fontA Density Matrix Renormalization Group Method for 2D Classical Models

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The density matrix renormalization group (DMRG) method is applied to the interaction round a face (IRF) model. When the transfer matrix is asymmetric, singular-value decomposition of the density matrix is required. A trial numerical calculation is performed on the square lattice Ising model, which is a special case of the IRF model.

KEYWORDS:

The renormalization group is one of the basic concepts in statistical mechanics.[1,2] Its real-space expression — the real-space renormalization group[3] — has been applied to various statistical models. Recently White proposed a precise numerical renormalization algorithm, which is known as the density matrix renormalization group (DMRG) method.[4,5] This method has been widely used for one-dimensional (1D) quantum lattice models[5–7] because of its numerical accuracy and portability.

The DMRG method was originally designed for 1D quantum lattice models. Since d-dimensional quantum systems are closely related to classical systems in d+1 dimensions,[8] the DMRG method is applicable to two-dimensional (2D) classical systems. In this paper we apply the DMRG method to the interaction round a face (IRF) model,[9] which contains various 2D statistical models such as the Ising model and the vertex models.

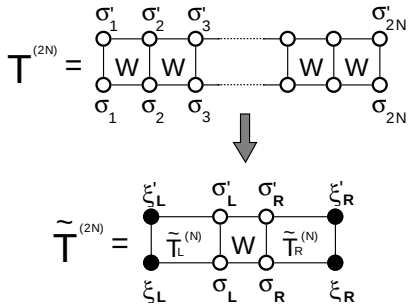

Fig. 1. Renormalization processes. We assume that the transfer matrix $T^{(2N)}$ can be renormalized as the product form $\tilde{T}^{(2N)}$ in eq.(2).

The IRF model is defined by a Boltzmann weight W on each face, which is surrounded by four n-state spins σ. The transfer matrix of the IRF model is given by

$$T^{(2N)}(\sigma'_1 \ldots \sigma'_{2N}|\sigma_1 \ldots \sigma_{2N}) = \prod_{i=1}^{2N-1} W(\sigma'_i\sigma'_{i+1}|\sigma_i\sigma_{i+1}), \quad (1)$$

where σ_i and $\sigma_i^{'}$ are n-state spins on adjacent rows with width $2N$. (Fig.1) We assume open boundary conditions. In general, the transfer matrix is not symmetric. If the Boltzmann weights satisfy a constraint — the Yang-Baxter relation[9,10] — the model is analytically solvable. Here, we consider a numerical analysis of $T^{(2N)}$ in view of the existence of unsolvable cases.

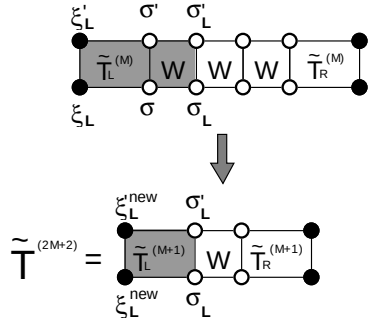

Fig. 2. The assumption in Eq.(2) is justified through the relation between $\tilde{T}_L^{(M)}$ and $\tilde{T}_L^{(M+1)}$ in eq.(7).

The DMRG method for the IRF model is expressed as a renormalization of the transfer matrix $T^{(2N)}$. Figures 1 and 2 show the method of renormalization. First of all, we assume that $T^{(2N)}$ can be renormalized into a product form

$$\tilde{T}^{(2N)}(\xi'_L\sigma'_L\sigma'_R\xi'_R|\xi_L\sigma_L\sigma_R\xi_R) = \tilde{T}_L^{(N)}(\xi'_L\sigma'_L|\xi_L\sigma_L)W(\sigma'_L\sigma'_R|\sigma_L\sigma_R)\tilde{T}_R^{(N)}(\sigma'_R\xi'_R|\sigma_R\xi_R), \quad (2)$$

where $\tilde{T}_L^{(N)}$ and $\tilde{T}_R^{(N)}$ represent renormalized transfer matrices for the left and the right half of the system,

