Transfer-matrix method and Monte Carlo simulation in quantum spin systems

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Transfer-matrix methods for quantum spin systems are formulated and their limiting properties are studied rigorously. The present formulation is applied explicitly to an exactly soluble transverse Ising model. A computer implementation of the two-dimensional triangular antiferromagnetic quantum Heisenberg model is also proposed to study Anderson's picture of the dynamic coherence of the phase of singlet pairs.

I. INTRODUCTION AND SOME USEFUL FORMULAS

Analytical methods, particularly the transfer-matrix method,[1,2] have been very useful in rigorously studying the statistical mechanics of classical systems such as the Ising model. The purpose of the present paper is to extend the transfer-matrix method to quantum spin systems, to investigate some general features of this "quantum transfer-matrix method," and to apply this method to the one-dimensional transverse Ising model.

The basis of the quantum transfer-matrix method comes from the following equivalence theorem.[3]

Equivalence theorem (Ref. 3): A d-dimensional quantum spin system is mapped into a $(d+1)$-dimensional Ising system with many-spin interactions as follows: The partition function Z of a Hamiltonian $\mathscr{H}=\mathscr{H}_0+\mathscr{H}_1+\cdots+\mathscr{H}_p$ is expressed by

$$Z=\mathrm{Tr}^{(d)}e^{-\beta\mathscr{H}}=\mathrm{Tr}^{(d+1)}\exp\mathscr{H}_{\mathrm{eff}}^{(d+1)}\ , \tag{1.1}$$

where $\mathscr{H}_{\mathrm{eff}}^{(d+1)}$ denotes an effective $(d+1)$-dimensional Hamiltonian.

An explicit expression of the effective Hamiltonian $\mathscr{H}_{\mathrm{eff}}^{(d+1)}$ can be obtained[3] by using the following formula.[4]

Formula 1: For any set of operators $\{A_j\}$ in a Banach algebra, we have

$$\left|\left|\exp\left[\sum_{j=1}^{p}A_j\right]-\left[\prod_{j=1}^{p}\exp\left[\frac{1}{n}A_j\right]\right]^n\right|\right| \le\frac{1}{n}\left[\sum_{j=1}^{p}||A_j||\right]^2\exp\left[\sum_{j=1}^{p}||A_j||\right]\ , \tag{1.2}$$

where p is an arbitrary positive integer. Namely, for bounded operators $\{A_j\}$ we have

$$\lim_{n\to\infty}\left[\prod_{j=1}^{p}\exp\frac{1}{n}A_j\right]^n=\exp\sum_{j=1}^{p}A_j\ . \tag{1.3}$$

A little weaker upper bound than (1.2) was given in a previous paper by the present author.[4] Thus it will be instructive to give here a brief proof of (1.2). If we set

$$g=\exp\left[\frac{1}{n}\sum_{j=1}^{p}A_j\right]\quad\text{and}\quad h=\prod_{j=1}^{p}\exp\left[\frac{1}{n}A_j\right]\ , \tag{1.4}$$

then we obtain

$$\begin{aligned}||g^n-h^n||&\le||g-h||(||g||^{n-1}+||g||^{n-2}||h||+\cdots+||h||^{n-1})\\&\le n||g-h||\exp\left[\frac{n-1}{n}\sum_{j=1}^{p}||A_j||\right]\ .\end{aligned} \tag{1.5}$$

Next, it is easy to show that

$$\begin{aligned}||g-h||&\le2\left[\exp\left[\frac{1}{n}\sum_{j=1}^{p}||A_j||\right]-\left[1+\frac{1}{n}\sum_{j=1}^{p}||A_j||\right]\right]\\&\le\frac{1}{n^2}\left[\sum_{j=1}^{p}||A_j||\right]^2\exp\left[\frac{1}{n}\sum_{j=1}^{p}||A_j||\right]\ ,\end{aligned} \tag{1.6}$$

where we have used the mean value theorem. Thus we arrive at (1.2).

