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A New Monte Carlo Power Method for the Eigenvalue Problem of Transfer Matrices

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We propose a new Monte Carlo method for calculating eigenvalues of transfer matrices leading to free energies and to correlation lengths of classical and quantum many-body systems. Generally, this method can be applied to the calculation of the maximum eigenvalue of a nonnegative matrix $\hat{A}$ such that all the matrix elements of $\hat{A}^k$ are strictly positive for an integer k. This method is based on a new representation of the maximum eigenvalue of the matrix $\hat{A}$ as the thermal average of a certain observable of a many-body system. Therefore one can easily calculate the maximum eigenvalue of a transfer matrix leading to the free energy in the standard Monte Carlo simulations, such as the Metropolis algorithm. As test cases, we calculate the free energies of the square-lattice Ising model and of the spin-1/2 XY Heisenberg chain. We also prove two useful theorems on the ergodicity in quantum Monte Carlo algorithms, or more generally, on the ergodicity of Monte Carlo algorithms using our new representation of the maximum eigenvalue of the matrix $\hat{A}$.

KEY WORDS: Monte Carlo simulations; power method; eigenvalue problems; transfer matrices; free energy calculation.

1. INTRODUCTION

Since Metropolis *et al.* introduced the Monte Carlo method based on the idea of importance sampling into the field of the statistical mechanics,[1] this method has been widely used to study not only classical many-body systems,[2-4] but also quantum ones.[5-7] In fact, this method is very useful for calculating thermal averages of local observables.

However, in the importance-sampling method, it is very hard to obtain partition functions or free energies, because these quantities are not local. The problem of calculating free energies in the Monte Carlo

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simulations has received considerable attention theoretically, and also practically,[2,3] and a number of approaches have been proposed,[2,3] among which the thermodynamic integration method is probably the most popular.[8]

In this paper, for the purpose of calculating the maximum eigenvalue of a given transfer matrix leading to free energies and correlation lengths, we propose a new Monte Carlo method that is a power method combined with the idea of importance sampling. More generally, this method can be applied to the calculation of the maximum eigenvalue of a nonnegative matrix $\hat{A}$ such that all the matrix elements of $\hat{A}^k$ are strictly positive for an integer k. (In most applications, the matrix $\hat{A}$ is chosen as the transfer matrix of a many-body system.)

We start from the Rayleigh quotient, which is the standard expression of the power method for calculating the maximum eigenvalue of the above matrix $\hat{A}$. Our basic observation is that, with an appropriate choice of the trial vector in the Rayleigh quotient, the expression for the Rayleigh quotient becomes the thermal average of an observable of a classical many-body system with free boundary conditions. Such a representation of the maximum eigenvalue in terms of the thermal average may be of interest in its own right, but can also be used as a basis of numerical analysis. By calculating the thermal average of the above observable by a suitable Monte Carlo method, one can easily obtain the desired maximum eigenvalue. In this sense, our method may be summarized as a combination of the power method with the idea of importance sampling.

The paper is organized as follows. In Section 2, we derive the basic representation of the maximum eigenvalue of the matrix $\hat{A}$ in terms of the thermal average of an observable in a many-body system. As test cases, we calculate the free energies of the square-lattice Ising model and of the spin-1/2 XY Heisenberg chain in Section 3 and Section 4, respectively. As the reader can quickly read off from Tables I and II, the numerical results are encouraging. For the latter case, we use the path integral idea of Suzuki[6,7] to transform the partition function of the quantum system into a partition of a classical system. However, for the system so obtained, the ergodicity of Monte Carlo sequences does not simply hold.[5,6] For the problem, in Section 5 we prove two useful theorems that guarantee the ergodicity of quantum Monte Carlo algorithms, or in more general terms, the ergodicity of Monte Carlo algorithms for our new representation of the maximum eigenvalue of the matrix $\hat{A}$, i.e., for the thermal average of an observable in a classical system with Boltzmann weights determined from the matrix elements of $\hat{A}$. As a demonstration, these theorems are used to determine updating procedures in the Monte Carlo simulations for the spin-1/2 XY Heisenberg chain in Section 4.

2. MONTE CARLO POWER METHOD

In this section, we derive a new representation for the maximum eigenvalue of a nonnegative matrix in terms of the thermal average in a many-body system. The representation will serve as the basis of our new Monte Carlo method.

For this purpose, we begin with a review of the power method which we will use in our new formalism.

Given a nonnegative matrix $\hat{A}$, for which there exists an integer k such that all the matrix elements of $\hat{A}^k$ are strictly positive in an orthonormal basis $\{u(n)\}_n$, we consider the Rayleigh quotient

$$\Lambda^{(L)} := \frac{\langle \psi, \hat{A}^{L+1}\psi \rangle}{\langle \psi, \hat{A}^{L}\psi \rangle} \qquad (L = 0, 1, 2, \ldots) \tag{2.1}$$

(the symbol := signifies definition) for a trial vector ψ with nonnegative elements in the orthonormal basis $\{u(n)\}_n$. Then the maximum eigenvalue $\Lambda^{\max}$ of the matrix $\hat{A}$ is written as

$$\Lambda^{\max} = \lim_{L \uparrow \infty} \Lambda^{(L)} \tag{2.2}$$

by the Perron–Frobenius theorem, because all the matrix elements of $\hat{A}^{k'}$ are strictly positive for any integer $k' \geqslant k$.

Generally, power methods depend on the idea that the eigenvector with the maximum eigenvalue $\Lambda^{\max}$ can be obtained by multiplying the trial vector ψ by the matrix $\hat{A}$ repeatedly. Therefore, it is difficult to apply the methods to a large matrix, in particular, to a transfer matrix whose size increases exponentially with the lattice size of a system, requiring a correspondingly large memory area.

Now we shall develop a new method which does not require such a large memory area, i.e., the difficulty can be circumvented in the following way.

We choose

$$\psi = \sum_n u(n) \tag{2.3}$$

for the trial vector. Then, the Rayleigh quotient (2.1) can be written as

$$\Lambda^{(L)} = \frac{1}{Z^{(L)}} \sum_{n_1, \ldots, n_{L+1}} A_S(n_1) \prod_{j=1}^{L} W(n_j, n_{j+1}) \tag{2.4}$$

with

$$A_S(n) := \langle \psi, \hat{A}u(n) \rangle \tag{2.5}$$

$$W(n, m) := \langle u(n), \hat{A}u(m) \rangle \tag{2.6}$$

and

$$Z^{(L)} := \sum_{n_1,\ldots,n_{L+1}} \prod_{j=1}^{L} W(n_j, n_{j+1}) \tag{2.7}$$

The outstanding feature of the representation (2.4) is that it has precisely the form of the thermal average of the observable $A_S(n_1)$ with respect to the configurations $\Omega := \{(n_1,\ldots, n_{L+1})\}$ on the lattice $\{1, 2,\ldots, L+1\}$ with the Boltzmann weights

$$\prod_{j=1}^{L} W(n_j, n_{j+1}) \tag{2.8}$$

because the definition of the matrix $\hat{A}$ guarantees that these Boltzmann weights are nonnegative.

Our representation (2.4) may be of interest in its own right, but (at present) is most useful as a basis of a new numerical method for calculating the maximum eigenvalues of transfer matrices. Since the right-hand side of (2.4) is the thermal average of a classical system, one can invoke any of one's favorite methods to calculate it.

For example, by using the importance-sampling method introduced by Metropolis *et al.*[1-3] (see Appendix B), one can calculate the L-approximate eigenvalue $\Lambda^{(L)}$ for the maximum eigenvalue $\Lambda^{\max}$ of the matrix $\hat{A}$. As is well known,[1-3] the size of the memory area necessary for the calculation with the Metropolis algorithm is roughly proportional to the lattice size of the system. In fact, as will be shown in the following sections, one has only to treat *several* of the matrix elements $W(n, m) = \langle u(n), \hat{A}u(m)\rangle$ in (2.4) per one updating procedure in Monte Carlo simulations in our method without calculating *all* the matrix elements $\langle u(n), \hat{A}^l u(m)\rangle$ $(l = 1, 2,\ldots)$ as in the above power method. Thus, the difficulty in the above power method can be circumvented by our Monte Carlo power method.

In addition, we emphasize that our method is different from the transfer-matrix Monte Carlo method introduced by Nightingale and Blöte,[9] which is a variant of the Green's-function Monte Carlo method by Ceperly and Kalos.[10] In fact, their method does not utilize the idea of importance sampling.[11]

3. APPLICATION TO THE SQUARE-LATTICE ISING MODEL

In this section, we shall calculate the free energy of the square-lattice Ising model with the nearest-neighbor interaction by using our Monte Carlo power method of trial. It will be shown that the free energy of the

square-lattice Ising model is represented as the thermal average of the observable (3.6) below in the square-lattice Ising model with free boundary conditions in one of the space directions.

