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Corner Transfer Matrix Renormalization Group Method

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We propose a new fast numerical renormalization group method — the corner transfer matrix renormalization group (CTMRG) method — which is based on a unified scheme involving 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 CTMRG as a renormalization group for 2D classical models.

KEYWORDS: density matrix, corner transfer matrix, renormalization group

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 (RSRG) — has been applied to various lattice models.[3,4] Recently, White established a numerical renormalization algorithm, which is referred to as the 'density matrix renormalization group (DMRG)'.[5,6] The method has been applied to various one-dimensional (1D) quantum lattice models,[6-12] because it is possible to treat large-scale systems by means of relatively small-scale numerical calculation. Quite recently Martín-Delgado and Sierra have obtained a unified analytic formulation including conventional RSRG and DMRG.[13,14]

Although DMRG was originally proposed as a renormalization group for 1D quantum systems, it has an implicit relationship with 2D classical models. Östlund and Rommer analyzed the thermodynamic limit of DMRG,[15] and pointed out that the method is a mapping from 1D quantum lattice models to effective classical lattice models; the ground state wave function obtained using DMRG can be expressed as a product of tensors.[16-19] What is the classical model, then? Roughly speaking, it corresponds to a 2D square-lattice model, which is obtained through the Trotter decomposition[20,21] of the statistical operator $\exp(-\beta\hat{H})$; 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, which is a product of two vertex operators.[22]

The relationship between DMRG and 2D classical systems leads to a new viewpoint. *We find that the density matrix can be expressed as a product of Baxter's corner transfer matrices* (CTMs).[23-25] Moreover, the DMRG method and Baxter's variational method for CTM have many aspects in common. Both of them are natural extensions of the Kramers-Wannier approximation[26] and Kikuchi's approximation.[27] From this unified viewpoint, we present a very fast numerical renormalization procedure for 2D classical systems: the corner transfer matrix renormalization group (CTMRG). First, we briefly review the method for applying DMRG to 2D classical systems[28] in order to see the advantage of the CTMRG. We choose the 'interaction round a face (IRF) model' [25] as an example of 2D classical models. We then present the theoretical background and the numerical algorithm of the CTMRG. The numerical superiority of CTMRG is demonstrated by a trial calculation for the Ising model. We finally discuss how to apply CTMRG to 1D quantum systems.

The IRF model includes various 2D lattice models such as the Ising model and the Potts model. 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

$$T_{a'b'c'\ldots y'z',abc\ldots yz} = W_{a'b',ab}W_{b'c',bc}\ldots W_{y'z',yz}, \quad (1)$$

where the positions 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 for the IRF model is expressed as a renormalization of the transfer matrix

$$T_{a'b'c'\ldots y'z',abc\ldots yz} \to P_{i'\xi',i\xi}P_{i'\eta',i\eta} \quad (2)$$

as shown in Fig. 1, where P represents a renormalized transfer matrix for the left/right-half 2D lattice; P is closely related to the so-called 'vertex operator'.[22] The Greek indices ξ, ξ', η and η' are m-state block-spin variables, which 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 '$\cdot$' denotes a scalar product. The eigenvalue equation for T' is

$$\sum_{\xi ijk\eta} P_{i'\xi',i\xi}W_{i'j',ij}W_{j'k',jk}P_{k'\eta',k\eta}V_{\xi ijk\eta} = \lambda V_{\xi'i'j'k'\eta'}, \quad (3)$$

where λ is the largest nondegenerate eigenvalue of T', and $\boldsymbol{V}$ is the corresponding eigenvector. (See Fig. 2.)

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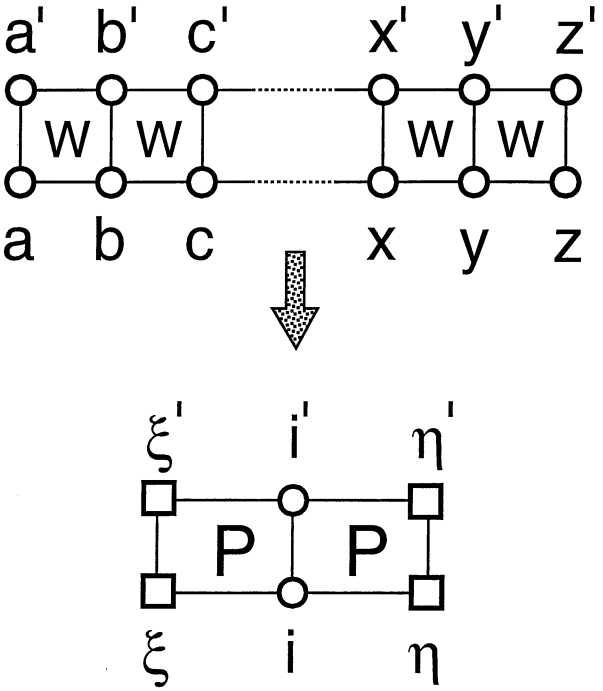