On the basis of the above equivalent theorem, Suzuki[3,4] proposed a systematic method of Monte Carlo simulation on quantum systems, and then there have been published many papers,[5–15] which applied the above Monte Carlo method of quantum systems to the quantum Heisenberg model, the XY model, and fermion systems. It is also of interest to note the following symmetry property of the approximant $f(n)$ defined by

$$f(n)=\mathrm{Tr}(e^{(1/n)A}e^{(1/n)B})^n\ . \tag{1.7}$$

Evenness of approximants: The approximant $f(n)$ defined by (1.7) is an even function of n. *Proof*: We have

$$f(-n)=\mathrm{Tr}(e^{-(1/n)A}e^{-(1/n)B})^{-n}=\mathrm{Tr}[(e^{-(1/n)A}e^{-(1/n)B})^{-1}]^{n}$$
$$=\mathrm{Tr}(e^{(1/n)B}e^{(1/n)A})^{n}=\mathrm{Tr}(e^{(1/n)A}e^{(1/n)B})^{n}=f(n)\ . \tag{1.8}$$

This symmetry property suggests that the correction of the approximant $f(n)$ to $\mathrm{Tr}\exp(A+B)$ is not of the order of $1/n$, but of the order of $1/n^2$. In fact, we can show the following inequality.

n^{-2}-correction law: For any operators A and B in a Banach algebra, we have

$$|\,\mathrm{Tr}\,e^{A+B}-\mathrm{Tr}(e^{(1/n)A}e^{(1/n)B})^{n}\,|\le\frac{d(||A||+||B||)^3}{3n^2}\exp(||A||+||B||)\ , \tag{1.9}$$

where d denotes the dimensionality of the operators A and B, and the norm $||Q||$ in (1.9) is defined by the maximum value of the absolute magnitude of the eigenvalue of a Hermitian operator Q.

This is a direct result of the following formula.

Formula 2: For any operators A and B in a Banach algebra, we have

$$||e^{A+B}-(e^{(1/2n)A}e^{(1/n)B}e^{(1/2n)A})^{n}||\le\frac{(||A||+||B||)^3}{3n^2}\exp(||A||+||B||)\ . \tag{1.10}$$

The proof is easily given in a way similar to (1.5) and (1.6), namely by noting that

$$||e^{1/n(A+B)}-e^{(1/2n)A}e^{(1/n)B}e^{(1/2n)A}||\le 2\left[e^{1/n(||A||+||B||)}-\left[1+\frac{||A||+||B||}{n}+\frac{(||A||+||B||)^2}{2n^2}\right]\right]$$
$$\le\frac{1}{3n^3}(||A||+||B||)^3\exp\frac{1}{n}(||A||+||B||)\ . \tag{1.11}$$

This n^{-2}-correction law on the trace of $[\exp(1/n)A\exp(1/n)B]^n$, not the operator itself, was pointed out to hold by Hirsch *et al.*[7] and by De Raedt *et al.*,[7] with the use of the properties that

$$\mathrm{Tr}(e^{(1/n)A}e^{(1/n)B})^{n}=\mathrm{Tr}(e^{(1/2n)A}e^{(1/n)B}e^{(1/2n)A})^{n}\ , \tag{1.12}$$

and that

$$e^{\tau(A+B)}-e^{(1/2)\tau A}e^{\tau B}e^{(1/2)\tau A}=O(\tau^3)\ . \tag{1.13}$$

The inequality (1.11) is only a rigorous statement of (1.13). The above n^{-2}-correction law has also been found numerically by many authors in performing Monte Carlo simulations of quantum systems. The present formulation gives rigorous proof of this n^{-2}-correction law for the partition function, namely for the trace of an exponential operator.

The above symmetry property, namely the evenness of the approximants, can be easily extended to any set of $\{A_j\}$ by the following.

Generalized evenness of approximants: The symmetrized approximant $f^{(s)}(n)$ defined by $f^{(s)}(n)=\mathrm{Tr}F^{(s)}(n)$ with

$$F^{(s)}(n)=(e^{(1/2n)A_1}e^{(1/2n)A_2}\cdots e^{(1/2n)A_{p-1}}e^{(1/n)A_p}e^{(1/2n)A_{p-1}}\cdots e^{(1/2n)A_1})^{n} \tag{1.14}$$

is an even function of n.

The proof is quite the same as in (1.8). Thus the correction of $f^{(s)}(n)$ is of the order of n^{-2}.

Similarly to (1.9) and (1.10), the following generalized inequalities hold.

Formula 3: For any set of operators $\{A_j\}$ in a Banach algebra, we have

$$\left|\left|\exp\sum_{j=1}^{p}A_j-F^{(s)}(n)\right|\right|\le\frac{1}{3n^2}\left[\sum_{j=1}^{p}||A_j||\right]^2\exp\left[\sum_{j=1}^{p}||A_j||\right] \tag{1.15}$$

with $F^{(s)}(n)$ defined by (1.14), and

$$\left|\mathrm{Tr}\exp\sum_{j=1}^{p}A_j-f^{(s)}(n)\right|\le\frac{d}{3n^2}\left[\sum_{j=1}^{p}||A_j||\right]^2\exp\left[\sum_{j=1}^{p}||A_j||\right]\ , \tag{1.16}$$

where the norm $||Q||$ in (1.16) is defined as in (1.9). It is worthwhile to note the following formula.

