Corner Transfer Matrix
Renormalization Group Method

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Abstract

We propose a new fast numerical renormalization group method, the corner transfer matrix renormalization group (CTMRG) method, which is based on a unified scheme of Baxter’s corner transfer matrix method and White’s density matrix renormalization group method. The key point is that a product of four corner transfer matrices coincides with the density matrix. We formulate the CTMRG method as a renormalization of 2D classical models.

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The renormalization group is one of the basic concepts in physics [1, 2]. Real space representation of the renormalization group — the real space renormalization group — has been applied to various lattice models [3]. Recently, White established a numerical renormalization algorithm, which is referred as ‘density matrix renormalization group (DMRG) method’ [4, 5]. The method has been applied to various one-dimensional (1D) quantum lattice models [5, 6, 7], because it is possible to treat large scale systems with relatively small numerical calculation.

Although DMRG method was originally proposed as a renormalization procedure for 1D quantum systems, the method has an implicit relation with 2D classical models. Östlund and Rommer analyzed the thermodynamic limit of the DMRG method [8], and pointed out that the method is a mapping from 1D quantum lattice models to effective classical lattice models. They show that the orthogonal matrix, which represents the block-spin transformation, plays a role of a transfer matrix of the classical model. What is the classical model, then? Roughly speaking, the model corresponds to a 2D square-lattice model, which is obtained through the Trotter decomposition [9, 10] of the operator \( \exp(-\beta \hat{H}) \) [11]; the row-to-row transfer matrix corresponds to the imaginary time shift operator \( \exp(-\Delta \beta \hat{H}) \); the transfer matrix discussed by Östlund and Rommer is a renormalized column-to-column transfer matrix.

The relation between the DMRG method and 2D classical systems leads a new view point. We find that the density matrix is expressed as a product of Baxter’s corner transfer matrices (CTMs) [12, 13, 14]. Moreover, the DMRG method and Baxter’s variational method on CTM have many aspects in common; both of them is a natural extension of the Kramers-Wannier approximation [15]. From this unified
view point, we present a very fast numerical renormalization procedure for 2D classical systems: the corner transfer matrix renormalization group (CTMRG) method. At first, we briefly review the way to apply the DMRG method to 2D classical systems [16] in order to see the advantage of the CTMRG method. We choose the ‘interaction round a face (IRF) model’ as an example of 2D classical models. We then present the theoretical background and the numerical algorithm of the CTMRG method. The numerical superiority of the CTMRG method is demonstrated by a trial calculation on the Ising model. We finally discuss the way to apply the CTMRG method to 1D quantum systems.

The IRF model includes various 2D lattice models such as the Ising model and the Potts model [14]. The IRF model is defined by the Boltzmann weight $W(a'b'|ab)$ on each face — a square surrounded by four $n$-state spins $a$, $a'$, $b$, and $b'$. The row-to-row transfer matrix of the IRF model is expressed as

$$T(a'b'c'...y'z'|abc...yz) = W(a'b'|ab)W(b'c'|bc)...W(y'z'|yz), \quad (1)$$

where the position of the spin variables are shown in Fig.1. Throughout this paper, we assume that $W$ is isotropic and symmetric — $W(ab|cd) = W(ba|dc) = W(ca|db) = W(dc|ba)$ — in order to simplify the discussion. Generalizations to anisotropic, and/or asymmetric cases are straightforward.

The DMRG method for the IRF model is expressed as a renormalization of the transfer matrix

$$T(a'b'c'...y'z'|abc...yz) \rightarrow P(i'\xi'|i\xi)P(i'\eta'|i\eta) \quad (2)$$

as shown in Fig.1, where $P$ represents a renormalized transfer matrix for the left/right-half 2D lattice. Hereafter, we call $P$ ‘partial transfer matrix’. The greek indices
ξ, ξ', η and η' are m-state block-spin variables, that are shown by open squares. The renormalized transfer matrix for the lattice with two additional columns is

\[ T' = P \cdot W \cdot W \cdot P, \]

where the dot '·' denotes a scalar product. The eigenvalue equation for \( T' \) is

\[
\sum_{\xiijk\eta} P(i'\xi'|i) W(i'j'|ij) W(j'k'|jk) P(k'\eta'|k\eta) V(\xiijk\eta) = \lambda V(\xi'i'j'k'\eta'),
\]

where \( \lambda \) is the non-degenerate largest eigenvalue of \( T' \), and \( V \) is the corresponding eigenvector. What is called ‘density matrix’ \( \rho \) is defined by a product

\[
\rho(\xi'\xi) = \sum_{jk\eta} V(\xi'\xi'j\eta) V(\xi\eta) \rho(\xi'\xi),
\]

where we have used the fact that \( V \) is real. The DMRG method is a systematic procedure to obtain \( P \) by using the information of \( \rho \).

