Product Wave Function
Renormalization Group

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Synopsis

The authors propose a fast numerical renormalization group method — the product wave function renormalization group (PWFRG) method — for 1D quantum lattice models and 2D classical ones. A variational wave function, which is expressed by a matrix product, is improved through a self-consistent calculation. The new method has the same fixed point as the density matrix renormalization group method.

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The real-space renormalization group\textsuperscript{1)} (RSRG) is a basic concept in statistical physics. One of the recent progress in the RSRG is the density matrix renormalization group (DMRG) method established by White.\textsuperscript{2,3)} The DMRG method has been applied to various one-dimensional (1D) quantum lattice models, such as the spin chains\textsuperscript{3)} and electron systems,\textsuperscript{4,5)} because the method gives precise results for large scale systems. The method is also applied to 2D classical models.\textsuperscript{6)} Recently, fixed point structure of the DMRG method has been analyzed by Östlund and Rommer.\textsuperscript{7)} They show that the ground state wave function obtained by the DMRG method is a product of matrices.

Quite recently, the authors have shown that the DMRG method is essentially the same as Baxter’s variational method on the corner transfer matrix.\textsuperscript{8)} On the basis of this fact, we have formulated a fast numerical method — the corner transfer matrix renormalization group (CTMRG) method\textsuperscript{9)} — for 2D classical systems. The CMTRG method is applicable to 1D quantum lattice models with the help of the Trotter formula.\textsuperscript{10)}

In this paper, we propose a new renormalization group method, which is an extension of the CTMRG method. The new method is applicable to 1D quantum systems with no reference of the Trotter formula.\textsuperscript{10)} Since the method renormalizes a wave function, which is expressed by a matrix product,\textsuperscript{11)} we call it ‘product wave function renormalization group (PWFRG) method.’ Since the PWFRG method and the DMRG method have many aspects in common, we review the DMRG method at first. We then show the numerical algorithm of the PWFRG method for 2D classical models. We accelerate the numerical calculation with the help of the
modified Lanczos method. Finally we discuss the way how to apply the PWFRG method to 1D quantum systems.

We choose the ‘interaction round a face (IRF) model’ as an example of the 2D classical model. The IRF model is defined by a Boltzmann weight \( W(a'b'|ab) \) on each face, that is surrounded by four \( n \)-state spins \( a, b, a', \) and \( b' \). The row-to-row transfer matrix is

\[
T(a'b'c' \ldots y'z'|abc \ldots yz) = W(a'b'|ab)W(b'c'|bc) \ldots W(y'z'|yz),
\]

where the variables \( \{a'b'c' \ldots y'z'\} \) and \( \{abc \ldots yz\} \) denote the \( n \)-state spins in subsequent rows. We assume that \( W(ab|cd) \) is symmetric — \( W(ab|cd) = W(ba|dc) = W(ca|db) = W(dc|ba) \) — in order to simplify the discussion. Generalizations for asymmetric cases are straightforward.

The DMRG method maps the transfer matrix \( T \) in Eq. 1 into the effective one

\[
\tilde{T}(\xi' \xi'|\eta' \eta) = P(i'|i)W(i'|j|j)P(j'|j),
\]

where \( P \) represents the effective transfer matrix for the left/right-half lattice. The greek indices \( \xi, \xi', \eta \) and \( \eta' \) denote \( m \)-state block-spin variables, that are shown by squares in Fig. 1. The eigenvector \( V \) that corresponds to the largest eigenvalue of \( \tilde{T} \) is well approximated by a matrix product

\[
V(i|j) = \sum_{\alpha} R(i|\alpha)(i) \omega_\alpha R^T(\alpha|j),
\]

where \( R \) is a \( n \times m \) orthogonal matrix, \( R^T \) is its transpose, and the relation \( \sum_{i} R^T(\alpha|i)(i|\beta) = \delta_\alpha^\beta \) is satisfied. We have expressed the \( (nm)^2 \)-dimensional vector \( V \), which we call ‘product wave function,’ as a
$nm$-dimensional square matrix. The r.h.s. of Eq.3 is actually the singular-value decomposition of the l.h.s of Eq.3, and therefore $\omega_\alpha$ is the singular value (or the eigenvalue) of the ‘matrix’ $V(i\xi|j\eta)$.

The PWFRG method gives the fixed point values of $P$ and $R$ — those in the thermodynamic limit — through successive improvements. We start from the 4-site system.\textsuperscript{2,3) The initial conditions for the system with open boundary conditions are $P = W$ (that means $\tilde{T} = WWW$), $R(i\alpha|\beta) = \delta^i_\alpha \delta^j_\beta$, $\omega_\alpha = 1/\sqrt{n}$, and $m = n$. We have to set appropriate initial values for $P$ and $\omega_\alpha$ when fixed boundary conditions are imposed. Starting from the initial status, we improve $P$ and $R$ by way of the following self-consistent calculations.