The Hamiltonian of the Ising model is given by

$$H := -\sum_{\langle i,j\rangle} \sigma_i \sigma_j \tag{3.1}$$

where the Ising spin σ_i at the ith site takes the values ± 1, and the summation runs over all the nearest-neighbor pairs of the sites i, j. As is well known, the free energy per spin in the $M \times N$ square lattice with the periodic boundary condition can be written as[12]

$$f_{M,N} := -\frac{1}{\beta MN} \log \mathrm{Tr}\, \hat{W}_N^M \tag{3.2}$$

in terms of the transfer matrix $\hat{W}_N$ with the matrix elements

$$\langle u(\sigma_1,..., \sigma_N), \hat{W}_N u(\sigma'_1,..., \sigma'_N)\rangle = \prod_{j=1}^{N} \exp[\beta\sigma_j(\sigma'_j + \sigma'_{j+1})] \tag{3.3}$$

with the periodic boundary condition

$$\sigma'_{N+1} = \sigma'_1 \tag{3.4}$$

in the orthonormal basis $\{u(\sigma_1,..., \sigma_N)\}$, where β is the inverse temperature and Tr denotes the trace over the spin states. Here, we use the so-called diagonal-to-diagonal transfer matrix $\hat{W}_N$, which is more convenient than the row-to-row transfer matrix[12] for the following calculations.

Then, the free energy per spin in the thermodynamic limit can be written as

$$f = -\lim_{N\uparrow\infty} \frac{1}{\beta N} \log \Lambda_N^{\max} \tag{3.5}$$

in terms of the maximum eigenvalue $\Lambda_N^{\max}$ of the diagonal-to-diagonal transfer matrix $\hat{W}_N$.

Now, in our formula (2.4), the L-approximate eigenvalue $\Lambda_N^{(L)}$ for the maximum eigenvalue $\Lambda_N^{\max}$ is obtained from the thermal average of the observable

$$\begin{aligned} W_{S,N}(\sigma'_1,..., \sigma'_N) &:= \sum_{\sigma_1,..., \sigma_N} \langle u(\sigma_1,..., \sigma_N), \hat{W}_N u(\sigma'_1,..., \sigma'_N)\rangle \\ &= (4\cosh 2\beta)^{N/2} \exp\left(J_S \sum_{j=1}^{N} \sigma'_j \sigma'_{j+1}\right) \\ &\quad (J_S := \tfrac{1}{2}\log\cosh 2\beta) \end{aligned} \tag{3.6}$$

on the surface in the $(L+1)\times N$ Ising system with the free boundary conditions in one space direction, and with the Boltzmann weights (3.3).

We have performed Monte Carlo simulations with the standard Metropolis algorithm on the $(L+1)\times N=16\times 16$ lattice using the personal computer NEC PC-9801F. After equilibration runs of 10^3 Monte Carlo steps per spin, the L-approximate eigenvalue $\Lambda_N^{(L)}$ was obtained with 10^6 Monte Carlo steps per spin.

The free energy f multiplied by $(-\beta)$,

$$-\beta f \sim \frac{1}{N}\log \Lambda_N^{(L)} \qquad (N=16,\ L=15) \tag{3.7}$$

is given in Table I. The statistical errors are estimated in the standard way (for example, see ref. 3). The exact values of Onsager[13] and the results obtained by Schlijper *et al.*[14] in 1990 are also given in the same table.

Schlijper *et al.* used a combination of the cluster-variation method and the local-state method in Monte Carlo simulations[14] on the 64×64 lattice on Cray 1S-2300 and Cray X-MP EA/164 computers. They calculated the free energy by counting the occurrences of various cluster configurations in 10^4 lattice-configuration sweeps. Their method does not work well at the critical temperature $T=T_C$. In fact, in spite of the fact that our size of the system is much smaller than theirs, our result at T_C is more precise than theirs. From our results, it seems that the finite-size corrections are relatively small in the present system. In fact, we were able to obtain satisfactory results in comparison with Onsager's exact values. Of course, it would be necessary for general systems to extrapolate a sequence of finite systems to an infinite one, as in the next section.

Table I. The Free Energy of the Square-Lattice Ising Model[a]

Temperature T/T_C	Free energy $-\beta f$		
	Present work	Exact	Schlijper *et al.* (1990)[14]
0.5	1.76363(4)	1.763668...	1.763668(1)
0.7	1.26684(7)	1.266894...	1.266894(1)
1.0	0.92967(5)	0.929694...	0.9295(1)
2.0	0.74376(1)	0.743754...	0.743753(1)
4.0	0.705402(3)	0.7054090...	0.705406(1)

[a] Numerals in parentheses give the statistical errors in the last digit in the Monte Carlo simulations. T_C denotes the exact critical temperature of Onsager.[13]

To conclude this section, we note that our Monte Carlo power method can be applied also to the calculation of the interface free energies in the two- and three-dimensional Ising models.[2]

4. APPLICATION TO THE SPIN-1/2 *XY* HEISENBERG CHAIN

In this section, we apply our Monte Carlo power method to the spin-1/2 *XY* Heisenberg chain as an example of quantum systems. We will show that the free energy is represented as the thermal average of an observable in a two-dimensional Ising system with free boundary conditions in one of the space directions.

4.1. Transfer Matrix for the Spin-1/2 *XY* Heisenberg Chain

The Hamiltonian is given by

$$\hat{H}_N := \sum_{j=1}^{N} \hat{H}_{j,j+1} \tag{4.1}$$

with

$$\hat{H}_{j,j+1} := -\tfrac{1}{2}(\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y) \tag{4.2}$$

and with the periodic boundary condition

$$\hat{\boldsymbol{\sigma}}_{N+1} = \hat{\boldsymbol{\sigma}}_1 \tag{4.3}$$

where $\hat{\boldsymbol{\sigma}}_j$ is the Pauli spin matrix for the site j ($j = 1,..., N$).

In order to calculate the free energy by our method, one has to define a transfer matrix whose maximum eigenvalue leads to the free energy.[15–21] For this purpose, in the same way as in our previous papers,[19–21] we use the path integral idea of Suzuki[6, 7] to transform the partition function of the model (4.1) with an even number of spins,

$$Z_{2n} := \mathrm{Tr} \exp(-\beta \hat{H}_{2n}) \qquad (n = 1, 2,...) \tag{4.4}$$

into a partition function of a two-dimensional Ising system, where Tr denotes the trace of the matrix.

By using the Trotter formula, we can approximate the partition function (4.4) by[15–20]

$$Z_{2n}^{(M)} := \mathrm{Tr} \left\{ \exp\left(-\frac{\beta \hat{H}_{2n}^{(1)}}{M} \right) \exp\left(-\frac{\beta \hat{H}_{2n}^{(2)}}{M} \right) \right\}^M \tag{4.5}$$

where

$$\hat{H}_{2n}^{(1)} := \sum_{l=1}^{n} \hat{H}_{2l-1,2l} \tag{4.6}$$

and

$$\hat{H}_{2n}^{(2)} := \sum_{l=1}^{n} \hat{H}_{2l,2l+1} \tag{4.7}$$

We call M the Trotter number. Further, by using the path integral idea, we can write the M-approximate partition function (4.5) as[19, 20]

$$Z_{2n}^{(M)} = \sum_{\Omega_n} \left\langle u_n^1, \exp\left(-\frac{\beta \hat{H}_{2n}^{(1)}}{M}\right) u_n^2 \right\rangle \times \left\langle u_n^2, \exp\left(-\frac{\beta \hat{H}_{2n}^{(2)}}{M}\right) u_n^3 \right\rangle \cdots \left\langle u_n^{2M}, \exp\left(-\frac{\beta \hat{H}_{2n}^{(2)}}{M}\right) u_n^1 \right\rangle \tag{4.8}$$

where

$$\Omega_n := \{(u_n^1, u_n^2, \ldots, u_n^{2M})\} \tag{4.9}$$

$$u_n^m := u(\sigma_1^m) \otimes u(\sigma_2^m) \otimes \cdots \otimes u(\sigma_{2n}^m) \qquad (m = 1, 2, \ldots, 2M) \tag{4.10}$$

and

$$u(\sigma) := \begin{cases} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & (\sigma = +1) \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} & (\sigma = -1) \end{cases} \tag{4.11}$$