Formula 2: For any operators A and B in a Banach algebra, we have

$$||e^{A+B}-(e^{(1/n)A}e^{(1/n)B})^n|| \le \frac{||[A,B]||}{2n}\exp(||A||+||B||) . \tag{1.17}$$

Proof: If we set

$$F(x)=\exp[x(A+B)]-\exp(xA)\exp(xB) ,$$

then we obtain the following expression:

$$F(x)=\int_0^x dt\int_0^t ds\, e^{tA}e^{(t-s)B}[B,A]e^{sB}e^{(x-t)(A+B)} \tag{1.18}$$

using Kubo's identity,[16]

$$[A,e^{tB}]=\int_0^t e^{(t-s)B}[A,B]e^{sB}ds . \tag{1.19}$$

Therefore, we obtain the following inequality:

$$||F(x)|| \le \frac{x^2}{2}||[A,B]||\exp[x(||A||+||B||)] . \tag{1.20}$$

By combining (1.5) with (1.20) for $x=1/n$, we arrive at (1.17).

II. TRANSFER-MATRIX METHODS IN QUANTUM SPIN SYSTEMS

As was mentioned in the preceding section, the transfer-matrix method can be applied to a $(d+1)$-dimensional effective classical Hamiltonian equivalent to the original system. This method was already used implicitly in a previous paper[3] to solve the one-dimensional transverse Ising model.[17,18] We start with the following Hamiltonian composed of two parts:

$$\mathscr{H}=\mathscr{H}_1+\mathscr{H}_2 , \tag{2.1}$$

where $\mathscr{H}_1$ and $\mathscr{H}_2$ are sums[3] of commutable local operators:

$$\mathscr{H}_1=\sum_{\underset{\sim}{r}}\mathscr{H}_1(\underset{\sim}{r}),\ [\mathscr{H}_1(\underset{\sim}{r}),\mathscr{H}_1(\underset{\sim}{r}')]=0 \tag{2.2}$$

and

$$\mathscr{H}_2=\sum_{\underset{\sim}{r}}\mathscr{H}_2(\underset{\sim}{r}),\ [\mathscr{H}_2(\underset{\sim}{r}),\mathscr{H}_2(\underset{\sim}{r}')]=0 . \tag{2.3}$$

The partition function of this system is expressed[3] as

$$\begin{aligned}Z=\mathrm{Tr}\,e^{-\beta\mathscr{H}}&=\lim_{n\to\infty}\mathrm{Tr}\left[\exp\left[-\frac{\beta}{n}\mathscr{H}_1\right]\exp\left[-\frac{\beta}{n}\mathscr{H}_2\right]\right]^n\\&=\lim_{n\to\infty}\sum_{\{\alpha_j\}\{\alpha_j'\}}\exp\left[\sum_{j=1}^n[\mathscr{H}_1(\alpha_j,\alpha_j')+\mathscr{H}_2(\alpha_j',\alpha_{j+1})]\right]\\&\equiv\sum_{\{\alpha_j\}\{\alpha_j'\}}\exp\mathscr{H}_{\mathrm{eff}} ,\end{aligned} \tag{2.4}$$

in terms of some appropriate representation $|\alpha_j\rangle$ with $|\alpha_{n+1}\rangle\equiv|\alpha_1\rangle$, where

$$\mathscr{H}_k(\alpha,\alpha')=\ln\left\langle\alpha\left|\exp\left[-\frac{\beta}{n}\mathscr{H}_k\right]\right|\alpha'\right\rangle \tag{2.5}$$

for $k=1$ and 2.

Now, the transfer-matrix method can be applied to the above equivalent effective classical Hamiltonian $\mathscr{H}_{\mathrm{eff}}$ in the following two ways.

A. Real-space transfer-matrix method

The above classical representation (2.4) is rewritten as

$$Z=\lim_{n\to\infty}\mathrm{Tr}_{\{\alpha_j\}}(T_1T_2)^n , \tag{2.6}$$

where $\{T_k\}$ denotes the following transfer matrices:

$$T_k=\left[\left\langle\alpha\left|\exp\left[-\frac{\beta}{n}\mathscr{H}_k\right]\right|\alpha'\right\rangle\right] . \tag{2.7}$$

See Fig. 1 for the direction of transfer. As was seen in Onsager's celebrated paper,[19,20] the symmetrized transfer-matrix $T=T_1^{1/2}T_2T_1^{1/2}$ can be diagonalized with eigenvalues $\{\lambda_j\}$ in some appropriate systems. In such lucky cases, the partition function of such quantum spin systems can be obtained analytically in a classical way as

$$Z=\lim_{n\to\infty}\mathrm{Tr}T^n=\lim_{n\to\infty}\sum_j\lambda_j^n . \tag{2.8}$$

Here it should be remarked that the eigenvalues $\{\lambda_j\}$ depend on n in a singular way, and consequently all the eigenvalues $\{\lambda_j\}$ have to be retained in the summation (2.8) in contrast to the ordinary transfer-matrix method in which the maximum eigenvalue gives an exact result in the thermodynamic limit.