Fig. 1. The row-to-row transfer matrix T of the IRF model is a product of the Boltzmann weights on each face. The DMRG maps T into a product form in eq. (2).

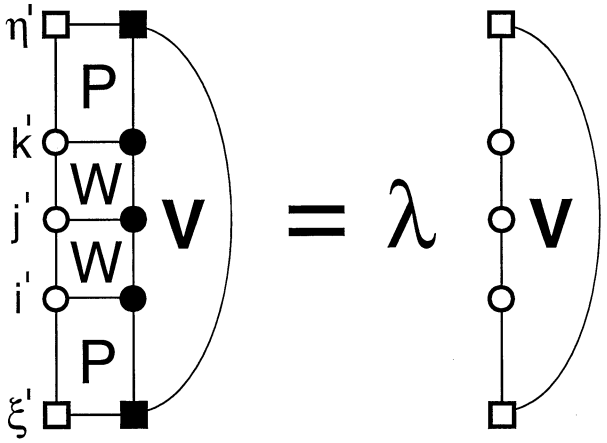

Fig. 2. Graphical representation of eq. (3). Filled symbols represent spin variables that are summed.

The so-called 'density matrix' ρ in DMRG is defined by a product

$$\rho_{\xi' i', \xi i} = \sum_{jk\eta} V'_{\xi' i' jk\eta} V_{\xi ijk\eta}, \tag{4}$$

where $\boldsymbol{V}'$ is the dual basis of $\boldsymbol{V}$;[29] $\boldsymbol{V}' = \boldsymbol{V}$ holds for the symmetric IRF model. The DMRG method is a systematic procedure for improving P by using the relevant information of ρ.

Here, we explain our physical view of the density matrix. Since λ in eq. (3) is the largest eigenvalue, $\boldsymbol{V}$ is given by the large L limit of $(T')^L \boldsymbol{X} / \|(T')^L \boldsymbol{X}\|$, where $\boldsymbol{X}$ is a vector that is not orthogonal to $\boldsymbol{V}$. Therefore, the vector element $V_{\xi ijk\eta}$ represents the Boltzmann weight for the lower (or the upper) half 2D lattice with the spin configuration $\{\xi ijk\eta\}$ on the horizontal boundary.

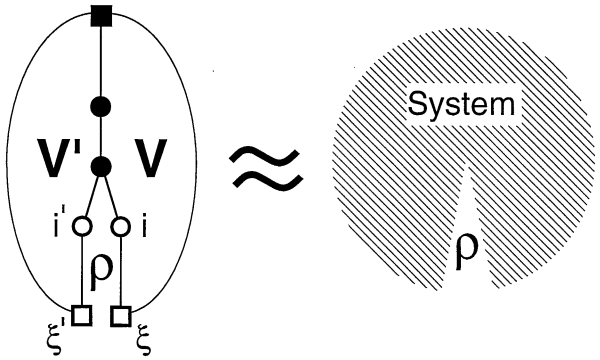

Fig. 3. The density matrix ρ as a product of $\boldsymbol{V}$. We regard ρ as a Boltzmann weight for the entire 2D lattice with a cut.

Equation (4) indicates that ρ is created by partially joining the two halves of the 2D lattice, as shown in Fig. 3; hence ρ represents the entire system with a cut. Alternatively, it is clear that a contraction of the matrix $\lim_{L\to\infty}(T')^L/\mathrm{Tr}\,(T')^L$ coincides with the r.h.s. of eq. (4), provided that the largest eigenvalue of T' is unique.