Therefore, by (4.6) and (4.7), it is easily shown that the partition function (4.8) is equivalent to one of a two dimensional Ising system with a four-Ising-spin interaction.[19, 20] For this two-dimensional Ising system, one can define two transfer matrices, one in the "time" direction, and the other in the "space" direction. In terms of the transfer matrix $\hat{U}_{2M}$ in the "space" direction, the M-approximate partition function (4.8) with $n = ML$ ($L = 1, 2, \ldots$) can be written as[19, 20]

$$Z_{2n}^{(M)} := \mathrm{Tr}(\hat{U}_{2M})^{2n} \qquad (n = ML;\ L = 1, 2, \ldots) \tag{4.12}$$

The explicit expression of $\hat{U}_{2M}$ is given by[19, 20]

$$\hat{U}_{2M} := \hat{T}_{2M}^{-1} \hat{R}_{2M} \tag{4.13}$$

with

$$\hat{R}_{2M} := \prod_{l=1}^{M} \hat{V}_{2l-1,2l} \tag{4.14}$$

and

$$\hat{V}_{i,j} := \tfrac{1}{2}(e^{\beta/M} + \hat{\tau}_i^x \hat{\tau}_j^x + \hat{\tau}_i^y \hat{\tau}_j^y - e^{-\beta/M} \hat{\tau}_i^z \hat{\tau}_j^z) \tag{4.15}$$

where $\hat{\tau}_j$ is the Pauli spin operator for the site with time j ($j = 1, 2, \ldots, 2M$), and $\hat{T}_{2M}$ is an operator that shifts any periodic array of the spin states by one lattice unit backward along the "time" direction.

The free energy per spin in the thermodynamic limit is given by

$$f := -\frac{1}{\beta} \lim_{m \uparrow \infty} \lim_{M \uparrow \infty} \frac{1}{2m} \log Z_{2m}^{(M)} \tag{4.16}$$

But the order of limits can be interchanged by the theorem.[16–21] Therefore, by (4.12), the free energy per spin in the thermodynamic limit can be written as

$$\begin{aligned} f &= -\frac{1}{\beta} \lim_{M \uparrow \infty} \lim_{L \uparrow \infty} \frac{1}{2ML} \log \operatorname{Tr}(\hat{U}_{2M})^{2ML} \\ &= -\frac{1}{\beta} \lim_{M \uparrow \infty} \log \Lambda_{2M}^{\max} \end{aligned} \tag{4.17}$$

in terms of the maximum eigenvalue $\Lambda_{2M}^{\max}$ of the transfer matrix $\hat{U}_{2M}$.

To apply our method to the transfer matrix $\hat{U}_{2M}$, we study the properties of this matrix.

From the definition $\hat{U}_{2M}$ in (4.13)–(4.15), one notices immediately that it commutes with

$$\hat{\tau}_{\text{tot}}^z := \sum_{j=1}^{2M} \hat{\tau}_j^z \tag{4.18}$$

We define $\hat{U}_{2M;k}$ to be the operator $\hat{U}_{2M}$ restricted to the k-down-spin subspace. We similarly define $\hat{R}_{2M;k}$.

Then, as we showed in a previous paper,[20] there exists an integer l such that $(\hat{U}_{2M;k})^l$ is strictly positive in the basis

$$\{u(\tau_1, \ldots, \tau_{2M})\} \tag{4.19}$$

restricted to the k-down-spin subspace, where

$$u(\tau_1, \ldots, \tau_{2M}) := u(\tau_1) \otimes \cdots \otimes u(\tau_{2M}) \tag{4.20}$$

and $u(\tau)$ is given by (4.11) with $\tau = \pm 1$. Further, we showed[20] that the maximum eigenvalue $\Lambda_{2M}^{\max}$ is equal to the maximum eigenvalue $\Lambda_{2M;M}^{\max}$ of $\hat{U}_{2M;M}$.

Therefore, it is sufficient to apply our method to the eigenvalue problem of the transfer matrix $\hat{U}_{2M;M}$ for calculating the free energy of the present model (4.1).

Now, by using our formula (2.4), we calculate the L-approximate eigenvalue $\Lambda_{2M;M}^{(L)}$ for the maximum eigenvalue $\Lambda_{2M;M}^{\max}$. It is obtained from the thermal average of the observable

$$\begin{aligned} U_{S,2M;M}(\tau'_1,\ldots,\tau'_{2M}) &:= \sum_{\tau_1,\ldots,\tau_{2M}} \langle u(\tau_1,\ldots,\tau_{2M}),\, \hat{U}_{2M;M} u(\tau'_1,\ldots,\tau'_{2M})\rangle \\ &= \prod_{l=1}^{M} \frac{1+e^{\beta/M}}{2\cosh K_S} \exp(K_S \tau'_{2l-1}\tau'_{2l}) \\ &\quad \left[K_S := \frac{1}{2}\log\tanh\left(\frac{\beta}{2M}\right)\right] \end{aligned} \tag{4.21}$$

on the surface in the $(L+1)\times 2M$ Ising system with the free boundary conditions in the "space" direction, and with the Boltzmann weights[15–21]

$$\begin{aligned} &\prod_{j=1}^{L} \langle u(\tau_1^j,\ldots,\tau_{2M}^j),\, \hat{U}_{2M;M} u(\tau_1^{j+1},\ldots,\tau_{2M}^{j+1})\rangle \\ &\quad = \prod_{j=1}^{L} \langle u(\mu_1^j,\ldots,\mu_{2M}^j),\, \hat{R}_{2M;M}(j)\, u(\mu_1^{j+1},\ldots,\mu_{2M}^{j+1})\rangle \end{aligned} \tag{4.22}$$

where

$$\mu_l^j := \tau_{l-j+1}^j \qquad (l=1,2,\ldots,2M) \tag{4.23}$$

with

$$\tau_l^j = \tau_{2M+l}^j \qquad (j=1,2,\ldots,L+1) \tag{4.24}$$

and

$$\hat{R}_{2M;M}(j) := \begin{cases} \hat{T}_{2M}^{-1}\hat{R}_{2M;M}\hat{T}_{2M} & (j=\text{odd}) \\ \hat{R}_{2M;M} & (j=\text{even}) \end{cases} \tag{4.25}$$

The right-hand side of (4.22) can be written as the product of

$$W(\mu_i,\mu_j;\mu'_i,\mu'_j) := \langle u(\mu_i,\mu_j),\, \hat{V}_{i,j} u(\mu'_i,\mu'_j)\rangle \tag{4.26}$$

that is, it equals the product of the Boltzmann weights for a four-Ising spin interaction.

4.2. Problems in Quantum Monte Carlo Simulations

Before applying our method to the system derived from the path integral formula, we note that the following three serious problems are known to exist generally in Monte Carlo simulations for quantum many-body systems.[5, 6]

(i) Negative Boltzmann weights.[5, 6]

(ii) Ergodicity of Monte Carlo sequences.[5, 22–24]

(iii) Wiesler freezing.[25]

These problems do not arise in the standard classical systems such as the Ising model in the previous section, i.e., these problems are peculiar to the systems derived from the path integral formula or our new formalism in general cases in Section 2.

However, in our present case, problem (i) does not arise, because all Boltzmann weights (4.26) are nonnegative, and problems (ii) and (iii) can be circumvented in the following way.

For problem (ii), we use the neighboring-four-spin flips for the bulk Ising spins,[5, 6] and the neighboring-two-spin flips for the Ising spins on the surface of the system with the free boundaries as the elementary updating procedures F. Then, we can show, following from the argument in the next Section 5, that the updating procedures F define an ergodic sequence (see Appendix A for the details).

In addition, we emphasize that our method does not use the often very costly global-spin-flip procedures[6, 22, 26] at all.

4.3. "n-Fold Way Algorithm"

To proceed to discuss problem (iii), we review briefly Wiesler freezing.[25]

To obtain the free energy per spin in the thermodynamic limit from the maximum eigenvalue $\Lambda_{2M}^{\max} = \Lambda_{2M;M}^{\max}$, one has to take the limit $M \uparrow \infty$ of M in (4.17). However, when M is sufficiently large for a given inverse temperature β, the transition probabilities become very small because the Boltzmann weights

$$W(+1, +1; +1, +1) = W(-1, -1; -1, -1) = \sinh\left(\frac{\beta}{M}\right) \tag{4.27}$$

in (4.26) become very small compared with other nonzero Boltzmann weights in (4.26). Therefore, the rate of generating new configurations becomes quite slow, and consequently, much time is wasted for rejected events in the standard Metropolis algorithm. This is the Wiesler freezing.

