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Density Matrix Renormalization Group
— Introduction from a variational point of view —

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The density matrix renormalization group theory is reviewed as a numerical variational method. The variational state, expressed as a product of local tensors, is improved through locally tuning each tensor. The first section is a tutorial with simplified discussions. Details are discussed in the subsequent sections. The review concludes with some recent developments and future directions

1. Tutorial

Density matrix renormalization group (DMRG) introduced by White in 1992 is a major progress in computational condensed-matter physics.[1] DMRG enables us to calculate ground states of relatively large scale one-dimensional (1D) quantum systems. DMRG has been applied to various topics in condensed matter physics,[2,3] such as Haldane systems,[4,5] spin ladders,[6] highly correlated electron systems,[7] and superconducting materials.[8] Two dimensional (2D) finite size systems have also been investigated,[9] with the aid of the zig-zag — snake like — decomposition of 2D clusters.[10,11]

Although the DMRG was originally developed for 1D quantum systems, it is also applicable to 2D classical systems. This is because the path integral representation of 1D quantum systems correspond to 2D classical systems.[12] For example, in quantum Monte Carlo simulations, they map a 1D quantum system at a finite temperature to a 2D classical system via the Trotter decomposition.[13,14] The applications of DMRG to 2D classical systems began with a trial calculation of the Ising model,[15] where the *infinite system algorithm* (§7) was employed. The DMRG thus applied to classical systems is often called the '*transfer matrix DMRG* (TMRG),' since the block-spin transformations are applied to transfer matrices. Recently, Car-

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lon *et al.* applied the *finite system algorithm* (§6) to the Potts models,[16,17,18] where their numerical results were precise enough to detect tiny corrections to the finite size scaling behavior.[19,20] Their results prove the power of DMRG when the method is applied to critical phenomena. More recently, the transfer matrix DMRG was applied to 1D quantum systems at finite temperatures,[21,22,23,24] where RG transformations are applied to the quantum transfer matrix.[25]

The purpose of this review is to answer the questions: 'What's DMRG?' and 'Why is DMRG so accurate?' Brief answers are, 'DMRG is a numerical variational method, whose trial state is a product of tensors,' and 'It maximizes the free energy efficiently using finite number of freedom.' The characteristic numerical properties of DMRG is (a) *small in computational memory size,* (b) *quick in numerical improvement for the variational state,* and (c) *accurate.* We explain the details of these points through a simple application to the Ising model. The principal aim of DMRG is to obtain the largest eigenvalue of the transfer matrix T,[26] through a numerical evaluation of the Rayleigh ratio

$$\lambda = \frac{\boldsymbol{v}^T\, T\, \boldsymbol{v}}{\boldsymbol{v}^T\, \boldsymbol{v}} = \frac{\langle v|T|v\rangle}{\langle v|v\rangle}\,, \tag{1}$$

where $\boldsymbol{v}$ is a variational state, and $\boldsymbol{v}^T$ is the conjugate ($\sim$ transpose) of $\boldsymbol{v}$. What we have to do is to find out the best variational state that maximizes λ, which is the approximate partition function per row (= unit transfer). From the numerical point of view, the variational state $\boldsymbol{v}$ should satisfy the following properties.

(a) The computations needed for both $\langle v|T|v\rangle = \boldsymbol{v}^T\, T\, \boldsymbol{v}$ and $\langle v|v\rangle = \boldsymbol{v}^T\, \boldsymbol{v}$ are *small sized* in numerical sense — the calculation does not require huge memory.

(b) Improvements of $\boldsymbol{v}$ can be done locally. Since a local improvement involves a small number of freedom, it can be done *quickly.* It is not hard to imagine that a global change in $\boldsymbol{v}$ is much more time consuming.[28] For this reason, $\boldsymbol{v}$ must be local in a certain sense.

(c) The variational state $\boldsymbol{v}$ is *accurate* enough to approximate the true eigenvector of T. This requirement tends to contradict (a) and (b).

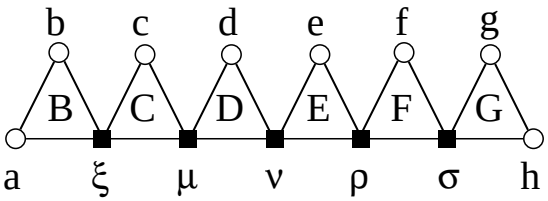

Fig. 1. Graphical representation of the variational state $\mathbf{v}$ in Eq. (2). We use the black marks for the variables that are summed up in the corresponding equation.

The secret of DMRG, that enables (a), (b), and (c) at the same time, is to write down the variational state $\boldsymbol{v}$ as a product of small-dimensional tensors. Let us see

a simple example. Consider a transfer matrix of the square lattice Ising model, whose width is $N = 8$. We choose such a small system for a tutorial purpose. (In realistic applications, N is of the order of $100 \sim 1000$, where no one can diagonalize T exactly.) The variational state is expressed as

$$v(abcdefgh) = \sum_{\xi\mu\nu\rho\sigma=1}^{\text{at most } m} B^b_{a\xi} C^c_{\xi\mu} D^d_{\mu\nu} E^e_{\nu\rho} F^f_{\rho\sigma} G^g_{\sigma h} \tag{2}$$

shown as Fig. 1,[29] where Roman indices a-h shown by white circles are Ising spins, and Greek indices ξ-σ by black squares are m-state auxiliary variables; we use a black mark when the summation is taken over the corresponding variable. The integer m is a small number compared with the dimension of the trial state $2^N = 256$. Such a variational state, which is written in the form of tensor product, has been known for more than 30 years. For the readers who are interested in the history of the tensor product formulation, we review the development in the next section. (If not, please skip §2.)

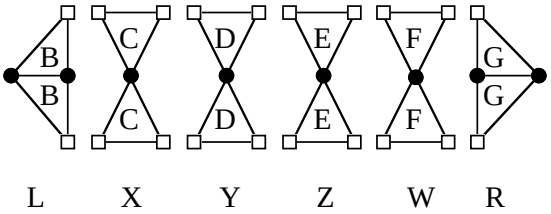

Fig. 2. The way to calculate the norm of the matrix product state. L, R, and X, Y, Z, W are m^2-dimensional vectors and matrices, respectively.

The tensor product state in Eq. (2) satisfies the conditions (a)-(c) because of the following reasons.

(i) First of all, the numerical calculation for the inner product $\boldsymbol{v}^T \boldsymbol{v} = \boldsymbol{v} \cdot \boldsymbol{v} = \langle v|v\rangle$ is *small in computational memory size*, because we do not have to create the 2^N-dimensional vector $\boldsymbol{v}$ explicitly. What we have to do is multiplications of m^2-dimensional matrices. For the case $N = 8$ shown in Figure 2, it is easily understood that $\boldsymbol{v}^T \boldsymbol{v}$ is obtained by multiplying the m^2-dimensional matrices $X_{(\xi\xi')(\mu\mu')} = \sum_c C^c_{\xi\mu} C^c_{\xi'\mu'}$, $Y_{(\mu\mu')(\nu\nu')} = \sum_d D^d_{\mu\nu} D^d_{\mu'\nu'}$, $Z_{(\nu\nu')(\rho\rho')} = \sum_e E^e_{\nu\rho} E^e_{\nu'\rho'}$, and $W_{(\rho\rho')(\sigma\sigma')} = \sum_f F^f_{\rho\sigma} F^f_{\rho'\sigma'}$ successively to the m^2-dimensional vector $(L| = L_{(\xi\xi')} = \sum_{ab} B^b_{a\xi} B^b_{a\xi'}$, and finally taking the inner product with the m^2 dimensional vector $|R) = R_{(\sigma\sigma')} = \sum_{gh} G^g_{\sigma h} G^g_{\sigma' h}$. As a result, we obtain $\langle v|v\rangle$ as $(L|XYZW|R)$. Thus the dimension of the matrix required to obtain $\langle v|v\rangle$ is always equal to m^2, independent of the system size N. We can expect the same *smallness* for the computation of $\boldsymbol{v}^T T \boldsymbol{v}$ in Eq. (1). We will explain the detail in §3.

(ii) Secondly, local improvements of $\boldsymbol{v}$ can be completed very *quickly*, because the variational state $\boldsymbol{v}$ is a product of local factors (= tensors); a local tuning for $\boldsymbol{v}$ is completed just by modifying one of the tensors. Let us consider the case

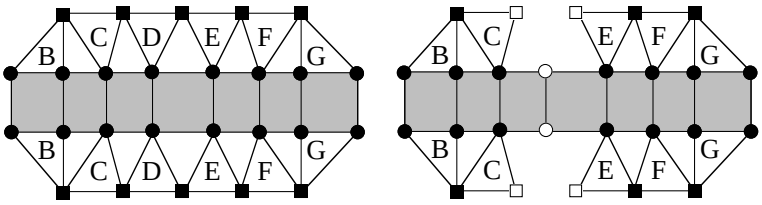

Fig. 3. Graphical representation of (a) $\langle v|T|v\rangle$ and (b) $\tilde{T}_{(\mu d\nu)(\mu' d' \nu')}$.