At this stage, we explain our physical view of the density matrix. Since \( \lambda \) in Eq.3 is the largest eigenvalue, \( V \) is given by the large \( L \) limit of \((T')^L X\), where \( X \) is a vector that is not orthogonal to \( V \). Therefore, the vector \( V(\xiijk\eta) \) represent the Boltzmann weight for the lower (or the upper) half 2D lattice with the spin configuration \{\( \xiijk\eta \)\} on the horizontal boundary. Equation 4 indicates that \( \rho \) is created by partially joining the two halves of the 2D lattice, as shown in Fig.2; The density matrix \( \rho \) represents the entire system with a cut.

The physical background of the density matrix enables us to skip the eigenvalue problem (Eq.3). What is really necessary in order to obtain \( \rho \) is not the eigenvector of \( T' \), but is the Boltzmann weight that stands for the upper/lower half lattice. How can we get \( \rho \), then? We employ Baxter’s corner transfer matrix (CTM) for this purpose. He expresses the half-infinite lattice as a product of CTMs

\[
V(\xiijk\eta) \approx \sum_{l\beta} A'(j\keta|jl\beta) A'(jl\beta|ji\xi),
\]

where
where \( A'(i'j'\alpha'|ij\alpha) \) is the CTM that represents the Boltzmann weight for a quadrant (or corner) of the 2D lattice. (See Fig.3.) The element \( A'(i'j'\alpha'|ij\alpha) \) is zero when \( i' \neq i \). The notation ‘\( \approx \)’ denotes that the r.h.s. of Eq.5 is not the same as the eigenvector in Eq.3, but is approximately exact. We further decompose \( V \) into a fine product form, \( V \approx (P \cdot W \cdot W \cdot P)(A \cdot P \cdot P \cdot A) \), as shown in Fig.3. The relation between \( A \) and \( A' \) is

\[
A'(jk\eta|jl\beta) = \sum_{m\mu\alpha} W(jk|lm)P(k\eta|m\mu)P(l\beta|ma)A(m\alpha|m\mu),
\]

where we have used the symmetry of the Boltzmann weight \( W \). The factor \( W \cdot P \cdot P \) in Eq.6 is a kind of transfer matrix that acts on \( A \), and increases the size of the corner. Substituting Eq.5 into Eq.4, we get a new expression of \( \rho \)

\[
\rho(\xi'\iota'|\xi\iota) \approx \sum_{jk\iota\eta\iota'} A(ji'\iota'|jk\iota)A(jk\iota|jl\iota)A(jl\iota|jm\iota)A(jm\iota|ji\iota).
\]

The density matrix is a product of four CTMs. The relation between \( \rho \) and \( A \) in Eq.7 unifies Baxter’s CTM method and White’s DMRG method.

Now we explain the key point of our new numerical method, which is a self-consistent relation between \( A \) and \( A' \). The relation consists of the mapping from \( A \) to \( A' \) (Eq.6) and the renormalization from \( A' \) to \( A \)

\[
\sum_{jj'\eta'\eta} O^T(\xi'|j'\eta')A'(i'j'\eta'|ij\eta)O(j\eta|\xi) \rightarrow A(i'\xi'|i\xi)
\]

together with the renormalization of \( P \)

\[
\sum_{jj'\eta'\eta} O^T(\xi'|j'\eta')W(i'j'|ij)P(j'\eta'|j\eta)O(j\eta|\xi) \rightarrow P(i'\xi'|i\xi).
\]