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respectively. (Fig.2) The block-spin variables ξ_L and ξ_R correspond to groups of the n-state spins $\{\sigma_1 \dots \sigma_{N-1}\}$ and $\{\sigma_{N+1} \dots \sigma_{2N}\}$, respectively. We assume that ξ_L and ξ_R take m different states, where m is much smaller than n^{N-1}. If there is a mapping from $\tilde{T}^{(2M)}$ to $\tilde{T}^{(2M+2)}$ for arbitrary M, then $\tilde{T}^{(2N)}$ in eq.(2) is obtained through successive mapping:

$$T^{(4)} = \tilde{T}^{(4)} \to \tilde{T}^{(6)} \dots \tilde{T}^{(2N-2)} \to \tilde{T}^{(2N)}. \tag{3}$$

In each step, block-spin transformations $\{\xi_L \sigma_L\} \to \xi_L^{\rm new}$ and $\{\sigma_R \xi_R\} \to \xi_R^{\rm new}$ are required. (Fig.2) The block-spin transformations are given in the following. Since the argument is common to both ξ_L and ξ_R, we discuss the renormalization for ξ_L only.

The matrix dimension of $\tilde{T}^{(2M)}$ is $(nm)^2$ for arbitrary M. If m is small enough, we can numerically solve the eigenvalue problem

$$\sum_{\xi_L \sigma_L \sigma_R \xi_R} \tilde{T}^{(2M)}(\xi'_L \sigma'_L \sigma'_R \xi'_R | \xi_L \sigma_L \sigma_R \xi_R) \Psi(\xi_L \sigma_L \sigma_R \xi_R) = \tilde{\lambda}^{(2M)} \Psi(\xi'_L \sigma'_L \sigma'_R \xi'_R), \tag{4}$$

and obtain the 'right' eigenvector Ψ that corresponds to the largest eigenvalue $\tilde{\lambda}^{(2M)}$. In the same way, we obtain the 'left' eigenvector Φ that satisfies $\Phi \tilde{T}^{(2M)} = \Phi \tilde{\lambda}^{(2M)}$. Note that if $\tilde{T}^{(2M)}$ is asymmetric, Φ is not the complex conjugate of Ψ. The density matrix[4,5] is then expressed as a partial product between Ψ and Φ:

$$\rho_L(\xi'_L \sigma'_L | \xi_L \sigma_L) = \sum_{\sigma''_R \xi''_R} \Phi(\xi'_L \sigma'_L \sigma''_R \xi''_R) \Psi(\xi_L \sigma_L \sigma''_R \xi''_R). \tag{5}$$

Apart from the density matrix for 1D quantum systems, ρ_L is not always Hermitian. Therefore we must perform the singular-value decomposition of ρ_L

$$\sum_{\xi'_L \sigma'_L \xi_L \sigma_L} O(i | \xi'_L \sigma'_L) \rho_L(\xi'_L \sigma'_L | \xi_L \sigma_L) Q(\xi_L \sigma_L | j) = \delta_{ij} \omega_j, \tag{6}$$

and obtain O and Q that satisfy $\sum_{\xi_L \sigma_L} O(i|\xi_L \sigma_L) Q(\xi_L \sigma_L | j) = \delta_{ij}$. We assume the decreasing order of the singular values: $\omega_1 \geq \omega_2 \geq \dots \omega_{nm}$. The m by nm matrix $O(\xi_L^{\rm new} | \xi_L \sigma_L)$ together with the the nm by m one $Q(\xi_L \sigma_L | \xi_L^{\rm new})$ represent the block-spin transformation from $\xi_L \sigma_L$ to a new m-state block-spin $\xi_L^{\rm new}$. The transformation naturally gives a relation between $\tilde{T}_L^{(M)}$ and $\tilde{T}_L^{(M+1)}$, which is a linear transformation

$$\tilde{T}_L^{(M+1)}(\xi'^{\rm new}_L \sigma'_L | \xi_L^{\rm new} \sigma_L) = \sum_{\xi'_L \sigma' \xi_L \sigma} O(\xi'^{\rm new}_L | \xi'_L \sigma') \tilde{T}_L^{(M)}(\xi'_L \sigma' | \xi_L \sigma) W(\sigma' \sigma'_L | \sigma \sigma_L) Q(\xi_L \sigma | \xi_L^{\rm new}). \tag{7}$$

We also obtain a similar relation between $\tilde{T}_R^{(M)}$ and $\tilde{T}_R^{(M+1)}$ in the same way. Now we obtain the renormalization processes in eq.(3).