$N = 8$ again, and try to maximize $\boldsymbol{v}^T T\, \boldsymbol{v}$ shown in Fig. 3(a). Suppose that we are, right now, trying to optimize the tensor $D^d_{\mu\nu}$ only. How can we determine the best $D^d_{\mu\nu}$? Well, we can obtain it by diagonalizing the $2m^2$-dimensional matrix $\tilde{T}_{(\mu d\nu)(\mu' d' \nu')}$ shown in Fig. 3(b), where the eigenvector $\tilde{V}_{\mu d\nu}$ that corresponds to the maximum eigenvalue of $\tilde{T}_{(\mu d\nu)(\mu' d' \nu')}$ coincides with the best $D^d_{\mu\nu}$. In the same way, we can improve each tensor just by repeating the same procedure. Note that the local improvement for $\boldsymbol{v}$ is *much quicker* than the global improvement, because the latter involves 2^N degrees of freedom. What we have mentioned here is rather oversimplified, but the idea is essentially correct. We explain the detail in §4.

(iii) Thirdly, the high numerical *accuracy* in the tensor product state is formally explained by the singular value decomposition (SVD) of matrices.[27] *The SVD of an N by M rectangular matrix A* is to express it as a product of three matrices. In the case $N \geq M$ the decomposition is written as

$$A_{ij} = \sum_{\xi=1}^{M} Q_{i\xi}\, \omega_\xi\, R_{\xi j}\,, \tag{3}$$

where Q is an N by M matrix, and R is an N-dimensional orthogonal matrix. (If $N < M$, Q is N by N and R is N by M.) The numbers ω_ξ are called the '*singular values*.' If A is real-symmetric, the SVD of A is equivalent to the diagonalization of A. Normally, a small number of singular values are dominant for most matrices, and the rest of them are very small. In such a case it is possible to approximate A by discarding the tiny singular values

$$A_{ij} \approx \sum_{\xi=1}^{m} Q_{i\xi}\, \omega_\xi\, R_{\xi j}\,, \tag{4}$$

where m is the number of dominant singular values. Now let us see how we can approximate an arbitrary vector $v(abcdefgh)$ by the tensor product. First of all, we regard $v(abcdefgh)$ as a 4 by 64 matrix $V_{(ab)(cdefgh)}$, and apply SVD as

$$V_{(ab)(cdefgh)} = \sum_{\xi=1}^{4} B_{(ab)\xi}\, \omega_\xi\, R_{\xi(cdefgh)}\,, \tag{5}$$

where $B_{(ab)\xi}$ corresponds to the tensor $B^b_{a\xi}$ in Eq. (2). We then regard the factor $\omega_\xi R_{\xi(cdefgh)}$ as an 8 by 32 matrix $V'_{(\xi c)(defgh)}$ and decompose it again

$$\omega_\xi R_{\xi(cdefgh)} = V'_{(\xi c)(defgh)} = \sum_{\mu=1}^{8} C_{(\xi c)\mu}\, \omega'_\mu\, R'_{\mu(cdefgh)} \tag{6}$$

to obtain the second tensor $C^c_{\xi\mu}$. In this way, we successively obtain the tensors $B^b_{a\xi}$, $C^c_{\xi\mu}$, $D^d_{\mu\nu}$, $E^e_{\nu\rho}$, $F^f_{\rho\sigma}$, and $G^g_{\sigma h}$ in Eq. (2). Keeping the dominant singular values in each SVD — restricting the freedom of Greek indices $(\xi, \mu, \nu, \rho, \sigma)$ down to m — we obtain the tensor product approximation for $v(abcdefgh)$. If m is sufficiently large, and the singular values decays sufficiently rapidly, the restricted tensor product in Eq. (2) is accurate enough to approximate the original vector $v(abcdefgh)$. Thus the distribution of the singular values for $\boldsymbol{v}$ (= the eigenvector of the transfer matrix T) is essential to the validity of the tensor product approximation. We consider this point in §5.

To summarize, DMRG is a numerical method that improves the tensor product state through optimizing each tensor individually. Such an iterative procedure is called a '*finite system algorithm.*' For the case $N = 8$, we improve the tensors in the order $A \to B \to C \to D \to E \to F \to G \to F \to E \to D \to C \to B \to A \to B \to C \to$, etc. To speak more precisely, pair of tensors are improved at a time, so it is better to rewrite the above order as $AB \to BC \to CD \to DE \to EF \to FG \to EF \to DE \to CD \to BC \to AB \to BC \to$, etc. We summarize the numerical procedure of the finite system algorithm in §6.

In the thermodynamic limit $N \to \infty$, we expect that the tensor product state is translationally invariant; the tensors lose the position dependence.[30] If we are only interested in the thermodynamic limit, to perform the finite system algorithm for a large N is a waist of time and money. There is a simple modification of the finite system algorithm, which is called '*infinite system algorithm.*' We explain this numerical algorithm in §7.

Numerical algorithm and applications of DMRG are still in progress; many developments are being achieved day by day. Not only the numerical efficiency but also the analytic structure of DMRG is one of the recent interests. There are so many riddles in DMRG. We list up current problems including theoretical questions in DMRG in the last section.

2. Tensor Product State before DMRG

The variational state written in a product of tensors had been known for long time. It is worth looking at the history of the tensor product formulation, though White established DMRG totally independent from the *classical* works. In 1941 Kramers and Wannier investigated a variational problem for the square lattice Ising model,[31,32] assuming that the eigenvector of the transfer matrix T is well approximated by the uniform matrix product

$$v(\ldots abcefgh\ldots) = \ldots F^{ab}F^{bc}F^{cd}F^{de}F^{ef}F^{fg}F^{gh}\ldots, \tag{7}$$

where $\ldots abcefgh\ldots$ denotes a row of Ising spins, and F^{ab} is a 2 by 2 symmetric matrix. Their approximation was superior to those approxoimations known in those days — the molecular field approximation, the Bethe approximation,[33] etc., — in the respect that the calculated transition temperature $T_{\rm c}$ and the specific heat are quite close to those obtained by Onsager's exact solution.[34] The Gutzwiller approximation using the Gutzwiller's variational wave function $\hat{P}|\Psi\rangle$,[35] which is one of the standard approximations for the Hubbard model,[35,36,37] can be regarded as a modification of the Kramers-Wannier approximation.

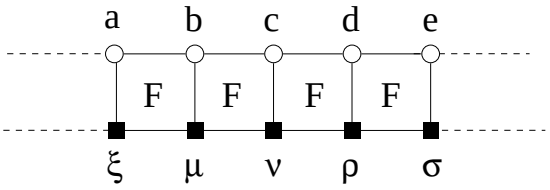

Fig. 4. Baxter's variational state in Eq. (8).

Around 1960-70 Baxter improved the Kramers-Wannier approximation by introducing additional degrees of freedom to the variational state.[38] His variational state is written as

$$v(\ldots abcdefgh\ldots) = \sum_{\ldots\xi\zeta\mu\nu\rho\sigma\tau\phi\ldots}^{m} \ldots F^{ab}_{\xi\zeta} F^{bc}_{\zeta\mu} F^{cd}_{\mu\nu} F^{de}_{\nu\rho} F^{ef}_{\rho\sigma} F^{fg}_{\sigma\tau} F^{gh}_{\tau\phi} \ldots , \tag{8}$$

where greek indices denote the additional m-state auxiliary variables. (See Fig. 4.) Since a tensor $F^{ab}_{\xi\zeta}$ contains $4m^2$ adjustable parameters — though there are a number of constraints between the tensor elements — the way of finding out the best element that maximizes $\lambda = (\boldsymbol{v}^T T\ \boldsymbol{v})/(\boldsymbol{v}^T \boldsymbol{v})$ is quite non trivial. He performed the maximization using a self-consistent equation for the corner transfer matrix (CTM).[38] Baxter's idea is very close to the infinite system algorithm in DMRG; one might be surprised to know that the concept of basis truncation with the help of density matrix was already mentioned in his well-known textbook '*Exactly Solved Models in Statistical Mechanics*.[39]'

Applications of the tensor product formulation to quantum systems began with the investigations of Haldane's conjecture. In 1985 Nightingale and Blöte used the Kramers-Wannier matrix product in Eq. (7) as the initial vector of their projector Monte Carlo simulation.[40] It is interesting that they further commented on the applicability of Baxter's formulation to quantum spin chains; if they realized what they commented, the infinite system DMRG would have been established earlier. In 1987 Affleck, Lieb, Kennedy, and Tasaki (AKLT)[41] showed that the ground-state wave function of a bilinear-biquadratic $S = 1$ spin chain can be exactly written as

$$\psi(\ldots abcde\ldots) = \sum_{\ldots\xi\mu\nu\rho\sigma\tau\ldots} \ldots M^{a}_{\xi\mu} M^{b}_{\mu\nu} M^{c}_{\nu\rho} M^{d}_{\rho\sigma} M^{e}_{\sigma\tau} \ldots , \tag{9}$$

where a, b, c, d, e, etc., are three-state spin variables that takes -1, 0, or 1, and the Greek indices represent 2-state auxiliary variables. If one introduces the notation

$$|\mu\nu\rangle = M^{-1}_{\mu\nu}|\downarrow\rangle + M^{0}_{\mu\nu}|0\rangle + M^{1}_{\mu\nu}|\uparrow\rangle\,, \tag{10}$$

the variational state ψ is written in the product form

$$\psi(\ldots abcde\ldots) = \sum_{\ldots\xi\mu\nu\rho\sigma\tau\ldots} \ldots|\xi\mu\rangle|\mu\nu\rangle|\nu\rho\rangle|\rho\sigma\rangle|\sigma\tau\rangle\ldots\,, \tag{11}$$

which is often referred as *matrix product state,* because it is possible to regard $|\mu\nu\rangle$ as the $\mu\nu$-element of a 2 by 2 matrix.