To avoid this problem, we use the "n-fold way" algorithm introduced by Bortz *et al.*[3, 27] (see Appendix B for the details). In this algorithm, once spins are selected, a flipping for the spins is immediately performed without wasting any time by rejecting events, because spins are selected in proportion to their probability of flipping. Of course, the computation time to generate a new configuration using the "n-fold way" algorithm is longer than the computation time to try a new configuration using the standard Metropolis algorithm. But, in situations in which the standard algorithm often rejects trial configurations, the "n-fold way" algorithm proceeds much faster.[27, 28]

4.4. Results for the Free Energy of the Spin-1/2 *XY* Heisenberg Chain

With the "n-fold way" algorithm and using the personal computer NEC PC-9801F, we performed Monte Carlo simulations for the present system defined by (4.22) with the length $L+1 \leqslant 63$ of the chain, and with the Trotter number $M \leqslant 16$. After equilibration runs of 10^4 Monte Carlo steps per spin, the L-approximate maximum eigenvalue $\Lambda_{2M;M}^{(L)}$ was obtained with 10^6 Monte Carlo steps per spin. The statistical errors are estimated in the standard way[2, 3] using the standard deviations which are defined by using the average (B.14).

The free energy per spin in the thermodynamic limit is given by

$$f = -\frac{1}{\beta} \lim_{M \uparrow \infty} \log \Lambda_{2M;M}^{\max} = -\frac{1}{\beta} \lim_{M \uparrow \infty} \lim_{L \uparrow \infty} \log \Lambda_{2M;M}^{(L)} \tag{4.28}$$

from (4.17). We take the double limits by using the least-square fitting combined with the AIC method.[19, 20, 29] Here, we remark that the limit

Table II. The Free Energy of the Spin-1/2 *XY* Heisenberg Chain[a]

Inverse temperature β	Free energy $-\beta f$	
	Present work	Exact
0.5	0.752(1)	0.7537...
1.0	0.918(1)	0.9174...
2.0	1.418(4)	1.4152...
10.0	6.396(5)	6.3924...

[a] Numerals in parentheses give the error in the last digit.

$M \uparrow \infty$ is effected by numerical extrapolation using the fact that maximum eigenvalue $\Lambda_{2M}^{\max} = \Lambda_{2M;M}^{\max}$ is a function of M.[6, 7, 16, 19, 20, 30]

The estimates of the free energy f multiplied by $(-\beta)$ and the exact values[31, 32] are given in Table II.

Our results agree very well with the exact values.

Thus, our Monte Carlo power method is useful for calculating the free energy of quantum systems as well as the one of classical systems as shown in Section 3.

To conclude the section, we note that our Monte Carlo power method can be applied also to the calculation of the correlation lengths of classical and quantum many-body systems.[12, 17–21, 33–37]

5. ERGODICITY OF MONTE CARLO SEQUENCES

As mentioned in the previous section, the ergodicity of Monte Carlo sequences does not simply hold for quantum systems, in more general, for our new representation (2.4) of the maximum eigenvalue of the matrix $\hat{A}$ in Section 2.

In this section, we study general properties of Monte Carlo sequences generated by the Monte Carlo algorithm for our system with the Boltzmann weights (2.8). In particular, Theorems 5.9 and 5.10 below guarantee the ergodicity of Monte Carlo sequences in our method. In fact, these theorems are very useful for determining updating procedures in Monte Carlo simulations of quantum systems as in Section 4.

In the following, we restrict the configuration space $\Omega = \{(n_1, n_2, ..., n_{L+1})\}$ in (2.4) to the subspace Ω^+ of all the configurations with nonzero Boltzmann weights (2.8).

We define B_i^+ to be the set of all the branchings of configurations $\{(n_i, n_{i+1}), (n_i, n'_{i+1})\}$ on the sublattice $\{i, i+1\} \subset \{1, 2, ..., L+1\}$ such that

$$n_{i+1} \neq n'_{i+1} \tag{5.1}$$

Further, we define B_j^- to be the set of all the branchings of configurations $\{(n_j, n_{j+1}), (n'_j, n_{j+1})\}$ on the sublattice $\{j, j+1\} \subset \{1, 2, ..., L+1\}$ such that

$$n_j \neq n'_j \tag{5.2}$$

If two configurations $\omega_{i,i+s} = (n_i, ..., n_{i+s})$ and $\omega'_{i,i+s} = (n'_i, ..., n'_{i+s})$ on the sublattice $\{i, ..., i+s\}$ $(1 \leqslant i \leqslant L-1,\ 2 \leqslant s \leqslant L+1-i)$ satisfy the conditions

$$n_i = n'_i, \qquad n_{i+1} \neq n'_{i+1}, \qquad n_{i+s-1} \neq n'_{i+s-1}, \qquad n_{i+s} = n'_{i+s} \tag{5.3}$$

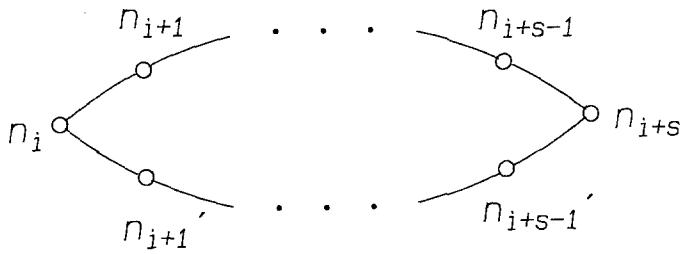

Fig. 1. The loop with length s on the sublattice $\{i, i+1,..., i+s\}$. The bonds represent nonzero Boltzmann weights.

then we say that $\{\omega_{i,i+s}, \omega'_{i,i+s}\}$ is the loop with the length s; this loop is represented in Fig. 1.

Clearly, this loop has the branching $\{(n_i, n_{i+1}), (n_i, n'_{i+1})\} \in B_i^+$, and also $\{(n_{i+s-1}, n_{i+s}), (n'_{i+s-1}, n_{i+s})\} \in B_{i+s-1}^-$.

For the branching $b_i^+ \in B_i^+$, we define

$$s(b_i^+) := \begin{cases} \min_{\rho \in E(b_i^+)} l(\rho) & [E(b_i^+) \neq \varnothing] \\ L+2-i & [E(b_i^+) = \varnothing] \end{cases} \qquad (i=1, 2,..., L) \qquad (5.4)$$

where $E(b)$ is the set of all loops having the branching b, $l(\rho)$ is the length of the loop ρ, and $\varnothing$ denotes the empty set.

Similarly, for the branching $b_j^- \in B_j^-$, we define

$$t(b_j^-) := \begin{cases} \min_{\rho \in E(b_j^-)} l(\rho) & [E(b_j^-) \neq \varnothing] \\ j+1 & [E(b_j^-) = \varnothing] \end{cases} \qquad (j=1, 2,..., L) \qquad (5.5)$$

Lemma 5.1. For any $b_i^+ = \{(n_i, n_{i+1}), (n_i, n'_{i+1})\} \in B_i^+$ $(i=1, 2,..., L)$, the integer $s(b_i^+)$ of (5.4) satisfies the inequality

$$2 \leqslant s(b_i^+) \leqslant k+1 \qquad (5.6)$$

where the integer k is determined by the condition that all the matrix elements of $\hat{A}^k$ are strictly positive (see the definition of the matrix $\hat{A}$ in Section 2). Therefore, k is independent of the linear dimension $L+1$ of the lattice $\{1, 2,..., L+1\}$.

Proof. Clearly, from the definition of $s(b_i^+)$ of (5.4), we have $2 \leqslant s(b_i^+)$. This is the lower bound of (5.6).

From the condition for the matrix $\hat{A}^k$, we have

$$\langle u(n_{i+1}), \hat{A}^k u(m) \rangle \neq 0 \qquad (5.7)$$

and

$$\langle u(n'_{i+1}), \hat{A}^k u(m) \rangle \neq 0 \qquad (5.8)$$

for any configuration m, and for the configurations n_{i+1} and n'_{i+1} in the branching b_i^+.

If $i+k \leqslant L$, then (5.7) and (5.8) imply that there exists a loop ρ with length $l(\rho) \leqslant k+1$ such that ρ has the branching b_i^+. Therefore, by (5.4), we have

$$s(b_i^+) \leqslant l(\rho) \leqslant k+1 \tag{5.9}$$

Conversely, if $i+k > L$, then we have

$$k > L-i \geqslant s(b_i^+) - 2 \tag{5.10}$$

by (5.4).