The physical background of the density matrix enables us to skip solving the eigenvalue problem eq. (3). *What is really necessary in order to obtain ρ is not the eigenvector of T', but the Boltzmann weight that represents the upper/lower half lattice.* Therefore we employ Baxter's corner transfer matrix (CTM)[23-25] in order to obtain ρ. He expresses the half-infinite lattice as a product of CTMs

$$V_{\xi ijk\eta} \approx \sum_{l\beta} A'_{jk\eta,jl\beta} A'_{jl\beta,ji\xi}, \tag{5}$$

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. 4.) The element $A'_{i'j'\alpha',ij\alpha}$ is zero when $i' \neq i$. The notation '$\approx$' indicates that the r.h.s. of eq. (5) is not the same as the eigenvector $\boldsymbol{V}$ in eq. (3), but is an approximation of $\boldsymbol{V}$. We further decompose the r.h.s. of eq. (5) into a fine product form, $\boldsymbol{V} \approx (P{\cdot}W{\cdot}W{\cdot}P)(A{\cdot}P{\cdot}P{\cdot}A)$, as shown in Fig. 4, where A is also a CTM. The relation between A and A' is

$$A'_{jk\eta,jl\beta} = \sum_{m\mu\alpha} W_{jk,lm} P_{k\eta,m\mu} P_{l\beta,m\alpha} A_{m\alpha,m\mu}, \tag{6}$$

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 linear size of the corner by one. Substituting eq. (5) into eq. (4), we get a new expression for ρ

$$\rho_{\xi' i', \xi i} \approx \sum_{jklm\alpha\beta\gamma} A'_{ji'\xi',jk\alpha} A'_{jk\alpha,jl\beta} A'_{jl\beta,jm\gamma} A'_{jm\gamma,ji\xi}. \tag{7}$$

In this way we express ρ as a product of CTMs. Now the difference between DMRG and our method is apparent: the DMRG treats an infinitely long 2D lattice with width N, i.e. a stripe, while we treat an N by N square cluster. Note that the thermodynamic limits $N \to \infty$ of both formulae are the same.

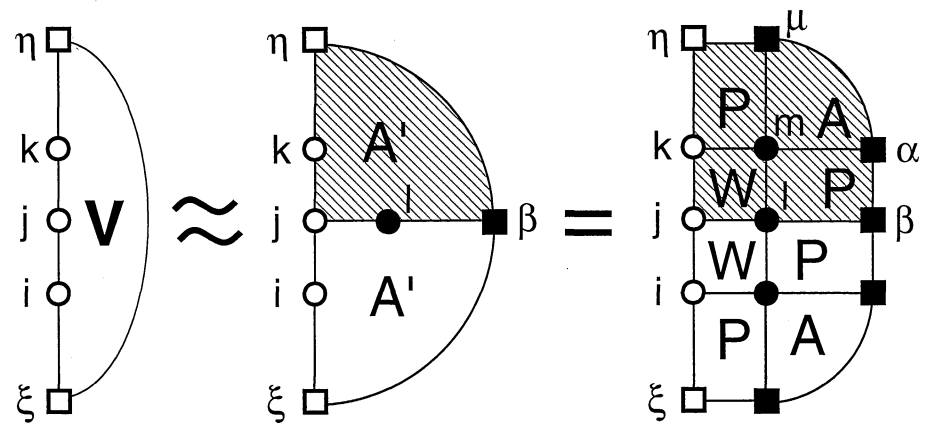

Fig. 4. The Boltzmann weight for the half-infinite lattice is constructed as a product of corner transfer matrices. The further decomposition in eq. (6) is also shown.

We explain the key point of our new numerical method: 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

$$\sum_{jj'\eta\eta'} O^T_{\xi',j'\eta'} A'_{i'j'\eta',ij\eta} O_{j\eta,\xi} \to A_{i'\xi',i\xi} \tag{8}$$

together with the renormalization of P

$$\sum_{jj'\eta\eta'} O^T_{\xi',j'\eta'} W_{i'j',ij} P_{j'\eta',j\eta} O_{j\eta,\xi} \to P_{i'\xi',i\xi}. \tag{9}$$

The orthogonal matrix O represents the block spin transformation, and is obtained from the diagonalization of ρ

$$\sum_{ii'\xi\xi'} O^T_{\eta,i'\xi'} \rho_{i'\xi',i\xi} O_{i\xi,\zeta} = \delta^\zeta_\eta \omega_\eta, \tag{10}$$

where O^T is the matrix transpose of O, and ω_η are the m-numbers of dominant eigenvalues of ρ.[5,6] (For the asymmetric IRF model, one has to perform the singular value decomposition[29] of ρ to obtain O and its dual-orthogonal matrix.) The self-consistent relation for CTM (eqs. (6)–(10)) has the same solution as that in Baxter's CTM method.[23-25]

