\hat{T}_1|\tilde{\Phi}_1\rangle \sim |\tilde{\Psi}_1\rangle$, $|\hat{T}_1^2|\tilde{\Phi}_1\rangle \sim |\hat{T}_1|\tilde{\Psi}_1\rangle$, $|\hat{T}_1^3|\tilde{\Phi}_1\rangle \sim |\hat{T}_1^2|\tilde{\Psi}_1\rangle$, etc., inside their numerical procedure, and therefore to start the diagonalization from $|\tilde{\Phi}_1\rangle$ is almost as efficient as to start from $|\tilde{\Psi}_1\rangle$.

Based on the above discussion about the initial vector, we find that the recursion relation Eq.(3.18) can be efficiently used for the numerical acceleration of the infinite system DMRG algorithm. The way is simply to replace the step (e) of the recursive calculations (a)-(e) by

\[(e')\] Using $|\tilde{\Phi}_1\rangle$ as the initial vector for the Lanczos diagonalization (or Davidson, Arnoldi diagonalization or the power method)\textsuperscript{28} of $\hat{T}_1$. Substitute the obtained largest-eigenvalue eigenvector of $\hat{T}_1$ to $|\tilde{\Psi}_1\rangle$ and proceed to the next iteration.

The modified recursive method, which consists of (a), (b), (c), (d), and (e’), is the numerical algorithm of the original version of the PWFRG method.\textsuperscript{15} So far the initial condition of this method — the matrix element of $A_2$ — was set empirically. What we have clarified here is that the initial condition $A_2$ is given by $V_1$ in Eq.(3.19), which represent the boundary condition of the system.\textsuperscript{29} One can easily verify that the calculation by (a)-(e’) gives the same result as the infinite system DMRG method, since the DMRG method consists of (a), (c), and the diagonalization of $\hat{T}_1$. Even with the use of the initial vector $\tilde{\Phi}_1$ the diagonalization step (e’) occasionally consume large amount of computational time. We can improve the situation, considering the half-way between (e) and (e’). For example, if we employ the Lanczos diagonalization, (e) or (e’) can be replaced by

\[(e’')\] Using $|\tilde{\Phi}_1\rangle$ as the initial vector for the Lanczos diagonalization of $\hat{T}_1$, perform only one or only a few Lanczos steps. Substitute the obtained Lanczos vector to $|\tilde{\Psi}_1\rangle$ and proceed to the next iteration.

This is a realistic choice if one already has a computational program of the infinite system DMRG method, and if only the physical quantities at the large system size limit $i \to \infty$ is required.\textsuperscript{18}

If we store all the block spin transformations $\hat{U}_2, \hat{U}_3, \ldots, \hat{U}_{i-1}$ obtained successively at the step(a), we implicitly have the variational MPS\textsuperscript{6,10}

\[
\left[ \hat{U}_2 \cdots \hat{U}_{i-1} \right] \Omega_{i-1} \left[ \hat{U}_{i-1}^\dagger \cdots \hat{U}_2^\dagger \right] ,
\]

which approximates $|\Psi_{i-1}\rangle$. The formulation can be obtained by considering the structure of $\langle \Psi_{i-1}|\hat{T}_{i-1}|\Psi_{i-1}\rangle$ which well approximates $\langle \Psi_{i-1}|\hat{T}_{i-1}|\Psi_{i-1}\rangle$. The fact enables us to use the iterative process of the PWFRG method (a)-(e’), combine with the finite size DMRG method. For example, the process (a)-(e’) can be used for the initial set-up of the variational MPS, that are further improved by the finite system DMRG sweeps. Equally, after finishing the finite system DMRG calculation for a certain system size $2N$, one can switch to the process (a)-(e’) again, and after $M$ iterations to obtain a good variational MPS for the next finite system DMRG sweep at the size $2(N+M)$. The step (e’) can be replaced by (e) or (e”), since the finite system DMRG sweep improves the extended MPS. Such a switching process is of use when precise numerical data calculated by the finite system DMRG method are required for finite size scaling analyses.

\section{Conclusions and Discussions}

We have explained the physical background of the PWFRG method from the view point of the MPS formalism. In section II, we first consider the calculation of the partition function of the IRF model on a finite size cluster. We observe the fact that the largest-eigenvalue eigenvector of a transfer matrix of width $2N$ can be approximated by the state vector that corresponds to lower half (in Fig.2(a)) of the system of width $2N$. By use of the fact, we construct an iterative numerical method to calculate the partition function up to arbitrary system size, which is equally of use as the CTMRG method.\textsuperscript{24,25} In Section III, we analyze the the whole structure of the renormalized transfer matrices, which appears in the formalism shown in §2. Observing the matrix product construction of the state vector, we find the way of increasing the number of matrices contained in MPS when we increment the system size. The extended MPS can be efficiently used as the initial vector for the diagonaliza-
tion of the renormalized transfer matrix, which appears in the infinite system DMRG method. As a result, we obtain the numerical algorithm of the PWFRG method. The initial condition for the PWFRG method, which has been set empirically, is clearly determined by Eq. (3.19) that corresponds to the boundary condition of the system.

The numerical method shown in §2 has clear physical meaning as the partition function calculation of finite size cluster of square shape. The same result can be obtained by the PWFRG method with the step (e) in the previous section. The PWFRG method with (e') gives exactly the same result as the infinite system DMRG method, where the calculation of the largest-eigenvalue eigenvector of the renormalized transfer matrix is faster than the conventional infinite system DMRG method. One can use the PWFRG method with (e'') if the convergence of the calculated physical quantities toward the large system size limit is slow with the use of (e) or (e'). The use of (e'') accelerates the convergence of the free energy per site, but the calculated data before completing the convergence do not have clear physical meaning. After the convergence, the PWFRG method with (e), (e') and (e'') give the same result about the thermodynamic limit of the system.

We comment that the PWFRG method can also be applied to 1D quantum systems, in addition to 2D classical systems. The simplest example is a uniform spin chain, whose Hamiltonian is written as a sum of po-

stantial independent local terms. In this case we obtain the superblock Hamiltonian \( H_i \equiv \tilde{R}^i + h + \tilde{H}^i \) using the recursive relation \( \tilde{R}^i_{i+1} = U_i^\dagger (h + \tilde{H}^i) U_i \) similar to the extension process of the renormalized transfer matrix \( \tilde{T}^i_{i+1} = U_i^\dagger (W \cdot \tilde{T}^i) U_i \). Implementing the diagonalization of \( H_i \) into the recursive procedure in the PWFRG method (a)-(e') in §3, one can obtain the ground state property of the quantum system in the thermodynamic limit. As for the classical systems, use of (a)-(e'') is efficient for the acceleration of the convergence toward the large system size limit.

About the recursive creation of variational state for infinite 1D quantum Hamiltonians, the CTMRG method can also be employed for this purpose. Consider the infinite size chess board system generated by the Trotter decomposition applied to 1D quantum systems, in addition to 2D clas-

ical systems. The formulation is similar to the recently proposed renormalization formalism for the corner Hamiltonian. The formulation is similar to the Trotter decomposition, one obtains a DMRG formalism for the corner Hamiltonian. The formulation is similar to the recently proposed renormalization formalism for the corner Hamiltonian by Okunishi, but the block spin transformation is obtained from the diagonalization of the density matrix, instead of the diagonalization of the corner Hamiltonian.

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