Fannes *et al.* generalized Baxter's tensor product state by assigning m-degrees of freedom to each auxiliary variable. Their variational state is known as '*finitely correlated state,*' since the correlation length of such state is always finite.[42,43] Although the construction of the ground state ψ in Eq. (9) does not look like that of $\boldsymbol{v}$ in Eq. (8), they are essentially the same. We can transform one to the other by mapping $M^{a}_{\xi\mu}$ in Eq. (9) into $F^{ab}_{\xi\mu}$ in Eq. (8) through a kind of duality transformation. Quite recently, the efficiency of the tensor product state is reported in the field of particle diffusion.[44,45,46]

Since the tensors are position independent in Eqs. (8)-(9), it is not straightforward to apply the above formulations to finite size systems, impurity systems, random systems, and any system that does not have the translational invariance. Compared with the uniform tensor product, the variational state used in DMRG

$$v(abcdefgh) = \sum_{\xi\mu\nu\rho\sigma=1}^{\text{at most } m} B^{b}_{a\xi}C^{c}_{\xi\mu}D^{d}_{\mu\nu}E^{e}_{\nu\rho}F^{f}_{\rho\sigma}G^{g}_{\sigma h} \tag{12}$$

is more flexible, because it allows the position dependence of the tensors.

3. Advantage of Tensor Product State

When a variational state is written in the tensor product, we can quickly calculate the inner product $\langle v|v\rangle = \boldsymbol{v}^T\boldsymbol{v}$ and the expectation value $\langle v|T|v\rangle = \boldsymbol{v}^T T\,\boldsymbol{v}$ with a small numerical calculation. Actually the variational state used in DMRG is normalized by definition, and thus we don't have to calculate $\boldsymbol{v}^T\boldsymbol{v}$. In order to explain this point, we introduce several new notations.

Let us consider the square lattice Ising model on a cylinder of width N. (See Fig. 5.) The system contains ℓ row of spins, where periodic boundary condition is imposed in the vertical direction.[47] We label the spins in a row as $s_1, s_2, \ldots, s_{N-1}, s_N$, where $s_j = \pm 1$ is the Ising spin at j-th site. The main subject is to find out the largest eigenvalue λ_0 of the transfer matrix $T_{(s'_1\cdots s'_N)(s_1\cdots s_N)}$. (We will soon give the definition of T in Eq. (20).)

In the formulation of DMRG, the variational state $\boldsymbol{v}$ for the transfer matrix T is expressed as a position dependent tensor product

$$v(s_{1\ldots}s_N) \tag{13}$$

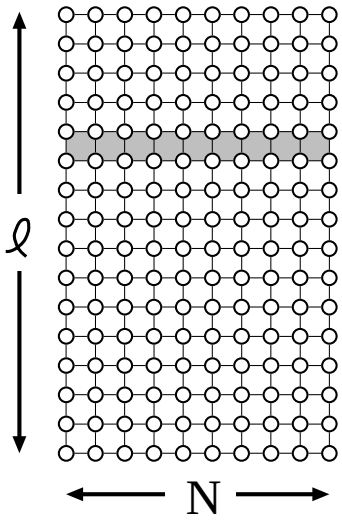

Fig. 5. Two-dimensional Ising model on a ℓ by N lattice, where periodic boundary condition is imposed to the vertical direction. The shaded region shows a row-to-row transfer matrix.

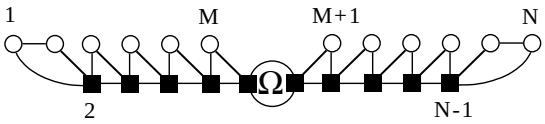

Fig. 6. The variational state used in the finite system DMRG, which is defined in Eq. (13).

$$= \sum_{\xi_2 \cdots \xi_{N-1}}^{m} A^{s_2}_{s_1 \xi_2} A^{s_3}_{\xi_2 \xi_3} \cdots A^{s_M}_{\xi_{M-1} \xi_M} \Omega_{\xi_M \xi_{M+1}} B_{\xi_{M+1}}{}^{s_{M+1}}_{\xi_{M+2}} \cdots B_{\xi_{N-2}}{}^{s_{N-2}}_{\xi_{N-1}} B_{\xi_{N-1}}{}^{s_{N-1}}_{s_N} ,$$

where $\xi_2 \cdots \xi_{N-1}$ denote the m-state auxiliary variables. (See Fig. 6.) Normally, m is of the order of $10 \sim 1000$, and is by far smaller than 2^N. The tensors $A^{s_i}_{\xi_{i-1} \xi_i}$ and $B_{\xi_j}{}^{s_j}_{\xi_{j+1}}$ are dependent on their positions i and j; we have distinguished the tensors by their spin indices. Each tensor satisfies the orthogonal relation

$$\begin{aligned} \sum_{\xi_{i-1} s_i} A^{s_i}_{\xi_{i-1} \xi_i} A^{s_i}_{\xi_{i-1} \xi'_i} &= \delta_{\xi_i \xi'_i} \\ \sum_{s_j \xi_{j+1}} B_{\xi_j}{}^{s_j}_{\xi_{j+1}} B_{\xi'_j}{}^{s_j}_{\xi_{j+1}} &= \delta_{\xi_j \xi'_j} , \end{aligned} \tag{14}$$

where we have written $A^{s_2}_{\xi_1 s_2}$ and $B_{\xi_{N-1}}{}^{s_{N-1}}_{s_N}$ as $A^{s_2}_{\xi_1 \xi_2}$ and $B_{\xi_{N-1}}{}^{s_{N-1}}_{\xi_N}$, respectively. Comparing Eq. (13) with Eq. (2), we have inserted an additional matrix $\Omega_{\xi_M \xi_{M+1}}$ at the M-th point, $(2 \le M \le N-2)$ which is an m-dimensional diagonal matrix

$$\Omega = \begin{pmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_m \end{pmatrix} . \tag{15}$$

We impose the normalization condition $\mathrm{Tr}\,\Omega^2 = \sum_\xi \omega_\xi^2 = 1$ and the decreasing order $|\omega_1| \ge |\omega_2| \ge \cdots |\omega_m|$ for convenience.

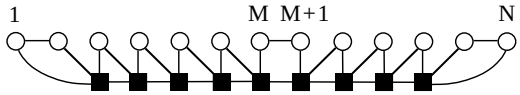

Fig. 7. Another standard form in Eq. (17) for the variational state.

The variational state in Eq. (13) is normalized by definition, because its inner product is equal to $\mathrm{Tr}\,\Omega^2$. (Use Eq. (14) repeatedly and finally use the fact $\mathrm{Tr}\,\Omega^2 = 1$.) Thus the variational relation in Eq. (1) can be simplified as

$$\lambda = \langle v|T|v\rangle = \boldsymbol{v}^T T \boldsymbol{v} . \tag{16}$$

They often rewrite the variational state as

$$v(s_{1 \cdots} s_N) = \sum_{\xi_2 \cdots \xi_{N-1}}^{m} A^{s_2}_{s_1 \xi_2} \cdots A^{s_{M-1}}_{\xi_{M-2} \xi_{M-1}} \tilde{V}^{s_M \; s_{M+1}}_{\xi_{M-1} \xi_{M+2}} B_{\xi_{M+2}}{}^{s_{M+2}}_{\xi_{M+3}} \cdots B_{\xi_{N-1}}{}^{s_{N-1}}_{s_N} , \tag{17}$$

(see Fig. 7,) where the new tensor $\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ correspond to the product[48]

$$\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}} = \sum_{\xi_M\xi_{M+1}} A^{s_M}_{\xi_{M-1}\xi_M}\,\Omega_{\xi_M\xi_{M+1}}\,B_{\xi_{M+1}}{}^{s_{M+1}}_{\xi_{M+2}} \tag{18}$$

which satisfies the normalization

$$\sum_{\xi_{M-1}s_Ms_{M+1}\xi_{M+2}} \left(\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}\right)^2 = 1\,. \tag{19}$$

The real advantage of expressing a variational state in the form of tensor product is that the numerical calculation of $\boldsymbol{v}^T\,T\,\boldsymbol{v}$ is very compact. This is because the transfer matrix T is also written in the product of local Boltzmann weights. For the Ising model, the transfer matrix — in order to save space we write $T_{(s'_1\ldots s'_N)(s_1\ldots s_N)}$ as $T^{s'_1\ldots s'_N}_{s_1\ldots s_N}$ — is expressed as

$$\begin{aligned} T^{s'_1\ldots s'_N}_{s_1\ldots s_N} &= \exp\left\{\frac{K}{2}\sum_{i=1}^{N-1}(s'_is'_{i+1}+s_is_{i+1})+K\sum_{i=1}^{N}s'_is_i\right\} \\ &= \exp\left\{\frac{K}{2}(s'_1s_1+s'_Ns_N)\right\}\prod_{i=1}^{N-1}W^{s'_is'_{i+1}}_{s_is_{i+1}}\,, \end{aligned} \tag{20}$$

where K is the parameter $-J/k_{\rm B}T$, and the tensor W represents the local Boltzmann weight

$$W^{s'_is'_{i+1}}_{s_is_{i+1}} = \exp\left\{\frac{K}{2}\left(s_is_{i+1}+s_{i+1}s'_{i+1}+s'_{i+1}s'_i+s'_is_i\right)\right\}\,. \tag{21}$$