Thus, we obtain (5.6). QED

Similarly, we have the following result:

Lemma 5.2. For any $b_j^- = \{(n_j, n_{j+1}), (n'_j, n_{j+1})\} \in B_j^-$ $(j = 1, 2, \ldots, L)$, the integer $t(b_j^-)$ of (5.5) satisfies the inequality

$$2 \leqslant t(b_j^+) \leqslant k+1 \tag{5.11}$$

where k is the same integer as in Lemma 5.1.

By using the integers $s(b_i^+)$ and $t(b_j^-)$ in Lemmas 5.1 and 5.2, we define the integer

$$r := \max\{r^+, r^-\} \tag{5.12}$$

with

$$r^+ := \max_{b^+ \in B^+} s(b^+) \tag{5.13}$$

and

$$r^- := \max_{b^- \in B^-} t(b^-) \tag{5.14}$$

where

$$B^+ := \bigcup_{i=1}^{L} B_i^+ \qquad \text{and} \qquad B^- := \bigcup_{j=1}^{L} B_j^- \tag{5.15}$$

By Lemmas 5.1 and 5.2, we have the following result:

Lemma 5.3. The integer r of (5.12) satisfies the inequality

$$2 \leqslant r \leqslant k+1 \tag{5.16}$$

where the integer k is determined by the condition that all the matrix elements of $\hat{A}^k$ are strictly positive. Therefore, the integer k is independent of the linear dimension $L+1$ of the lattice $\{1, 2,..., L+1\}$.

For the configuration $\omega = (n_1,..., n_{L+1})$, we define the q-neighborhood $U_q(\omega)$ $(q \geqslant 2)$ of ω to be the set of all the configurations of three types ω'_a, ω'_b, ω'_c, where

$$\omega'_a := (n_1,..., n_i, n'_{i+1},..., n'_{i+q-1}, n_{i+q},..., n_{L+1}) \qquad (1 \leqslant i, \quad i+q \leqslant L+1) \tag{5.17}$$

$$\omega'_b := (n'_1,..., n'_{i-1}, n_i,..., n_{L+1}) \qquad (1 \leqslant i \leqslant q \leqslant L+1) \tag{5.18}$$

and

$$\omega'_c := (n_1,..., n_i, n'_{i+1},..., n'_{L+1}) \qquad (1 \leqslant L+2-q \leqslant i \leqslant L+1) \tag{5.19}$$

These configurations ω, ω'_a, ω'_b, and ω'_c are represented in Fig. 2.

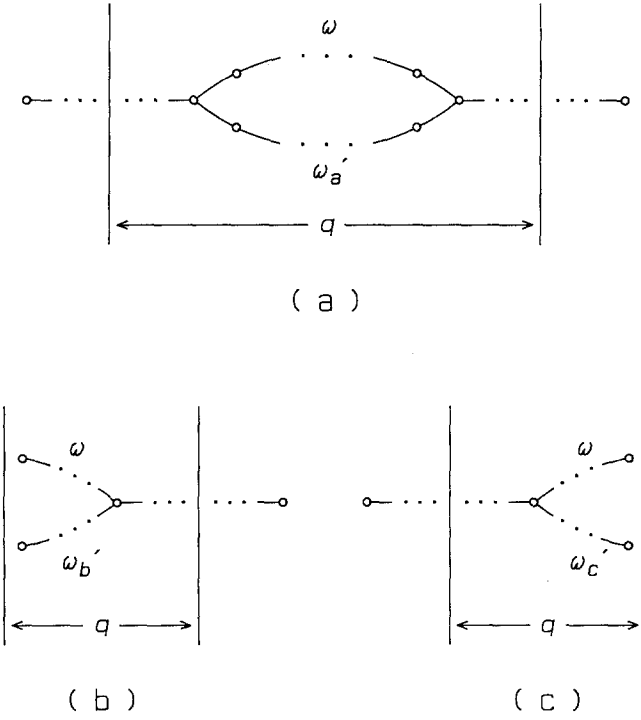

Fig. 2. The configuration pairs (a) $\{\omega, \omega'_a\}$, (b) $\{\omega, \omega'_b\}$, and (c) $\{\omega, \omega'_c\}$.

Further, we define the branching with tails

$$b^+_{1\sim i} := \{(n_1,..., n_i, n_{i+1}), (n_1,..., n_i, n'_{i+1})\} \qquad (n_{i+1} \neq n'_{i+1}) \tag{5.20}$$

$$b^-_{j\sim L+1} := \{(n_j, n_{j+1},..., n_{L+1}), (n'_j, n_{j+1},..., n_{L+1})\} \qquad (n_j \neq n'_j) \tag{5.21}$$

$$B^+_\sim := \bigcup_{i=1}^{L} b^+_{1\sim i} \tag{5.22}$$

and

$$B^-_\sim := \bigcup_{j=1}^{L} b^-_{j\sim L+1} \tag{5.23}$$

That is, $b^+_{1\sim i}$ is the branching $\{(n_i, n_{i+1}), (n_i, n'_{i+1})\}$ with the tail $(n_1,..., n_{i-1})$, and $b^-_{j\sim L+1}$ is the branching $\{(n_j, n_{j+1}), (n'_j, n_{j+1})\}$ with the tail $(n_{j+2},..., n_{L+1})$.

For $b_\sim \in B^+_\sim \cup B^-_\sim$ and $q \geqslant 2$, we define $C_q(b_\sim)$ to be a set of all the pairs of configurations $\{\omega, \omega'\} = \{(n_1,..., n_{L+1}), (n'_1,..., n'_{L+1})\}$ such that $\omega' \in U_q(\omega)$ and that $\{\omega, \omega'\}$ contains the branching $b_\sim$.

Lemma 5.4. Let $q \geqslant r$, where r is given by (5.12). Then, we have $C_q(b_\sim) \neq \varnothing$ for any branching $b_\sim \in B^+_\sim \cup B^-_\sim$.

Proof. If $b_\sim \in B^+_\sim$, then $b_\sim$ contains a branching $b^+_i \in B^+_i$. Therefore, from the definitions of (5.12)–(5.15) for r, we have $s(b^+_i) \leqslant r \leqslant q$. This implies, by (5.4), that there exists a loop ρ with the length $l(\rho) \leqslant q$ and having the branching b^+_i, or $L+2-i \leqslant q$. By combining this with the definitions (5.17) and (5.19) for $U_q(\omega)$, we can easily find a pair of configurations $\{\omega, \omega'\} \in C_q(b_\sim)$.

The case of $b_\sim \in B^-_\sim$ can be treated in the same way. QED

Definition 5.5. Let ω and ω' be two configurations, and let F be a set of updating procedures in a Monte Carlo algorithm. We define

$$\omega \sim_F \omega'$$

if and only if ω and ω' can be connected by applications of elements w's in F, i.e., updating procedures w's define the nonzero transition probabilities, which can be written as

$$w(\omega \to \omega') = w(\omega_0 \to \omega_1)\, w(\omega_1 \to \omega_2) \cdots w(\omega_{k-1} \to \omega_k = \omega') \tag{5.24}$$

and

$$w(\omega' \to \omega) = w(\omega' = \omega_k \to \omega_{k-1}) \cdots w(\omega_1 \to \omega_0 = \omega) \tag{5.25}$$

in terms of elements

$$w(\omega_i \to \omega_{i+1}),\ w(\omega_{i+1} \to \omega_i) \in F \qquad (i = 0, 1, \ldots, k-1) \tag{5.26}$$

Definition 5.6. Let F be a set of updating procedures in a Monte Carlo algorithm. We say that F has the updating range $q \geqslant 2$ if and only if, for any given branching $b_{\sim} \in B^{+}_{\sim} \cup B^{-}_{\sim}$, there exists a pair of configurations $\{\omega, \omega'\}$ such that $\omega \sim_F \omega'$ and $\{\omega, \omega'\} \in C_q(b_{\sim})$.