We solve the self-consistent relation using the following iterative procedures. (I) Set appropriate initial values for P and A according to the boundary conditions. (II) Obtain A' using eq. (6). (III) Construct ρ using eq. (7). (IV) Diagonalize ρ and obtain O as in eq. (10). (V) Renormalize P and A according to eqs. (8) and (9). (VI) Repeat (II)–(V) until A and P reach their fixed points. We call the method the 'corner transfer matrix renormalization group (CTMRG)', since the renormalization is done for CTM. After we obtain P and A at the fixed point, we calculate thermodynamic functions. For example, two-point spin correlation functions along a row (or column) are 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 using the fixed point value of O in eq. (10).[15]

Every time we repeat the procedures (I)–(V) shown above, the size of the corner increases by one. The situation is similar to the 'infinite chain method' of DMRG, and therefore we can apply these procedures only for infinitely large translationally invariant systems. For finite and/or random systems, we have to modify our algorithm by introducing the concept of the 'finite chain method' of DMRG.

We apply CTMRG to the square lattice Ising model, which is a especial case of the IRF model. Figure 5 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 10–1000 iterations, and deviate from the exact ones[30] by 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 — the number of iterations. (See inset of Fig. 5.) A simple $1/N$ fitting gives $E(T_c) = 0.70704$, which is close to the exact value $1/\sqrt{2} = 0.70711$. The $1/N$ dependence of the finite-size correction is related to scale invariance of the critical system;[31,32] the details of the applications of CTMRG at criticality will be discussed elsewhere.[33] It should be noted that the computation of CTMRG is

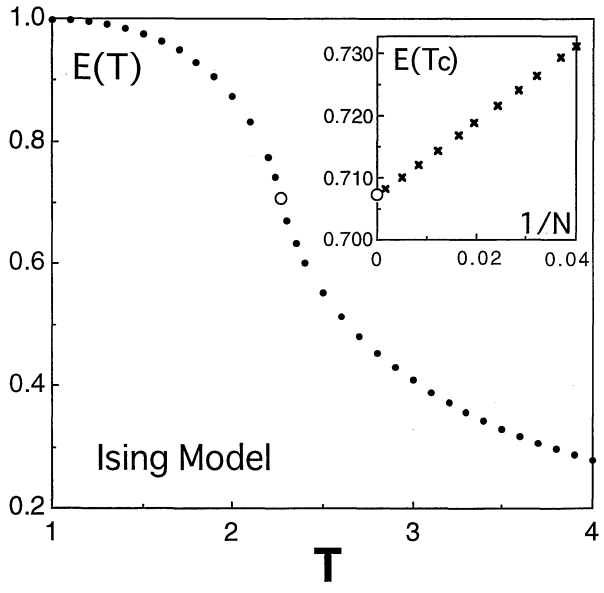

Fig. 5. Local energy $E(T)$ of the Ising model. We determine $E(T_c)$ by observing the convergence with respect to N, which is the number of iterations of the CTMRG procedure.

much faster than that of DMRG; the CTMRG requires 8.7 seconds to obtain $E(T)$ at $T = 2.2$ using the NEC SX-3/14R supercomputer, while the DMRG consumes 149.8s to yield data with comparable numerical precision.[28] The CTMRG runs faster because it creates ρ using eq. (7), which involves a few n^2m-dimensional matrix multiplications. In contrast, the DMRG requires the solution of the n^2m^2-dimensional eigenvalue problem.

We have presented CTMRG as a fast numerical renormalization group method for 2D classical models. We finally discuss two different ways of applying the CTMRG 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.[20,21] The corresponding 2D model is a checkerboard type, which is a kind of anisotropic IRF model. Therefore, it is possible to apply the CTMRG to the 1D quantum models that have been analyzed by quantum Monte Carlo (QMC) simulations. It should be noted that DMRG and CTMRG are free from the sign problem that occasionally makes QMC simulations difficult. In principle, correlation functions for both space and imaginary time directions can be calculated, since the formulation of the CTMRG is symmetric for both space and imaginary time directions. Another extension is the 'product wave function renormalization group', which we have obtained quite recently.[34] This does not require the Trotter formula, and is written in terms of a renormalization group for matrix product wave functions.[16-18]

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