Since the boundary factor $\exp\left\{\frac{K}{2}(s'_1s_1+s'_Ns_N)\right\}$ is not essential — at least for the explanation of DMRG — we employ the simplified transfer matrix

$$T^{s'_1\ldots s'_N}_{s_1\ldots s_N} = \prod_{i=1}^{N-1}W^{s'_is'_{i+1}}_{s_is_{i+1}} = W^{s'_1s'_2}_{s_1s_2}\,W^{s'_2s'_3}_{s_2s_3}\cdots W^{s'_{N-1}s'_N}_{s_{N-1}s_N} \tag{22}$$

in the following. Note that the transfer matrix is symmetric.[26]

Do we have to create a 2^N dimensional matrix $T^{s'_1\ldots s'_N}_{s_1\ldots s_N}$ for the computation of $\lambda = \boldsymbol{v}^T\,T\,\boldsymbol{v}$? As we have discussed in §1, the answer is no. We can obtain λ just by repeating matrix operations of a small dimension. What we have to perform are the following procedures;

(a) First, consider the Boltzmann weights at the both end of the transfer matrix. Rewrite them as

$$\begin{aligned} L^{s'_1s'_2}_{s_1s_2} &\equiv W^{s'_1s'_2}_{s_1s_2} \\ R^{s'_{N-1}s'_N}_{s_{N-1}s_N} &\equiv W^{s'_{N-1}s'_N}_{s_{N-1}s_N}\,. \end{aligned} \tag{23}$$

(b) Increase the length of L and R by joining a local weight

$$\begin{aligned} L^{s_1' s_2' s_3'}_{s_1 s_2 s_3} &= L^{s_1' s_2'}_{s_1 s_2} W^{s_2' s_3'}_{s_2 s_3} \\ R^{s_{N-2}' s_{N-1}' s_N'}_{s_{N-2} s_{N-1} s_N} &= W^{s_{N-2}' s_{N-1}'}_{s_{N-2} s_{N-1}} R^{s_{N-1}' s_N'}_{s_{N-1} s_N} . \end{aligned} \tag{24}$$

(c) Take contractions with A and B

$$\begin{aligned} L^{\xi_2' s_3'}_{\xi_2 s_3} &= \sum_{s_1' s_1 s_2' s_2} L^{s_1' s_2' s_3'}_{s_1 s_2 s_3} A^{s_2}_{s_1 \xi_2} A^{s_2'}_{s_1' \xi_2'} \\ R^{s_{N-2}' \xi_{N-1}'}_{s_{N-2} \xi_{N-1}} &= \sum_{s_{N-1}' s_{N-1} s_N' s_N} B_{\xi_{N-1} s_N}^{\quad s_{N-1}} B_{\xi_{N-1}' s_N'}^{\quad s_{N-1}'} R^{s_{N-2}' s_{N-1}' s_N'}_{s_{N-2} s_{N-1} s_N} . \end{aligned} \tag{25}$$

(d) As (b), increase the length of L and R as

$$\begin{aligned} L^{\xi_2' s_3' s_4'}_{\xi_2 s_3 s_4} &= L^{\xi_2' s_3'}_{\xi_2 s_3} W^{s_3' s_4'}_{s_3 s_4} \\ R^{s_{N-3}' s_{N-2}' \xi_{N-1}'}_{s_{N-3} s_{N-2} \xi_{N-1}} &= W^{s_{N-3}' s_{N-2}'}_{s_{N-3} s_{N-2}} R^{s_{N-2}' \xi_{N-1}'}_{s_{N-2} \xi_{N-1}} . \end{aligned} \tag{26}$$

(e) As (c), take contractions with A and B

$$\begin{aligned} L^{\xi_3' s_4'}_{\xi_3 s_4} &= \sum_{\xi_2' \xi_2 s_3' s_3} L^{\xi_2' s_3' s_4'}_{\xi_2 s_3 s_4} A^{s_3}_{\xi_2 \xi_3} A^{s_3'}_{\xi_2' \xi_3'} \\ R^{s_{N-3}' \xi_{N-2}'}_{s_{N-3} \xi_{N-2}} &= \sum_{s_{N-2}' s_{N-2} \xi_{N-1}' \xi_{N-1}} B_{\xi_{N-2} \xi_{N-1}}^{\quad s_{N-2}} B_{\xi_{N-2}' \xi_{N-1}'}^{\quad s_{N-2}'} R^{s_{N-3}' s_{N-2}' \xi_{N-1}'}_{s_{N-3} s_{N-2} \xi_{N-1}} . \end{aligned} \tag{27}$$

(f) Repeat (d) and (e) till we get $L^{\xi_{M-1}' s_M'}_{\xi_{M-1} s_M}$ and $R^{s_{M+1}' \xi_{M+2}'}_{s_{M+1} \xi_{M+2}}$. The λ in Eq. (16) is then obtained as

$$\lambda = \sum \tilde{V}^{s_M' \quad s_{M+1}'}_{\xi_{M-1}' \xi_{M+2}'} L^{\xi_{M-1}' s_M'}_{\xi_{M-1} s_M} W^{s_M' s_{M+1}'}_{s_M s_{M+1}} R^{s_{M+1}' \xi_{M+2}'}_{s_{M+1} \xi_{M+2}} \tilde{V}^{s_M \quad s_{M+1}}_{\xi_{M-1} \xi_{M+2}} , \tag{28}$$

where the sum is taken over for all spin indices in the right hand side. (See Fig. 8.)

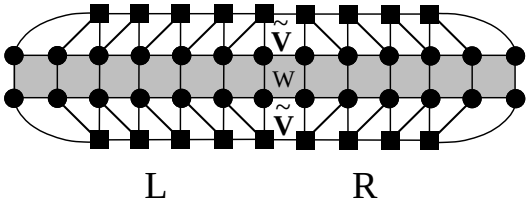

Fig. 8. Graphical representation of $\langle v|T|v\rangle$. The shaded region represents the transfer matrix. We calculate it from the left and the right end.

To summarize, we can obtain $\lambda = \boldsymbol{v}^T T \boldsymbol{v}$ without directly creating the 2^N-dimensional matrix T. This is because both variational state $\boldsymbol{v}$ and the transfer

matrix T are given by products of local factors. The computer storage space for the calculation of λ is linear in Nm^2.

4. Rapid Local Improvement

The second advantage of the tensor product state is that its improvement can be done very quickly. This is because we can improve the trial state locally, by just modifying each tensor independently. To see this point, let us consider the local improvement of a factor $\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ in the normalized variational state

$$v(s_{1\cdots}s_N) = \sum_{\xi_2\cdots\xi_{N-1}}^{m} A^{s_2}_{s_1\xi_2}\cdots A^{s_{M-1}}_{\xi_{M-2}\xi_{M-1}}\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}B_{\xi_{M+2}}^{\ \ s_{M+2}\ \ \xi_{M+3}}\cdots B_{\xi_{N-1}}^{\ \ s_{N-1}\ \ s_N}. \quad (29)$$

Do not ask for the improvements of $A^{s_i}_{\xi_{i-1}\xi_i}$ and $B_{\xi_j}^{\ \ s_j\ \ \xi_{j+1}}$ at this moment; we will discuss them later. The subject is to maximize $\lambda = \boldsymbol{v}^T T\,\boldsymbol{v}$ just by tuning the $4m^2$ numbers of elements in $\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ under the constraint $\sum\left(\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}\right)^2 = 1$. (See Eq. (19).) The notations that we have defined in the last section are of use. Equation (28) tells us that λ is written as

$$\lambda = \sum_{\text{all indices in the r.h.s}} \tilde{V}^{s'_M\ s'_{M+1}}_{\xi'_{M-1}\xi'_{M+2}}\,\tilde{T}^{\xi'_{M-1}s'_Ms'_{M+1}\xi'_{M+2}}_{\xi_{M-1}s_Ms_{M+1}\xi_{M+2}}\,\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}, \quad (30)$$

where the $4m^2$-dimensional matrix $\tilde{T}$ — the renormalized transfer matrix — is defined as

$$\tilde{T}^{\xi'_{M-1}s'_Ms'_{M+1}\xi'_{M+2}}_{\xi_{M-1}s_Ms_{M+1}\xi_{M+2}} = L^{\xi'_{M-1}s'_M}_{\xi_{M-1}s_M}\,W^{s'_Ms'_{M+1}}_{s_Ms_{M+1}}\,R^{s'_{M+1}\xi'_{M+2}}_{s_{M+1}\xi_{M+2}}. \quad (31)$$

Now , it is obvious that λ is maximized when $\tilde{V}_{\xi_{M-1}s_Ms_{M+1}\xi_{M+2}} \equiv \tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ is the eigenvector of $\tilde{T}^{\xi'_{M-1}s'_Ms'_{M+1}\xi'_{M+2}}_{\xi_{M-1}s_Ms_{M+1}\xi_{M+2}}$.