Lemma 5.7. Let ω_i and ω'_i be two configurations which can be written as

$$\omega_i = (n_1, \ldots, n_i, n_{i+1}, \ldots, n_{L+1}) \tag{5.27}$$

and

$$\omega'_i = (n_1, \ldots, n_i, n'_{i+1}, \ldots, n'_{L+1}) \tag{5.28}$$

with

$$n_{i+1} \neq n'_{i+1} \qquad (i = 1, 2, \ldots, L) \tag{5.29}$$

that is, $\{\omega_i, \omega'_i\}$ has the branching $b^{+}_{1 \sim i} = \{(n_1, \ldots, n_i, n_{i+1}), (n_1, \ldots, n_i, n'_{i+1})\} \in B^{+}_{\sim}$ (see Fig. 3), and let F be a set of updating procedures that has the updating range $q = r$, where r is given by (5.12). Then

$$\omega_i \sim_F \omega'_i \qquad (i = 1, \ldots, L)$$

Proof. Clearly, $\{\omega_L, \omega'_L\} \in B^{+}_{\sim}$ by the definitions of (5.20) and (5.22). Therefore, by Definition 5.6, there exists $\{\omega, \omega'\}$ such that $\omega \sim_F \omega'$ and $\{\omega, \omega'\} \in C_q(\{\omega_L, \omega'_L\})$. By the definition of $C_q(\cdots)$, $\{\omega, \omega'\}$ contains

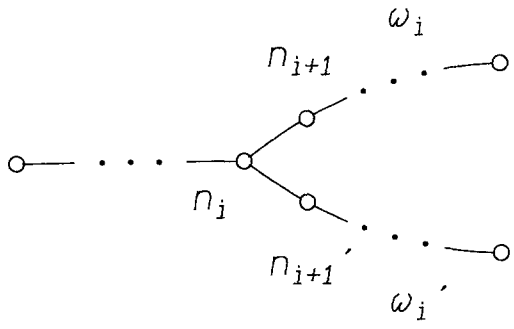

Fig. 3. The configuration pair $\{\omega_i, \omega'_i\}$ with the branching $\{(n_i, n_{i+1}), (n_i, n'_{i+1})\}$.

$\{\omega_L, \omega'_L\}$. This implies $\{\omega, \omega'\} = \{\omega_L, \omega'_L\}$. Combining this with $\omega \sim_F \omega'$ gives $\omega_L \sim_F \omega'_L$.

Therefore, it is sufficient to show that if $\omega_{i+1} \sim_F \omega'_{i+1}$ for any ω_{i+1} and ω'_{i+1}, then $\omega_i \sim_F \omega'_i$ for any ω_i and ω'_i.

As shown in Fig. 3, the pair of configurations $\{\omega_i, \omega'_i\}$ of (5.27) and (5.28) contains the branching $b^+_{1\sim i}$. Therefore, by the assumption for F, there exist two configurations

$$\omega_i^+ = \begin{cases} (n_1, \ldots, n_i, n_{i+1}, n^+_{i+2}, \ldots, n^+_{i+s-1}, n^*_{i+s}, \ldots, n^*_{L+1}) & (L+1-i \geqslant r) \\ (n_1, \ldots, n_i, n_{i+1}, n^+_{i+2}, \ldots, n^+_{L+1}) & (L+1-i < r) \end{cases} \tag{5.30}$$

and

$$\omega_i^- = \begin{cases} (n_1, \ldots, n_i, n'_{i+1}, n^-_{i+2}, \ldots, n^-_{i+s-1}, n^*_{i+s}, \ldots, n^*_{L+1}) & (L+1-i \geqslant r) \\ (n_1, \ldots, n_i, n'_{i+1}, n^-_{i+2}, \ldots, n^-_{L+1}) & (L+1-i < r) \end{cases} \tag{5.31}$$

with an integer s $(s \leqslant r)$ (see Fig. 4).

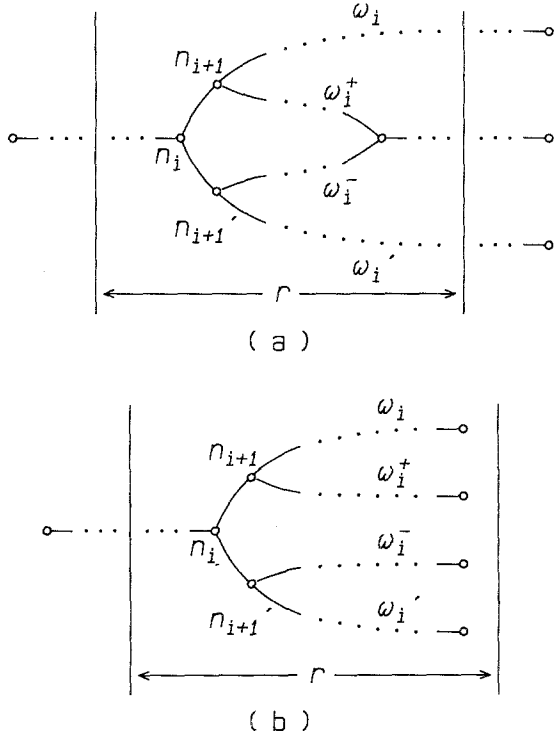

Fig. 4. The configurations ω_i, ω'_i, ω_i^+, and ω_i^- in the cases of (a) $L+1-i \geqslant r$ and of (b) $L+1-i < r$.

These satisfy

$$\omega_i^+ \sim_F \omega_i^- \tag{5.32}$$

Further, from the assumption that $\omega_{i+1} \sim_F \omega'_{i+1}$ for any ω_{i+1} and ω'_{i+1}, we have

$$\omega_i \sim_F \omega_i^+ \qquad \text{and} \qquad \omega_i^- \sim_F \omega'_i \tag{5.33}$$

The relations (5.32) and (5.33) imply

$$\omega_i \sim_F \omega'_i \tag{5.34}$$

Thus, the lemma has been proved. QED

Similarly, we have the following result:

Lemma 5.8. Let ω_j and ω'_j be two configurations which can be written as

$$\omega_j = (n_1, ..., n_{j-1}, n_j, ..., n_{L+1}) \tag{5.35}$$

and

$$\omega'_j = (n'_1, ..., n'_{j-1}, n_j, ..., n_{L+1}) \tag{5.36}$$

with

$$n_{j-1} \neq n'_{j-1} \qquad (j = 2, 3, ..., L+1) \tag{5.37}$$

(see Fig. 5), and let F be a set of updating procedures that has the updating range $q = r$, where r is given by (5.12). Then

$$\omega_j \sim_F \omega'_j \qquad (j = 2, 3, ..., L+1)$$

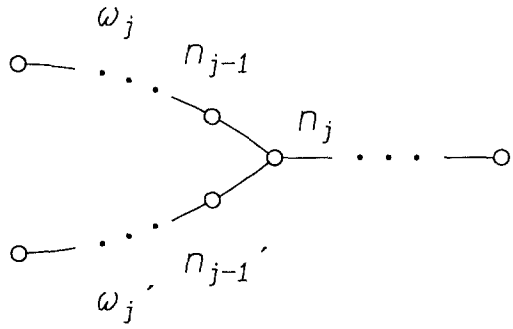

Fig. 5. The configuration pair $\{\omega_j, \omega'_j\}$ with the branching $\{(n_{j-1}, n_j), (n'_{j-1}, n_j)\}$.

Theorem 5.9. Let F be a set of updating procedures that has the updating range $q = r$, where r is given by (5.12). Then, F defines an ergodic Monte Carlo sequence if the linear dimension $L+1$ of the lattice in (2.4) is sufficiently large, i.e., $\hat{A}^L$ is positive in the basis $\{u(n)\}_n$.

Proof. It is sufficient to show that any two configurations $\omega = (n_1, ..., n_{L+1})$ and $\omega' = (n'_1, ..., n'_{L+1})$ can be connected by applications of elements of F, i.e., $\omega \sim_F \omega'$.

By the assumption on the linear dimension L and the definition of the matrix $\hat{A}$, we have

$$\langle u(n_1), \hat{A}^L u(n'_{L+1}) \rangle \neq 0 \tag{5.38}$$

This implies that there exists a configuration ω^* that can be written as

$$\omega^* = (n_1, n_2^*, ..., n_L^*, n'_{L+1}) \tag{5.39}$$

Therefore, by Lemmas 5.7 and 5.8, we have

$$\omega \sim_F \omega^* \qquad \text{and} \qquad \omega^* \sim_F \omega' \tag{5.40}$$

Thus, we obtain

$$\omega \sim_F \omega' \qquad \text{QED} \tag{5.41}$$

Theorem 5.10. Let F be a set of updating procedures that has the updating range $q = r$, where r is given by (5.12). Then, F defines an ergodic Monte Carlo sequence if the matrix $\hat{A}$ is symmetric in the basis $\{u(n)\}_n$, i.e., the transposed matrix ${}^t\hat{A}$ equals $\hat{A}$ itself.