The orthogonal matrix \( O \) represents the block spin transformation, and is obtained from the diagonalization of \( \rho \) [18]

\[
\sum_{ii'\iota\iota'} O^T(\eta|i'\iota')\rho(i'\iota'|i\iota)O(i\iota'|\iota) = \delta_{\eta\iota}\omega_{\eta},
\]
where $O^T$ is the matrix transpose of $O$, and $\omega_m$ is the $m$-numbers of eigenvalues of $\rho$ from the largest $[4, 5]$. The self-consistent relation for CTM (Eq.6-10) has the same solution as Baxter’s CTM method [12, 13, 14]. We solve the self-consistent relation by way of the following numerical procedure: (I) Set appropriate initial values for $P$ and $A$ according to the boundary conditions: (II) Obtain $A'$ by using Eq.6; (III) Create $\rho$ by Eq.7; (IV) Diagonalize $\rho$ and obtain $O$ (Eq.10); (V) Renormalize $P$ and $A$ according to Eq.8 and Eq.9; (VI) Repeat (II)-(V) until $A$ and $P$ reach their fixed point. We call the method ‘corner transfer matrix renormalization group (CTMRG) method’, since the renormalization is done for CTM. After we obtain $P$ and $A$ at the fixed point, we calculate spin correlation functions. For example, two-point spin correlation functions along a row (or column) is obtained from several large eigenvalues of $P \cdot P$ in the r.h.s. of Eq.2. It is also possible to calculate correlation functions by using the fixed point value of $O$ in Eq.10 [8].

We apply the CTMRG method to square lattice Ising model, which is a special case of the IRF model. Figure 4 shows the calculated local energy $E(T)$ — the nearest-neighbor spin correlation function — when $m = 98$. The data shown by the black dots are obtained after $10 \sim 1000$ iterations, where the data deviate from the exact ones [13] at most $10^{-7}$. The numerical precision can be improved by additional iterations. At the critical temperature, we estimate $E(T_c)$ by observing its convergence with respect to $N$, which is the number of iteration. (See inset of Fig.4.) A simple $1/N$ fitting gives $E(T_c) = 0.70704$, which is close to the exact one $1/\sqrt{2} = 0.70711$. It should be noted that the CTMRG method is much faster than the DMRG method. The CTMRG method requires 8.7sec to obtain $E(T)$ at $T = 2.2$ by the NEC SX-3 super computer, while the DMRG method consumes 149.8sec to deduce the data of the comparable numerical precision [16]. The CTMRG method
runs faster because it crates $\rho$ by using Eq.7, which consists of a few $n^2m$-dimensional matrix multiplication. On the contrary, the DMRG method requires the solution of the $n^2m^2$-dimensional eigenvalue problem.

We have presented the CTMRG method as a fast numerical renormalization group method for 2D classical models. We finally discuss a way to apply the CTMRG method to 1D quantum lattice models. A natural extension is given through a mapping from 1D quantum models to 2D classical ones via the Trotter formula [9, 10]. The corresponding 2D model is a checkerboard type one, which is an anisotropic IRF model. Therefore, it is possible to apply the CTMRG method to the 1D quantum models that have been analyzed by QMC simulations. It should be noted that the CTMRG method is free from the sign problem that occasionally makes the QMC simulation difficult. In principle, correlation functions for both space and imaginary time directions can be calculated, since the formulation of the CTMRG method is symmetric for both space and imaginary time directions. We have obtain another extension of the CTMRG method for 1D quantum systems. This one does not require the Trotter formula, and is written in a renomalization group on wave functions. The detail will be discussed elsewhere [20].

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Figure 1: The row-to-row transfer matrix $T$ of the IRF model is a product of the Boltzmann weights on each face. The DMRG method maps $T$ into a product form in Eq.2.

Figure 2: The density matrix $\rho$ as a product of $V$. We regard $\rho$ as a Boltzmann weight for the entire 2D lattice with a cut.

Figure 3: The Boltzmann weight for the half-infinite lattice is constructed as a product of corner transfer matrices. The further decomposition in Eq.6 is also shown.

Figure 4: Local energy $E(T)$ of the Ising model. We determine $E(T_c)$ by observing the convergence with respect to $N$, the number of iterations of the CTMRG procedure.
$$\rho = \text{System}$$
\[ \eta \quad \xi \quad j \quad k \quad A' \quad = \quad \eta \quad j \quad i \quad A' \quad = \quad \eta \quad k \quad l \quad \beta \quad = \quad \eta \quad k \quad W \quad P \quad A \quad = \quad \eta \quad i \quad P \quad W \quad P \quad A \quad = \quad \eta \quad i \quad \mu \quad \alpha \quad \beta \]