From the numerical point of view, to find out the largest eigenvalue of $4m^2$-dimensional matrix $\tilde{T}$ by the Lanczos method[49] is not time consuming at all, partially because the matrix dimension is not so huge for a modest $m \sim 100$. (We may also use the power method, or the look ahead Lanczos, that are simpler than Lanczos method.) Another reason for the quickness in the Lanczos diagonalization is that the matrix $\tilde{T}$ is written in the product of three factors L, W, and R. (See Eq. (31).) For example, when we multiply $\tilde{T}$ to an arbitrary vector $\boldsymbol{x}$, what we do is the following procedures;

$$\begin{aligned}
x'(\xi'_{M-1}s'_Ms_Ms_{M+1}\xi_{M+2}) &= \sum_{\xi_{M-1}} L^{\xi'_{M-1}s'_M}_{\xi_{M-1}s_M}\,x(\xi_{M-1}s_Ms_{M+1}\xi_{M+2})\\
x''(\xi'_{M-1}s'_Ms'_{M+1}s_{M+1}\xi_{M+2}) &= \sum_{s_M} W^{s'_Ms'_{M+1}}_{s_Ms_{M+1}}\,x'(\xi'_{M-1}s'_Ms_Ms_{M+1}\xi_{M+2}) \quad (32)\\
x'''(\xi'_{M-1}s'_Ms'_{M+1}\xi'_{M+2}) &= \sum_{s_{M+1}\xi_{M+2}} R^{s'_{M+1}\xi'_{M+2}}_{s_{M+1}\xi_{M+2}}\,x''(\xi'_{M-1}s'_Ms'_{M+1}s_{M+1}\xi_{M+2}).
\end{aligned}$$

(See Fig. 9.) We have to prepare $8m^2$-dimensional vector as the work space for each step.

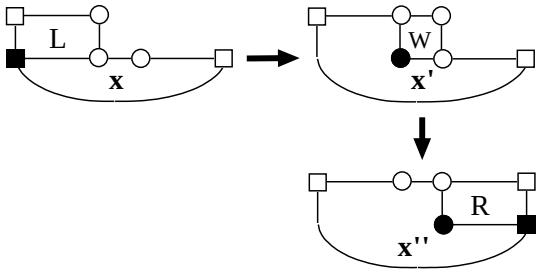

Fig. 9. A way to multiply the renormalized transfer matrix in Eq. (31) to a vector. (See Eq. (32).)

Improvements of local factors other than $\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ — $A^{s_i}_{\xi_{i-1}\xi_i}$ and $B_{\xi_j}{}^{s_j}{}_{\xi_{j+1}}$ for arbitrary position i — are performed by rewriting the variational state $v(s_{1\cdots}s_N)$ into the new form

$$v(s_{1\cdots}s_N) = \sum_{\xi_2\cdots\xi_{N-1}}^{m} A^{s_2}_{s_1\xi_2}\cdots A^{s_M}_{\xi_{M-1}\xi_M}\tilde{V}^{s_{M+1}\,s_{M+2}}_{\xi_M\quad\xi_{M+3}} B_{\xi_{M+3}}{}^{s_{M+3}}{}_{\xi_{M+4}}\cdots B_{\xi_{N-1}}{}^{s_{N-1}}{}_{s_N}\,. \tag{33}$$

The intention of the transformation Eq. (29) $\rightarrow$ Eq. (33) is to shift the place of $\tilde{V}$ by one lattice spacing, and then improve $v(s_{1\cdots}s_N)$ around the sites s_{M+1} and s_{M+2}; it is equivalent to improving $A^{s_{M+1}}_{\xi_M\xi_{M+1}}$ and $B_{\xi_{M+2}}{}^{s_{M+2}}{}_{\xi_{M+3}}$. The transformation from Eq. (29) to Eq. (33) is mediated by the extended local factor

$$\begin{aligned}\tilde{U}^{s_M\ s_{M+1}\ s_{M+2}}_{\xi_{M-1}\qquad\xi_{M+3}} &\equiv \sum_{\xi_{M+2}} \tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}} B_{\xi_{M+2}}{}^{s_{M+2}}{}_{\xi_{M+3}} \\ &= \sum_{\xi_M} A^{s_M}_{\xi_{M-1}\xi_M}\tilde{V}^{s_{M+1}\,s_{M+2}}_{\xi_M\quad\xi_{M+3}}\,,\end{aligned} \tag{34}$$

where the new tensor $A^{s_M}_{\xi_{M-1}\xi_M}$ is obtained by the SVD of $\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$ as follows.
(a) Create a $2m$-dimensional matrix

$$\tilde{\rho}_{(\xi'_{M-1}s'_M)(\xi_{M-1}s_M)} = \sum_{s_{M+1}\xi_{M+2}} \tilde{V}^{s'_M\ s_{M+1}}_{\xi'_{M-1}\xi_{M+2}}\tilde{V}^{s_M\ s_{M+1}}_{\xi_{M-1}\xi_{M+2}}\,, \tag{35}$$

that is normalized $\mathrm{Tr}\,\tilde{\rho} = 1$. The normalization comes from the normalization of $\tilde{V}$ in Eq. (19).
(b) Diagonalize $\tilde{\rho}$

$$\tilde{\rho}_{(\xi'_{M-1}s'_M)(\xi_{M-1}s_M)} = \sum_{\xi_M}^{2m} A^{s'_M}_{\xi'_{M-1}\xi_M}\,\omega^2_{\xi_M}\,A^{s_M}_{\xi_{M-1}\xi_M}\,, \tag{36}$$

where we assume the decreasing order for the eigenvalues. Note that the new variable ξ_M runs from 1 to $2m$.
(c) Restrict the degree of freedom of ξ_M down to m.
(d) Create $\tilde{V}^{s_{M+1}s_{M+2}}_{\xi_M\xi_{M+3}}$ by way of a fusion process

$$\tilde{V}^{s_{M+1}s_{M+2}}_{\xi_M\quad\xi_{M+3}} = \sum_{\xi_{M-1}s_M\xi_{M+2}} A^{s_M}_{\xi_{M-1}\xi_M}\tilde{V}^{s_M\quad s_{M+1}}_{\xi_{M-1}\quad\xi_{M+2}} B_{\xi_{M+2}\xi_{M+3}}^{\quad s_{M+2}} . \tag{37}$$

(See Fig. 10.) In such a way we can shift the place of $\tilde{V}$ to any place as we like.[50]

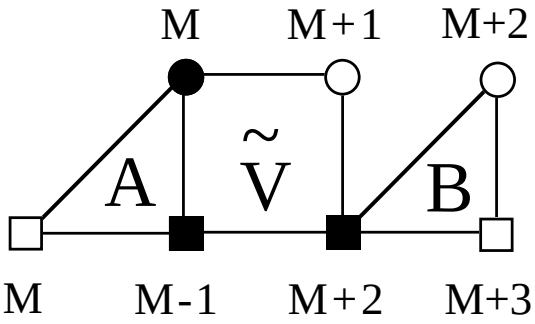

Fig. 10. Shift of $\tilde{V}$ from the M-th point to $M+1$. (See Eq. (37).)

Now , it is obvious that the local improvement for $\tilde{V}^{s_{M+1}s_{M+2}}_{\xi_M\quad\xi_{M+3}}$ is performed by the Lanczos diagonalization of the $4m^2$-dimensional matrix

$$\tilde{T}^{\xi'_M s'_{M+1}s'_{M+2}\xi'_{M+3}}_{\xi_M s_{M+1}s_{M+2}\xi_{M+3}} = L^{\xi'_M s'_{M+1}}_{\xi_M s_{M+1}} W^{s'_{M+1}s'_{M+2}}_{s_{M+1}s_{M+2}} R^{s'_{M+2}\xi'_{M+3}}_{s_{M+2}\xi_{M+3}} , \tag{38}$$

where we have obtained $R^{s'_{M+2}\xi'_{M+3}}_{s_{M+2}\xi_{M+3}}$ when we calculated $R^{s'_{M+1}\xi'_{M+2}}_{s_{M+1}\xi_{M+2}}$ in Eqs. (25)-(27), and $L^{\xi'_M s'_{M+1}}_{\xi_M s_{M+1}}$ is immediately obtained as

$$L^{\xi'_M s'_{M+1}}_{\xi_M s_{M+1}} = \sum_{\xi'_{M-1}\xi_{M-1}s'_M s_M} L^{\xi'_{M-1}s'_M s'_{M+1}}_{\xi_{M-1}s_M s_{M+1}} A^{s_M}_{\xi_{M-1}\xi_M} A^{s'_M}_{\xi'_{M-1}\xi'_M} \tag{39}$$

together with

$$L^{\xi'_{M-1}s'_M s'_{M+1}}_{\xi_{M-1}s_M s_{M+1}} = L^{\xi'_{M-1}s'_M}_{\xi_{M-1}s_M} W^{s'_M s'_{M+1}}_{s_M s_{M+1}} . \tag{40}$$

Thus the construction of $\tilde{T}^{\xi'_M s'_{M+1}s'_{M+2}\xi'_{M+3}}_{\xi_M s_{M+1}s_{M+2}\xi_{M+3}}$ is very easy and quick.