Proof. Let $\omega = (n_1, ..., n_{L+1})$ and $\omega' = (n'_1, ..., n'_{L+1})$ be two configurations. Then, by the definition of the matrix $\hat{A}$, there exists an integer k such that

$$\langle u(n_1), \hat{A}^{2kL} u(n'_1) \rangle \neq 0 \tag{5.42}$$

This implies that there exist configurations $n_{L+1}^{(1)}, ..., n_{L+1}^{(k)}$ and $n_1^{(1)}, ..., n_1^{(k-1)}$ such that

$$\begin{aligned} &\langle u(n_1), \hat{A}^L u(n_{L+1}^{(1)}) \rangle \times \langle u(n_{L+1}^{(1)}), \hat{A}^L u(n_1^{(1)}) \rangle \\ &\quad \times \langle u(n_1^{(1)}), \hat{A}^L u(n_{L+1}^{(2)}) \rangle \times \cdots \times \langle u(n_{L+1}^{(k-1)}), \hat{A}^L u(n_1^{(k-1)}) \rangle \\ &\quad \times \langle u(n_1^{(k-1)}), \hat{A}^L u(n_{L+1}^{(k)}) \rangle \times \langle u(n_{L+1}^{(k)}), \hat{A}^L u(n'_1) \rangle \neq 0 \end{aligned} \tag{5.43}$$

We note that, for any two configurations m and m',

$$\langle u(m), \hat{A}^L u(m') \rangle = \langle u(m'), \hat{A}^L u(m) \rangle \tag{5.44}$$

by ${}^t\hat{A} = \hat{A}$ in the basis $\{u(n)\}_n$. Further, note that if, for two configurations m and m',

$$\langle u(m), \hat{A}^L u(m') \rangle \neq 0 \qquad (L \geqslant 1) \tag{5.45}$$

then there exists a configuration ω^* that can be written as

$$\omega^* = (m, n_1^*, ..., n_{L-1}^*, m') \tag{5.46}$$

Therefore, there exist two configurations $\omega^{(1)}$ and $\omega^{(k)}$ that can be written as

$$\omega^{(1)} = (n_1, n_2^{(1)}, ..., n_{L+1}^{(1)}) \tag{5.47}$$

and

$$\omega^{(k)} = (n_1', n_2^{(k)}, ..., n_{L+1}^{(k)}) \tag{5.48}$$

and that satisfy

$$\omega^{(1)} \sim_F \omega^{(k)} \tag{5.49}$$

by Lemmas 5.7 and 5.8.

Further, by Lemmas 5.7 and 5.8, we obtain

$$\omega \sim_F \omega^{(1)} \qquad \text{and} \qquad \omega' \sim_F \omega^{(k)} \tag{5.50}$$

These relations (5.49) and (5.50) imply

$$\omega \sim_F \omega' \qquad \text{QED} \tag{5.51}$$

The applications to the spin-1/2 XY Heisenberg chain in the previous section are given in Appendix A.

To conclude this section, we emphasize that in our method, there exists no such difficulty as in the standard power methods mentioned in Section 2. In fact, one can calculate the Rayleigh quotient $\Lambda^{(L)}$ without calculating the matrix elements $\langle u(n), \hat{A}^k u(m) \rangle$ $(k = 1, 2, ...)$, i.e., one has only to treat several of the matrix elements $W(n, m) = \langle u(n), \hat{A} u(m) \rangle$ in (2.4) in each updating procedure in the Metropolis algorithm; the number of elements $W(n, m)$ per one updating can be determined by the integer r of (5.12), which is independent of the linear dimension $L+1$ of the lattice in our formula (2.4) (see Lemma 5.3).

APPENDIX A. PROOF OF THE ERGODICITY OF THE MONTE CARLO SEQUENCES FOR THE SPIN-1/2 *XY* HEISENBERG CHAIN

In this appendix, we show, following from the argument in Section 5, that the updating procedures F introduced in Section 4.2 define an ergodic sequence.

First, we calculate r of (5.12), which will be equal to the updating range of the procedures F which consist of the neighboring-four- and neighboring-two-spin flips.

Consider the branching $b_i^+ := \{(\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1}), (\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1'})\}$, where

$$\boldsymbol{\mu} := \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_{2M} \end{pmatrix} \tag{A.1}$$

It satisfies

$$\langle u(\boldsymbol{\mu}^i), \hat{R}_{2M;M}(i)\, u(\boldsymbol{\mu}^{i+1}) \rangle \neq 0 \tag{A.2}$$

and

$$\langle u(\boldsymbol{\mu}^i), \hat{R}_{2M;M}(i)\, u(\boldsymbol{\mu}^{i+1'}) \rangle \neq 0 \tag{A.3}$$

by the definition of the branching and (4.22)–(4.25).

We note that

$$\langle u(\boldsymbol{\mu}^{i+1}), \hat{R}_{2M;M}(i+1)\, u(\boldsymbol{\mu}^{i+1}) \rangle \neq 0 \tag{A.4}$$

and

$$\langle u(\boldsymbol{\mu}^{i+1'}), \hat{R}_{2M;M}(i+1)\, u(\boldsymbol{\mu}^{i+1'}) \rangle \neq 0 \tag{A.5}$$

by (4.14), (4.15), and (4.25). Further, since the matrices $\hat{R}_{2M;M}(\cdots)$ are symmetric, we have

$$\langle u(\boldsymbol{\mu}^{i+1}), \hat{R}_{2M;M}(i+2)\, u(\boldsymbol{\mu}^i) \rangle \neq 0 \tag{A.6}$$

and

$$\langle u(\boldsymbol{\mu}^{i+1'}), \hat{R}_{2M;M}(i+2)\, u(\boldsymbol{\mu}^i) \rangle \neq 0 \tag{A.7}$$

by (A.2), (A.3), and (4.25).

The relations (A.2)–(A.7) imply that the loop $\rho_{i,i+3}$ has the length 3, where

$$\rho_{i,i+3} := \{(\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1}, \boldsymbol{\mu}^{i+1}, \boldsymbol{\mu}^i), (\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1'}, \boldsymbol{\mu}^{i+1'}, \boldsymbol{\mu}^i)\} \tag{A.8}$$

Further, one can immediately notice that this loop has the branching

$$b_{i+2}^- = \{(\boldsymbol{\mu}^{i+1}, \boldsymbol{\mu}^i)(\boldsymbol{\mu}^{i+1'}, \boldsymbol{\mu}^i)\}$$

On the other hand, there is no loop with the length $s \leqslant 2$ by (4.14), (4.15), (4.22), and (4.25).

Therefore, we have $r=3$ by (5.4), (5.5), and (5.12)–(5.15).

Next, we show that the updating procedures F (the neighboring-four-spin flips) connect

$$\omega_{i,i+3} := (\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1}, \boldsymbol{\mu}^{i+1}, \boldsymbol{\mu}^i)$$

with

$$\omega'_{i,i+3} := (\boldsymbol{\mu}^i, \boldsymbol{\mu}^{i+1'}, \boldsymbol{\mu}^{i+1'}, \boldsymbol{\mu}^i)$$

in the loop $\rho_{i,i+3}$ of (A.8).

We proceed by classifying the cases as follows.

(1) $i=$ even.

By (4.14) and (4.25), we have

$$\langle u(\boldsymbol{\mu}^i), \hat{R}_{2M;M}(i)\, u(\boldsymbol{\mu}^{i+1})\rangle = \prod_{l=1}^{M} \langle u(\mu^i_{2l-1}, \mu^i_{2l}), \hat{V}_{2l-1,2l} u(\mu^{i+1}_{2l-1}, \mu^{i+1}_{2l})\rangle \tag{A.9}$$

and

$$\langle u(\boldsymbol{\mu}^i), \hat{R}_{2M;M}(i)\, u(\boldsymbol{\mu}^{i+1'})\rangle = \prod_{l=1}^{M} \langle u(\mu^i_{2l-1}, \mu^i_{2l}), \hat{V}_{2l-1,2l} u(\mu^{i+1'}_{2l-1}, \mu^{i+1'}_{2l})\rangle \tag{A.10}$$

Therefore, if $\mu^i_{2l-1} = \mu^i_{2l}$, then we have

$$\mu^{i+1}_{2l-1} = \mu^{i+1}_{2l} = \mu^{i+1'}_{2l-1} = \mu^{i+1'}_{2l} \tag{A.11}$$

by (4.15).