As one repeats the mapping in eq.(3) with the aid of eqs.(4)-(7), the eigenvectors of the renormalized transfer matrix $\tilde{T}^{(2M)}$ approach their fixed-point values. After Φ and Ψ have converged, we can obtain local thermodynamic quantities in the large-N limit. For example, the nearest-neighbor spin correlation is expressed as

$$\langle \sigma_i \sigma_{i+1} \rangle \sim \langle \sigma_L \sigma_R \rangle = \sum_{\xi_L \sigma_L \sigma_R \xi_R} \Phi(\xi_L \sigma_L \sigma_R \xi_R) \sigma_L \sigma_R \Psi(\xi_L \sigma_L \sigma_R \xi_R) \tag{8}$$

when the inner product (Φ, Ψ) is unity. In the same way, we can obtain the internal energy, susceptibilities, and specific heat. Observations of correlation functions and surface tensions are possible with the use of the 'finite chain algorithm' of the DMRG method.[5]

We examine efficiency of the DMRG method. As a reference, we calculate specific heat of the nearest-neighbor Ising model, where the Boltzmann weight is

$$W(\sigma'_i \sigma'_{i+1} | \sigma_i \sigma_{i+1}) = \exp\left\{ \frac{K}{2} (\sigma'_i \sigma'_{i+1} + \sigma'_i \sigma_i + \sigma'_{i+1} \sigma_{i+1} + \sigma_i \sigma_{i+1}) \right\} \tag{9}$$

for $\sigma = \pm 1$. In this case, the renormalized transfer matrix $\tilde{T}^{(2N)}$ is real-symmetric for arbitrary N, and therefore the eigenvectors Φ and Ψ in eq.(5) are the same. The specific heat C_v is obtained from a numerical differential of the nearest-neighbor spin correlation $\langle \sigma_i \sigma_{i+1} \rangle$ in eq.(8). The numerical error ϵ in C_v is obtained through a comparison between calculated data and the exact value.[11]

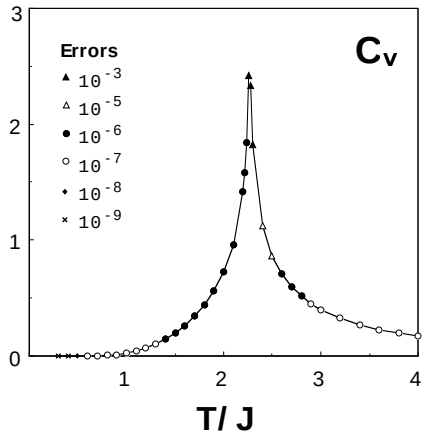

Fig. 3. Numerically calculated specific heat of the Ising model. The plotted data are obtained within 1024 iterations ($2N = 2048$) under the condition $m = 60$. The numerical error ϵ in each data point is indicated by the symbols.

Figure 3 shows the calculated specific heat. The plotted data are obtained within 1024 iterations ($2N = 2048$) when $m = 60$. The numerical error ϵ in C_v is non-negligible near T_c, partly because the numerical convergence of the bond energy $\langle \sigma_i \sigma_{i+1} \rangle$ with respect to N and m becomes worse as the parameter $K = J/k_B T$ approaches its critical value $K^* = J/k_B T_c$. The calculated energy per site at $T = T_c$ is -1.41398 when $m = 60$, which is comparable in accuracy to a recent numerical estimate[12] $-1.419(1)$ by a microcanonical Monte Carlo simulation; the exact value[11] is $-\sqrt{2} = -1.414213$. An-

other source of error is in the numerical differential of $\langle\sigma_i\sigma_{i+1}\rangle$ with respect to T. Since the derivative diverges at T_c, a slight error in $\langle\sigma_i\sigma_{i+1}\rangle$ reduces the accuracy in C_v near T_c.

The numerical result shows that the DMRG method is quite efficient in the off-critical — high- and low-temperature — regions. On the other hand, it is difficult to maintain good numerical accuracy near the critical point, because long-range spin correlations prevent us from obtaining good renormalized transfer matrix, whose size ($= 2m$) is limited by computational restrictions. This convergence property of the DMRG method for the Ising model is in accordance with the fact that the DMRG method works more efficiently for 1D quantum systems with a finite excitation gap.[5)]

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