5. Validity of the Approximation

One might be skeptical about the validity of the tensor product approximation. The point is whether we can approximate the eigenvector $v(s_{1\ldots}s_N)$ of the transfer matrix T precise enough or not by using the restricted tensor product. (People who

believe in this point can skip this section.) This problem is deeply related to the eigenvalue distribution of the density matrix[52]

$$\rho_{(s'_1\cdots s'_M)(s_1\cdots s_M)} = \sum_{s_{M+1}\cdots s_N} v(s'_{1\ldots}s'_M s_{M+1}s_N)v(s_{1\ldots}s_M s_{M+1}s_N)\,, \tag{41}$$

which is diagonalized as

$$\rho_{(s'_1\cdots s'_M)(s_1\cdots s_M)} = \sum_{\xi_M}^{2^M} A_{(s'_1\cdots s'_M)\xi_M}\,\omega^2_{\xi_M}\,A_{(s_1\cdots s_M)\xi_M}\,. \tag{42}$$

Here, we have assumed that T is symmetric, and that the density matrix is positive semi-definite. We also assume that $\omega^2_{\xi_M}$ is in the decreasing order $\omega_1 \geq \omega_2 \geq \cdots \omega_{2^M}$. In addition to $\rho_{(s'_1\cdots s'_M)(s_1\cdots s_M)}$, by considering the density matrix for the right side

$$\begin{aligned}\rho_{(s'_{M+1}\cdots s'_N)(s_{M+1}\cdots s_N)} &= \sum_{s_{1\ldots}s_M} v(s_{1\ldots}s_M s'_{M+1}s'_N)v(s_{1\ldots}s_M s_{M+1}s_N) \\ &= \sum_{\xi_{M+1}}^{2^{N-M}} B_{\xi_M(s'_{M+1}\cdots s'_N)}\,\omega^2_{\xi_{M+1}}\,B_{\xi_{M+1}(s_{M+1}\cdots s_N)}\,,\end{aligned} \tag{43}$$

we reach the SVD for the eigenvector

$$v(s_{1\ldots}s_N) = \sum_{\xi_M\xi_{M+1}} A_{(s_1\cdots s_M)\xi_M}\Omega_{\xi_M\xi_{M+1}}B_{\xi_{M+1}(s_{M+1}\cdots s_N)}\,, \tag{44}$$

where $\Omega_{\xi_M\xi_{M+1}}$ is equal to $\delta_{\xi_M\xi_{M+1}}\omega_{\xi_M}$. (See Eq. (15).)

If $|\omega_{\xi_M}|$ decreases rapidly with respect to ξ_M, we can well approximate $v(s_{1\ldots}s_N)$ by restricting the range of ξ_M and ξ_{M+1} down to m

$$v(s_1\cdots s_N) \sim \sum_{\xi_M\xi_{M+1}}^{m} A_{(s_1\cdots s_M)\xi_M}\Omega_{\xi_M\xi_{M+1}}B_{\xi_{M+1}(s_{M+1}\cdots s_N)} \tag{45}$$

without loss of numerical accuracy. It is easy to imagine that by repeating SVD and freedom restriction ($2m \to m$) for both $A_{(s_1\cdots s_M)\xi_M}$ and $B_{\xi_{M+1}(s_{M+1}\cdots s_N)}$, we finally obtain the matrix product representation (or approximation) for $v(s_{1\ldots}s_N)$. Thus the essential problem is, whether $|\omega_{\xi_M}|$ really decreases rapidly enough or not.

In order to answer this question, let us look at the SVD for $v(s_{1\ldots}s_N)$ in Eq. (15) again. We find that the factor $\Omega_{\xi_M\xi_{M+1}}$ is a *joint* between the left half of the system $\{s_1\cdots s_M\}$ and the right half $\{s_{M+1}\cdots s_N\}$. If the system is off critical — if there is finite excitation energy — only the spin fluctuations within the correlation length pass through the joint $\Omega_{\xi_M\xi_{M+1}}$. In that case ω_{ξ_M} shows quasi exponential dumping; for the Ising model, exact formulation for ω_{ξ_M} in the limit $N \to \infty$ was obtained

by Baxter,[38] where ω_ξ actually decays nearly exponentially.[53,54] It should be noted that finite size systems are always off critical, and therefore we can approximate $v(s_{1\cdots}s_N)$ precisely enough in the form of tensor product. On the other hand, the tensor product approximation does not work for (infinitely large) critical systems.[55]

There is a way to check the efficiency of the tensor product approximation without knowing the detail of the system. That is, to observe the quantity

$$P_m = \sum_{\xi_M}^{m} \omega_{\xi_M}^2 \tag{46}$$

during the numerical calculation, and check whether $1 - P_m$ is close enough to 0 or not. If not, one has to increase m to keep the numerical precision of the variational state.

6. Finite System Algorithm

The numerical algorithm of the finite system DMRG is summarized as follows:

(a) Prepare the initial tensors $A^{s_i}_{\xi_{i-1}\xi_i}$ for $2 \le i \le M$ and $B_{\xi_j}{}^{s_j}_{\xi_{j+1}}$ for $M+1 \le j \le N-1$, where the tensor elements can be chosen arbitrarily. (A more efficient starting point is given by the infinite system algorithm; see §7.)

(b) Create $L^{\xi'_{M-1}s'_M}_{\xi_{M-1}s_M}$ and $R^{s'_{M+1}\xi'_{M+2}}_{s_{M+1}\xi_{M+2}}$ using Eqs. (23)-(27) successively.

(c) Diagonalize $\tilde{T}_M \equiv \tilde{T}^{\xi'_{M-1}s'_M s'_{M+1}\xi'_{M+2}}_{\xi_{M-1}s_M s_{M+1}\xi_{M+2}}$ in Eq. (31), using the Lanczos method to obtain the eigenvector $\tilde{V}_M \equiv \tilde{V}^{s_M \quad s_{M+1}}_{\xi_{M-1}\xi_{M+2}}$.

(d) Shift the position of $\tilde{V}_M$ to the right direction: $\tilde{V}_M \to \tilde{V}_{M+1}$ via Eqs. (34)-(37). At the same time, create $\tilde{T}_{M+1}$ following Eqs. (38)-(40). (Increment M: $M \to M+1$.)

(e) Repeat (c) and (d) until $\tilde{V}_M$ reaches at the right end of the system.

(f) Shift the position of $\tilde{V}_M$ to the left direction: $\tilde{V}_M \to \tilde{V}_{M-1}$. At the same time, create $\tilde{T}_{M-1}$. (Decrement M: $M \to M-1$.)

(g) Improve $\tilde{V}_M$ by the diagonalization of $\tilde{T}_M$, and repeat (f)-(g) until $\tilde{V}_M$ reaches at the left end of the system.

(h) Shuttle (or zip) $\tilde{V}_M$ from the left to right by repeating the steps (c)-(g), and improve the all the parts of the variational state.

(i) Stop the iteration when λ converges to its maximum value. It is recommended to stop when $M = N/2$.

The numerical algorithm in this table is referred as '*zone burning process*' or '*zipper process.*[56] '

In the above sequence, the Lanczos diagonalizations in step (c) and (g) always come after the shift of $\tilde{V}_M \to \tilde{V}_{M\pm1}$ in (d) and (f). White showed that $\tilde{V}_{M\pm1}$ obtained by Eqs. (34)-(37) is a good candidate for the eigenvector of $\tilde{T}_{M\pm1}$, and therefore we can reduce the computation time of the Lanczos diagonalization for $\tilde{T}_{M\pm1}$.[50,51]

After we stop at the step (i), we obtain the maximized λ and the corresponding optimized variational state $v(s_{1\ldots}s_N)$. The approximate free energy per site is then expressed as

$$f = -\frac{1}{N} k_{\rm B} T \, \log \lambda \,, \tag{47}$$

and we can calculate thermodynamic quantities from f. Since we have the variational state explicitly, we can directly calculate the spin correlation functions. For example, the spin polarization at the i-th site is obtained as

$$\langle s_i \rangle \;=\; \sum_{s_1 \cdots s_N} v(s_{1\ldots}s_N)\, s_i \, v(s_{1\ldots}s_N) = \sum_{\xi_{i-1} s_i s_{i+1} \xi_{i+2}} s_i \left(\tilde{V}^{s_i s_{i+1}}_{\xi_{i-1}\xi_{i+2}} \right)^2 , \tag{48}$$

and the diagonal two-spin correlation function is expressed in the same way

$$\langle s_i s_j \rangle \;=\; \sum_{s_1 \cdots s_N} v(s_{1\ldots}s_N)\, s_i s_j \, v(s_{1\ldots}s_N) \,. \tag{49}$$

(See Fig. 11.) Calculations for $\langle s_i \rangle$ and $\langle s_i s_j \rangle$ can be worked out without creating $v(s_{1\ldots}s_N)$ explicitly, as we have evaluated λ without creating the 2^N-dimensional vectors. In the same way, off-diagonal correlations are calculated as

$$\langle \hat{O}_i \hat{O}_j \rangle \;=\; \sum_{s_1 \cdots s_N, s'_i s'_j} v(s_{1\ldots} s_{i-1} s'_i s_{i+1\ldots} s_{j-1} s'_j s_{j+1\ldots} s_N)\, O_{s'_i s_i} O_{s'_j s_j} \, v(s_{1\ldots}s_N) \,, \tag{50}$$

where $O_{s'_i s_i}$ is a matrix representation of an operator $\hat{O}_i$ that contains spin flip processes.