As a first step, we create a trial product wave function by using $R$ and $\omega$: $V(i\xi|j\eta) = \sum_\alpha R(i\xi|\alpha) \omega_\alpha R^T(\alpha|j\eta)$. The vector $V$ is not usually the eigenvector of $\tilde{T} = PWP$ in Eq.2. We then multiply $\tilde{T}$ on $V$ in order to obtain the improved Ritz vector

$$V'(i'\xi'|j'\eta') = \sum_{\xi ij\eta} P(i'\xi'|i\xi)W(i'j'|ij)P(j'\eta'|j\eta)V(i\xi|j\eta)$$

(4)

of the effective transfer matrix $\tilde{T}$, where the inequality $(V', \tilde{T}V')/(V', V') \geq (V, \tilde{T}V)/(V, V)$ is satisfied.

Second, we decompose $V'$ into a matrix product

$$V'(i'\xi'|j'\eta') \rightarrow \sum_\alpha A(i'\xi'|\alpha) \omega_\alpha A^T(\alpha|j'\eta')$$

(5)

via the singular-value decomposition (or the matrix diagonalization), where $A$ is a $nm$ by $m'$ orthogonal matrix. We decide the new dimension $m'$ for
the block-spin variable $\alpha \leq m'$ so that the new singular values $\omega_\alpha$ in Eq.5 are greater than a certain threshold.

The third step is the renormalization of the effective transfer matrix

$$\sum_{jj'} A^T(\xi'|j'\eta') W(i'j'|ij) P(j'\eta'|j\eta) A(j\eta|\xi) \rightarrow P(i'\xi'|i\xi),$$

(6)

and that of the orthogonal matrix $R$

$$\sum_{j\zeta} A^T(\xi|j\zeta) R(j\zeta|\rho) A(i\rho|\eta) \rightarrow R(i\zeta|\eta),$$

(7)

where the graphical representation of these equations are shown in Fig.2. Equation 7 is actually the renormalization of the product wave function, because the new $R$ gives a new product wave function. After the renormalization by Eq.6 and Eq.7, $P$ is a $nm'$-dimensional matrix, and $R$ is a $nm'$ by $m'$ orthogonal matrix. At this point, we return to the first step by setting $m = m'$.

We repeat the iteration shown above until $R$ becomes invariant under the renormalization in Eq.7; this means $A = R$. At the fixed point of the DMRG method, the orthogonal matrix $R$ satisfies the relation $R(i\alpha|\beta) \omega_\beta = \omega_\alpha R^T(\alpha|i\beta)$, where the matrix $R(i\alpha|\beta) \omega_\beta$ is proportional to the square of the corner transfer matrix. After $R$ is converged to its fixed point value, we calculate physical quantities by using the fixed-point value of the product wave function $V$. Östlund and Rommer have shown that the largest eigenvalue of the matrix $t(\alpha\beta|\gamma\eta) \equiv \sum_i R(i\alpha|\gamma) R(i\beta|\eta)$ is equal to unity, and the second one gives the correlation length.
The convergence of $R$ is rather slow when the correlation length is very long. In such a case, we modify Eq.4 to accelerate the convergence. In addition to $V' = \tilde{T}V$ in Eq.4, let us create another vector $V'' = \tilde{T}V'$. It is apparent that a certain linear-combination between $V'$ and $V''$ gives a better Ritz vector. Such an improvement is called ‘modified Lanczos method.'\textsuperscript{12,13} What we have to do is to substitute the best linear combination $V''' = aV' + bV''$ into the l.h.s. of Eq.5, where $a$ and $b$ are adjusted so that $(V''', \tilde{T}V''')/(V''', V''')$ takes its maximum value.

The PWFRG method and the DMRG method gives the same result at their common fixed point. The main difference between them is that the PWFRG method renormalizes the product wave function, while the DMRG method does not. With the use of the wave function renormalization (Eq.7), the PWFRG method avoid the numerical diagonalization of $\tilde{T}$. As a result, the PWFRG method runs much faster than the DMRG method.

As a test case, we apply the PWFRG method to the square lattice Ising model. Figure 3 shows the nearest-neighbor spin correlation function of the Ising model. Numerical error in the data when $m = 40$ is less than $10^{-7}$ outside the region $2.2 \leq T/J \leq 2.3$, where $J$ is the coupling constant. The result agrees with that obtained by the DMRG\textsuperscript{6} and the CTMRG\textsuperscript{9} methods.

Finally, we discuss the way how to apply the PWFRG method to 1D quantum lattice models. The transfer matrix of a 2D classical model is a product of Boltzmann factors, while the Hamiltonian of a 1D quantum lattice model is a sum of local operators. Thus we can apply the PWFRG method to 1D quantum models by replacing the transfer matrix renormalization in Eq.6 by the renormalization of the effective Hamiltonian. Such a
renormalization algorithm for the effective Hamiltonian is already given by
the DMRG method\textsuperscript{2,3)}.

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**Figure Captions**

Fig. 1. Graphical representation of the effective transfer matrix $\tilde{T}$ in Eq.2 and the product wave function $V$ in Eq.3.

Fig. 2. Graphical representation of the renormalization for $P$ and $R$ in Eq.6 and 7, respectively.

Fig. 3. Nearest neighbor spin correlation function of the Ising model.
\[ \langle \sigma_i \sigma_{i+1} \rangle \]

- Fig. 3 -

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