Conversely, if $\mu^i_{2l-1} \neq \mu^i_{2l}$, then we have

$$\mu^{i+1}_{2l-1} = -\mu^{i+1}_{2l} = \mu^{i+1'}_{2l-1} = -\mu^{i+1'}_{2l} \tag{A.12}$$

or

$$\mu^{i+1}_{2l-1} = -\mu^{i+1}_{2l} = -\mu^{i+1'}_{2l-1} = \mu^{i+1'}_{2l} \tag{A.13}$$

In the case of (A.13), the four-spin flip changes

$$\left(\begin{pmatrix}\mu^{i+1}_{2l-1}\\ \mu^{i+1}_{2l}\end{pmatrix}, \begin{pmatrix}\mu^{i+1}_{2l-1}\\ \mu^{i+1}_{2l}\end{pmatrix}\right) \tag{A.14}$$

into

$$\left(\begin{pmatrix}\mu^{i+1'}_{2l-1}\\ \mu^{i+1'}_{2l}\end{pmatrix}, \begin{pmatrix}\mu^{i+1'}_{2l-1}\\ \mu^{i+1'}_{2l}\end{pmatrix}\right) \tag{A.15}$$

The results (A.11)–(A.15) imply that one can connect $\omega_{i,i+3}$ with $\omega'_{i,i+3}$ by many applications of the four-spin flips.

(2) $i =$ odd.

This case can be treated in the same way in the above.

Thus, the updating procedures F connect $\omega_{i,i+3}$ with $\omega'_{i,i+3}$.

Further, if the branchings are in the free boundaries, i.e.,

$$b_i^+ = b_L^+ = \{(\boldsymbol{\mu}^L, \boldsymbol{\mu}^{L+1}), (\boldsymbol{\mu}^L, \boldsymbol{\mu}^{L+1'})\} \tag{A.16}$$

or

$$b_{i+1}^- = b_1^- = \{(\boldsymbol{\mu}^1, \boldsymbol{\mu}^2), (\boldsymbol{\mu}^{1'}, \boldsymbol{\mu}^2)\} \tag{A.17}$$

then, in the same way, one can connect $\boldsymbol{\mu}^{L+1}$ with $\boldsymbol{\mu}^{L+1'}$, and also $\boldsymbol{\mu}^1$ with $\boldsymbol{\mu}^{1'}$ by many applications of the two-spin flips.

Therefore, for any given branching $b_\sim$ with tails, one can easily find a pair of configurations $\{\omega, \omega'\} \in C_{q=r=3}(b_\sim)$ in Definition 5.6 in Section 5, i.e., the updating procedures F have the range 3.

Combining this with Theorem 5.9, we have that the updating procedures F define an ergodic sequence if the linear dimension $L+1$ of the lattice in (4.22) is sufficiently large.

Further, we note that one can easily extend Theorem 5.10 to the one for the present system (4.22), which can be rewritten in terms of two symmetric matrices $\hat{R}_{2M;M}(\cdots)$. That is, the updating procedures F define an ergodic sequence for the present system with any size $L+1$ of the linear dimension.

APPENDIX B. "n-FOLD WAY" ALGORITHM[3, 27, 28]

We first review the standard Metropolis algorithm.[1–3]

Consider the master equation for the probability $P_n(\omega)$ that configuration ω occurs at the nth step,

$$P_n(\omega) = \sum_{\omega' \neq \omega} P_{n-1}(\omega')\, w(\omega' \to \omega) + P_{n-1}(\omega)\, w(\omega \to \omega) \qquad (n = 1, 2, \ldots) \tag{B.1}$$

where

$$w(\omega \to \omega) := 1 - Q(\omega) \tag{B.2}$$

with

$$Q(\omega) := \sum_{\omega' \neq \omega} w(\omega \to \omega') \tag{B.3}$$

and $w(\omega \to \omega')$ $(\omega \neq \omega')$ is the transition probability from ω to ω' that satisfies the detailed balance condition

$$P_{eq}(\omega)\, w(\omega \to \omega') = P_{eq}(\omega')\, w(\omega' \to \omega) \tag{B.4}$$

with the canonical distribution

$$P_{eq}(\omega) := \frac{1}{Z} \exp[-\beta H(\omega)] \tag{B.5}$$

Here, H is the Hamiltonian and Z is the partition function, i.e.,

$$Z := \sum_{\omega} \exp[-\beta H(\omega)] \tag{B.6}$$

Clearly, there exists an arbitrariness in the choice of the transition probability w. Metropolis *et al.*[1] proposed

$$w(\omega \to \omega') = \begin{cases} \tau^{-1} \exp\{-\beta[H(\omega') - H(\omega)]\}, & H(\omega') > H(\omega) \\ \tau^{-1}, & \text{otherwise} \end{cases} \tag{B.7}$$

for $\omega \neq \omega'$, where τ is an arbitrary time unit that does not affect the detailed balance condition (B.4), and that satisfies the condition such that

$$\sum_{\omega' \neq \omega} w(\omega \to \omega') \leqslant 1 \tag{B.8}$$

for any configuration ω. In passing, we note that another way is the so-called "heat-bath" method,[38, 39]

$$w(\omega \to \omega') = \frac{\tau^{-1} \exp\{-\beta[H(\omega') - H(\omega)]\}}{1 + \exp\{-\beta[H(\omega') - H(\omega)]\}} \tag{B.9}$$

for ω, where τ satisfies the same condition as above.

Starting from an initial configuration ω_0, one can construct a Markov sequence $\{\omega_0, \omega_1, \omega_2, \ldots\}$ by the master equation (B.1), then the thermal average of an observable O,

$$\langle O \rangle := \sum_{\omega} O(\omega)\, P_{eq}(\omega) \tag{B.10}$$

can be written in terms of an arithmetic average

$$\langle O \rangle = \lim_{T \uparrow \infty} \frac{1}{T} \sum_{j=0}^{T} O(\omega_j) \tag{B.11}$$

However, the usefulness of this standard algorithm is limited by the low transition probability (B.7) or (B.9) of generating new configurations.

To avoid this difficulty, Bortz *et al.* proposed the "n-fold way" algorithm.[3, 27, 28] In their method, a Markov sequence is generated by the master equation[28]

$$P_n^*(\omega) = \sum_{\omega'} P_{n-1}^*(\omega')\, w^*(\omega' \to \omega) \tag{B.12}$$

with

$$w^*(\omega \to \omega') := \begin{cases} w(\omega \to \omega')/Q(\omega) & (\omega \neq \omega') \\ 0 & (\omega = \omega') \end{cases} \tag{B.13}$$

That is, in their Monte Carlo simulations, once one event $\omega \to \omega'$ is selected, the updating is immediately performed without wasting any time by rejected events. Of course, because of Q in (B.13), the computation time to generate a new configuration using the "n-fold way" algorithm is longer than the computation time to try a new configuration using the standard Metropolis algorithm. But in situations in which the standard algorithm often rejects trial configurations, the "n-fold way" algorithm proceeds much faster.[27, 28]

The thermal average of the observable O is given by an average,

$$\langle O \rangle = \lim_{T \uparrow \infty} \frac{\sum_{j=0}^{T} O(\omega_j^*)\, Q^{-1}(\omega_j^*)}{\sum_{j=0}^{T} Q^{-1}(\omega_j^*)} \tag{B.14}$$

where $\{\omega_j^*\}$ is a Markov sequence generated by the master equation (B.12).

To show (B.14), we note that, by (B.1)–(B.5), (B.12), and (B.13),

$$\sum_{\omega} w^*(\omega' \to \omega) = 1 \tag{B.15}$$

$$Q(\omega)\, P_{\text{eq}}(\omega) = \sum_{\omega'} Q(\omega')\, P_{\text{eq}}(\omega')\, w^*(\omega' \to \omega) \tag{B.16}$$

and

$$P_{\text{eq}}^*(\omega) = \sum_{\omega'} P_{\text{eq}}^*(\omega')\, w^*(\omega' \to \omega) \tag{B.17}$$

where P_{eq}^* is the equilibrium distribution for the master equation (B.12). Equation (B.15) implies that the vector with all components 1 is the right eigenvector with the eigenvalue 1 of the matrix $w^*(\omega' \to \omega)$. Therefore, the maximum eigenvalue of this matrix is 1 by the Perron–Frobenius theorem.

On the other hand, Eqs. (B.16) and (B.17) imply that both of the vectors $Q(\omega) P_{eq}(\omega)$ and $P^*_{eq}(\omega)$ are left eigenvectors with the eigenvalue 1 of the matrix $w^*(\omega' \to \omega)$. Therefore, again by the Perron–Frobenius theorem, we have

$$N \times P^*_{eq}(\omega) = Q(\omega) P_{eq}(\omega) \tag{B.18}$$

where N is a positive constant that is independent of the configuration ω. Thus, with (B.10), we obtain (B.14).

Finally, we note that the detailed balance condition

$$P^*_{eq}(\omega) w^*(\omega \to \omega') = P^*_{eq}(\omega') w^*(\omega' \to \omega) \tag{B.19}$$

holds from (B.4), (B.13), and (B.18).

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