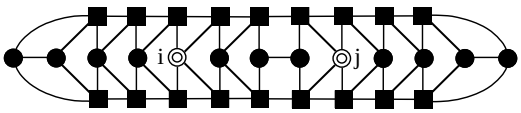

Fig. 11. Correlation function between s_i and s_j, that are shown by double circles.

One might not be happy about the construction of initial variational state in the initial step (a). Roughly speaking, we may put *arbitrary random numbers*

to the initial tensors; the tensors do not have to satisfy the orthogonal relations in Eq. (14), because they are automatically orthogonalized during the first sweep of $\tilde{V}_M$. Actually, we can create the initial variational state more efficiently; the numerical procedure is called the infinite system DMRG algorithm.

7. Infinite System Algorithm

When the system is off critical, the tensors in the variational state

$$v(s_{1\cdots}s_N) = \sum_{\xi_2\cdots\xi_{N-1}^m} A^{s_2}_{s_1\xi_2}\cdots A^{s_M}_{\xi_{M-1}\xi_M}\Omega_{\xi_M\xi_{M+1}}B_{\xi_{M+1}}{}^{s_{M+1}}{}_{\xi_{M+2}}\cdots B_{\xi_{N-1}}{}^{s_{N-1}}{}_{s_N}, \qquad (51)$$

lose position dependence, except for those near the both boundaries, under the condition that the system size N is far larger than the correlation length ℓ_0.[57] If we are only interested in the bulk properties of the system, we don't have to obtain the entire tensor product state so accurately. What we need is only one pair of the (representative) tensors, say $A^{s_M}_{\xi_{M-1}\xi_M}$ and $B_{\xi_{M+1}}{}^{s_{M+1}}{}_{\xi_{M+2}}$, at the center of the system. The infinite system algorithm is a numerical tool to obtain such a pair of tensors, by using a kind of simplification of the finite system algorithm.

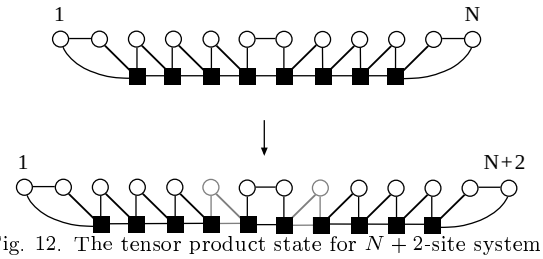

Fig. 12. The tensor product state for $N+2$-site system can be obtained by simply inserting two tensors at the center of the state for N-site system.

Let us compare the variational state $v(s_{1\cdots}s_N)$ and $v(s_{1\cdots}s_{N+2})$, where N is much longer than the correlation length ℓ_0. (See Fig. 12.) It is obvious that we get the latter by just inserting two matrices to the center. The correspondence between N and $N+2$ plays an important role in the infinite system algorithm. It might be better to show the first several (numerical) steps in order to see the basic idea of this algorithm. The calculation starts from the case $N=4$. The transfer matrix is constructed as

$$T^{s_1' s_2' s_{\overline{2}}' s_{\overline{1}}'}_{s_1 s_2 s_{\overline{2}} s_{\overline{1}}} = L^{s_1' s_2'}_{s_1 s_2} W^{s_2' s_{\overline{2}}'}_{s_2 s_{\overline{2}}} R^{s_{\overline{2}}' s_{\overline{1}}'}_{s_{\overline{2}} s_{\overline{1}}}, \qquad (52)$$

where we use the site indices $(1,2,\overline{2},\overline{1})$ instead of $(1,2,3,4)$ in order to stress the similarity between the left and the right. Diagonalizing the transfer matrix, we obtain the largest eigenvalue $\lambda^{(4)}$ and the corresponding eigenvector $v(s_1 s_2 s_{\overline{2}} s_{\overline{1}})$. Let us decompose it using SVD

$$v(s_1 s_2 s_{\overline{2}} s_{\overline{1}}) = \sum_{\xi_2} A^{s_2}_{s_1\xi_2}\,\omega_{\xi_2}\,B_{\xi_2}{}^{s_{\overline{2}}}{}_{s_{\overline{1}}}, \qquad (53)$$

where $A^{s_2}_{s_1\xi_2}$ is identical to $B^{s_{\overline{2}}}_{\xi_{\overline{2}}s_{\overline{1}}}$, if the transfer matrix is invariant under the space reflection.

The trick of the infinite system DMRG is to use the tensors $A^{s_2}_{s_1\xi_2}$ *and* $B^{s_{\overline{2}}}_{\xi_{\overline{2}}s_{\overline{1}}}$ *as a part of variational state for* $N = 6$. This is equivalent to use them as a RG transformation for the transfer matrix for $N = 6$. The RG transformation is done by increasing the length of transfer matrices

$$\begin{aligned} L^{s_1's_2's_3'}_{s_1s_2s_3} &= L^{s_1's_2'}_{s_1s_2} W^{s_2's_3'}_{s_2s_3} \\ R^{s_{\overline{3}}'s_{\overline{2}}'s_{\overline{1}}'}_{s_{\overline{3}}s_{\overline{2}}s_{\overline{1}}} &= W^{s_{\overline{3}}'s_{\overline{2}}'}_{s_{\overline{3}}s_{\overline{2}}} R^{s_{\overline{2}}'s_{\overline{1}}'}_{s_{\overline{2}}s_{\overline{1}}} \end{aligned} \tag{54}$$

and by performing the block spin transformation

$$\begin{aligned} L^{\xi_2's_3'}_{\xi_2s_3} &= \sum_{s_1's_1s_2's_2} L^{s_1's_2's_3'}_{s_1s_2s_3} A^{s_2'}_{s_1'\xi_2'} A^{s_2}_{s_1\xi_2} \\ R^{s_{\overline{3}}'\xi_{\overline{2}}'}_{s_{\overline{3}}\xi_{\overline{2}}} &= \sum_{s_{\overline{2}}'s_{\overline{2}}s_{\overline{1}}'s_{\overline{1}}} B^{s_{\overline{2}}'}_{\xi_{\overline{2}}'s_{\overline{1}}'} B^{s_{\overline{2}}}_{\xi_{\overline{2}}s_{\overline{1}}} R^{s_{\overline{3}}'s_{\overline{2}}'s_{\overline{1}}'}_{s_{\overline{3}}s_{\overline{2}}s_{\overline{1}}} \end{aligned} \tag{55}$$

to obtained the renormalized transfer matrix for $N = 6$

$$\tilde{T}^{\xi_2's_3's_{\overline{3}}'\xi_{\overline{2}}'}_{\xi_2s_3s_{\overline{3}}\xi_{\overline{2}}} = L^{\xi_2's_3'}_{\xi_2s_3} W^{s_3's_{\overline{3}}'}_{s_3s_{\overline{3}}} R^{s_{\overline{3}}'\xi_{\overline{2}}'}_{s_{\overline{3}}\xi_{\overline{2}}}. \tag{56}$$

These are the first iteration of the infinite system algorithm.

The next step is simply to increase the subscripts of each spin variables. Diagonalizing $\tilde{T}^{\xi_2's_3's_{\overline{3}}'\xi_{\overline{2}}'}_{\xi_2s_3s_{\overline{3}}\xi_{\overline{2}}}$, we obtain the eigenvector

$$v(\xi_2s_3s_{\overline{3}}\xi_{\overline{2}}) = \sum_{\xi_3} A^{s_3}_{\xi_2\xi_3}\, \omega_{\xi_3}\, B^{s_{\overline{3}}}_{\xi_{\overline{3}}\xi_{\overline{2}}}. \tag{57}$$

If ξ_3 can exceed m, we restrict the its range up to m by keeping the important states that correspond to the large singular values. Using the obtained tensors $A^{s_3}_{\xi_2\xi_3}$ and $B^{s_{\overline{3}}}_{\xi_{\overline{3}}\xi_{\overline{2}}}$, we create $\tilde{T}^{\xi_3's_4's_{\overline{4}}'\xi_{\overline{3}}'}_{\xi_3s_4s_{\overline{4}}\xi_{\overline{3}}}$ through the linear (or, RG) transformations

$$\begin{aligned} L^{\xi_3's_4'}_{\xi_3s_4} &= \sum_{\xi_2'\xi_2s_3's_3} L^{\xi_2's_3's_4'}_{\xi_2s_3s_4} A^{s_3'}_{\xi_2'\xi_3'} A^{s_3}_{\xi_2\xi_3} \\ R^{s_{\overline{4}}'\xi_{\overline{3}}'}_{s_{\overline{4}}\xi_{\overline{3}}} &= \sum_{s_{\overline{3}}'s_{\overline{3}}\xi_{\overline{2}}'\xi_{\overline{2}}} B^{s_{\overline{3}}'}_{\xi_{\overline{3}}'\xi_{\overline{2}}'} B^{s_{\overline{3}}}_{\xi_{\overline{3}}\xi_{\overline{2}}} R^{s_{\overline{4}}'s_{\overline{3}}'\xi_{\overline{2}}'}_{s_{\overline{4}}s_{\overline{3}}\xi_{\overline{2}}} \end{aligned} \tag{58}$$

and so on.

It is clear that the further iterations successively produces $\tilde{T}^{\xi_2's_3's_{\overline{3}}'\xi_{\overline{2}}'}_{\xi_2s_3s_{\overline{3}}\xi_{\overline{2}}} \to v(\xi_2s_3s_{\overline{3}}\xi_{\overline{2}})$ $\to \tilde{T}^{\xi_3's_4's_{\overline{4}}'\xi_{\overline{3}}'}_{\xi_3s_4s_{\overline{4}}\xi_{\overline{3}}} \to v(\xi_3s_4s_{\overline{4}}\xi_{\overline{3}}) \to \cdots \to \tilde{T}^{\xi_i's_{i+1}'s_{\overline{i+1}}'\xi_{\overline{i}}'}_{\xi_i\, s_{i+1}s_{\overline{i+1}}\xi_{\overline{i}}} \to v(\xi_i\, s_{i+1}s_{\overline{i+1}}\xi_{\overline{i}})$ up to an arbitrary size i.[59] This is a kind of self consistent equation, and finally we get the fixed

point values $\tilde{T}^{\xi'_\infty s'_{\infty+1} s'_{\overline{\infty+1}} \xi'_{\overline{\infty}}}_{\xi_\infty s_{\infty+1} s_{\overline{\infty+1}} \xi_{\overline{\infty}}}$ and $v(\xi_\infty s_{\infty+1} s_{\overline{\infty+1}} \xi_{\overline{\infty}})$. By decomposing the latter via SVD

$$v(\xi_\infty s_{\infty+1} s_{\overline{\infty+1}} \xi_{\overline{\infty}}) = \sum_{\xi_{\infty+1}} A^{s_{\infty+1}}_{s_\infty \xi_{\infty+1}} \omega_{\xi_{\infty+1}} B_{\xi_{\overline{\infty+1}} s_{\overline{\infty}}}^{\quad s_{\overline{\infty+1}}}, \tag{59}$$

we finally get the position independent tensor in the thermodynamic limit $N \to \infty$.

There are two usages of the infinite system algorithm. One is to use it in order to prepare the tensors that are necessary for the initial step (a) in §6 of the finite system algorithm.[1] After repeating the above iteration for $N/2$ times, and renaming the spin indices $\overline{i} \to N\text{-}i{+}1$, we obtain a good start point for the variational state $v(s_{1\ldots} s_{N/2} s_{N/2+1 \ldots} s_N)$.

The other usage is, as we have intended, to use it purely in order to observe expectation values of local operators (= thermodynamic quantities) in the thermodynamic limit. For example, the spin polarization is obtained as

$$\langle s \rangle = \sum_{\xi s \bar{s} \bar{\xi}} v(\xi s \bar{s} \bar{\xi})\, s\, v(\xi s \bar{s} \bar{\xi}), \tag{60}$$

where $v(\xi s \bar{s} \bar{\xi})$ is the vector $v(\xi_\infty s_{\infty+1} s_{\overline{\infty+1}} \xi_{\overline{\infty}})$ defined in Eq. (59). In the same way, the nearest neighbor spin correlation function is obtained as

$$\langle s \bar{s} \rangle = \sum_{\xi s \bar{s} \bar{\xi}} v(\xi s \bar{s} \bar{\xi})\, s \bar{s}\, v(\xi s \bar{s} \bar{\xi}). \tag{61}$$

We can also calculate spin correlation functions between distant sites, since the variational state is position independent, and we already have the tensors $A^{s_{\infty+1}}_{s_\infty \xi_{\infty+1}}$ and $B_{\xi_{\overline{\infty+1}} s_{\overline{\infty}}}^{\quad s_{\overline{\infty+1}}}$; remember the correspondence between N and $N+2$ in Fig. 12.

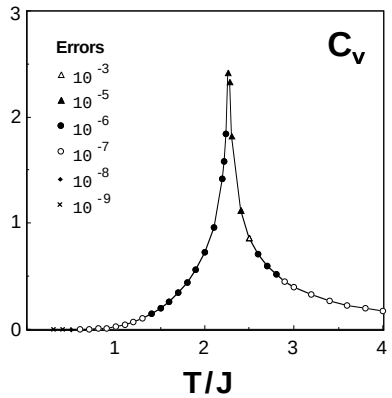

Fig. 13. Specific heat of the Ising model calculated by the infinite system algorithm.

Let us see how precise the infinite DMRG is. Figure 13 shows the specific heat $\mathrm{C_v}(T)$ of the square lattice Ising model, which is obtained by taking the temperature

derivative of the nearest neighbor correlation function $E(T) = \langle s\overline{s} \rangle$ in Eq. (61). We calculate $E(T)$ for the system with $N = 2048$, which is sufficiently larger than the correlation length for each plotted temperature. The m dependence for $E(T)$ is not conspicuous around $m = 60$. Since we know the exact solution of this model,[34] we can directly evaluate the numerical error in $\mathrm{C_v}(T)$. The difference between calculated $\mathrm{C_v}(T)$ and the exact one is indicated by several marks. The numerical error is non-negligible near the critical temperature T_c, partially because $E(T)$ is singular at T_c, and because numerical derivative

$$\frac{E(T + \Delta T/2) - E(T - \Delta T/2)}{\Delta T} \tag{62}$$

is sensitive to ΔT; typically, we set $\Delta T = 10^{-4}$. The other source of numerical error is that the increase of the cut-off energy scale ϵ_m near T_c, that spoils the numerical precision in the block spin transformation. The latter error source can be suppressed by the scaling analysis with respect to m.[58]

For a tutorial purpose we have consider the Ising model throughout this review. From the variational interpretation of DMRG, it is apparent that the method can be applied to more general classical models, such as (a) the models that have *discrete spin symmetry and short range interactions*, as the q-state Potts Model or n-vector models, and (b) the interaction round a face (IRF) model whose Boltzmann weight $W^{s_i' s_{i+1}'}_{s_i s_{i+1}}$ is expressed by *arbitrary square matrices*, where the Boltzmann weight can be even negative or complex. The transfer matrix need not be symmetric.[26]

8. Discussion

The DMRG for 2D classical systems is formulated for the row-to-row transfer matrix. The formulation is therefore anisotropic, since the distinction between horizontal and vertical directions is formally introduced. More isotropic treatment of 2D lattice has been developed by Baxter, using the corner transfer matrix (CTM).[38] It is a small surprise that we encounter the principle of DMRG — the basis truncation assisted by density submatrix, variational relation for partition function, and iterative use of block spin transformation — when we read Baxter's textbook.[38] It is possible to introduce the infinite system algorithm to Baxter's formulation, and to obtain a more isotropic expression of DMRG for 2D classical systems: the corner transfer matrix renormalization group (CTMRG).[62] The advantage of CTMRG is that the numerical calculation is faster than the infinite system DMRG algorithm.

Not only applications, but also the formalism in DMRG are still in progress. We finally pick up several new topics in DMRG. Since in DMRG the ground state is precisely obtained as a product of tensors, it is natural to consider the *analytic formulation of DMRG,*[57,63] whose aim is to obtain the appropriate tensors purely analytically, without any numerical calculation; this attempt is similar to the tensor product Ansatz that had been known before DMRG.[42,43,44,45,46] Quite recently , Sierra *et al* . proposed the '*recurrent variational Ansatz,*[64]' which quantitatively agrees with numerical results by DMRG, and the Ansatz clarifies the physical inter-

pretation of the matrix product state. The extension of the tensor product Ansatz to 2D quantum (or 3D classical) systems is one of the hot subjects that would tell us something about the DMRG for higher dimensional systems.[65,66,67] Finally , we list up several unsolved problems.

- **Periodic Boundary Condition:** It is natural to imagine that the variational state for the system with periodic boundary condition is a uniform (= position independent) tensor product. However, the current finite system algorithm does not produce such a uniform tensor product.[68]
- **Long Range Interactions (LRI):** It is rather hard to treat 1D quantum systems with LRI. It is much harder to treat 2D classical systems with long range interactions; consider how hard to define the transfer matrix is. It is even non-trivial to apply DMRG to 1D classical systems with LRI.
- **Continuous Variable:** Since DMRG is defined for lattice models with discrete site variables, we have to introduce discretization (= regularization) in order to treat models with continuous spin symmetry or field models in continuous space.[69] We don't have any general principle for such a discretization.[70]
- **Random 2D Classical System:** Formally speaking, it is possible to apply DMRG to random 2D classical systems. There are, however, two major problems: (a) Since the transfer matrix and the density matrix are dependent to the position of the spin row, we have to perform RG transformations independently for each row; the procedure is much more time consuming than DMRG for uniform system. (b) Eigenvalues of the density submatrix are not always positive. Therefore , the calculation is not *variational* any more.
- **Free Fermion and Free Boson Systems:** One might think that it is easy to obtain an analytic (or exact) formulation of DMRG for free fermions and bosons on 1D lattice. However, no one has actually diagonalized the density submatrix of such systems in the thermodynamic limit. Similarly, in 2D classical systems, analytic formulation for the Gaussian model or the Ising model at the massless point is not known.[71,72]
- **Solvability:** For exactly solved models,[38] there should be *exact analytic expression for DMRG*, that is not known so far. What is the relation between the R-matrix and the RG transformation matrices in DMRG?
- **Density Matrix Formulation in higher dimensions:** We know the exponential damping of the eigenvalues of the density submatrix for 1D quantum and 2D classical systems. The property enables the precise calculation in DMRG. Can we expect the same damping trend in higher dimensions, including the infinite dimension?[73]

The DMRG is not only a powerful numerical method, but is also a new gate for the analytical study of the statistical systems. We hope that these points will be clarified near future.

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