In the case when the transfer matrix cannot be diagonalized analytically (as in most cases), direct numerical calculations of the product $(T_1T_2)^n$ are useful for small finite lattices and Monte Carlo simulation is also practical[3–15] for larger finite lattices, as was mentioned in Sec. II. We have the following theorem concerning the limit of the free energy per spin $f_{m,n}$ defined by

$$f_{m,n}=\frac{-k_BT}{\Omega}\ln\mathrm{Tr}[T(m)]^n,\quad \Omega\equiv m^d \tag{2.9}$$

where $T(m)$ denotes the transfer matrix for the lattice size m, and d denotes the dimensionality of the system.

Theorem 1: For spin systems described by the Hamiltonian (2.1) with (2.2) and (2.3), the following limit exists:

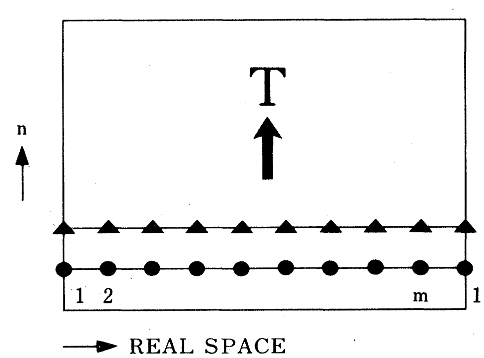

FIG. 1. Transfer matrix T in d-dimensional real space.

$$\lim_{n\to\infty} f_{m,n} \equiv f_m \ . \qquad (2.10)$$

The proof is easily given for formula 1, (1.2). The existence of the thermodynamic limit

$$\lim_{m\to\infty} f_m \equiv f \qquad (2.11)$$

has been proved by Griffiths.[21] Therefore, we have

$$\lim_{m\to\infty} \lim_{n\to\infty} f_{m,n} = f \ . \qquad (2.12)$$

B. Virtual-space transfer-matrix method

The second formulation is to apply the transfer-matrix method to the virtual space, as shown in Fig. 2. The partition function is expressed by

$$Z = \lim_{n\to\infty} \mathrm{Tr}[T'(n)]^m \ , \qquad (2.13)$$

where the transfer matrix $T'(n)$ is easily obtained explicitly from the classical representation (2.4). The dimensionality D' of T'_n is given by

$$D' = 2^{nm^{d-1}} \ , \qquad (2.14)$$

where another extra factor of 2 may appear owing to the structure of $T'(n)$, while the dimensionality D of the real-space transfer matrix $T(m)$ is

$$D = 2^{m^d} \ . \qquad (2.15)$$

Thus we have $D' \ll D$ when $n \ll m$. As was seen in Refs. 5—15, a small value of n might be enough to obtain reliable results for the partition function except at very low temperatures. In such a situation, this second formulation will be more useful for numerical calculation by a high-speed computer. It will be possible to perform numerical calculation[22] for a very large (practically infinite) value of m.

The free energy per spin $f_{m,n}$ is now given by

$$f_{m,n} = \frac{-k_B T}{\Omega} \ln \mathrm{Tr}[T'(n)]^m \ . \qquad (2.16)$$

The following relation should hold:

$$\mathrm{Tr}[T'(n)]^m = \mathrm{Tr}[T(m)]^n \ , \qquad (2.17)$$

from the definition of $f_{m,n}$, though it is not easy to confirm this relation for explicit expressions of $T(m)$ and $T'(n)$.

An important question concerning the above two limits

$$\lim_{m\to\infty} \lim_{n\to\infty} f_{m,n} = f \ \text{ and } \lim_{n\to\infty} \lim_{n\to\infty} f_{m,n} = \tilde{f} \ , \qquad (2.18)$$

and concerning the double limit

$$\lim_{\substack{m\to\infty \\ n\to\infty}} f_{m,n} = \hat{f} \ , \qquad (2.19)$$

is, do they exist? If they exist, do they agree with each other?

An answer to the above question is given by the following theorem.

Theorem 2: For the free energy defined by (2.16) with the Hamiltonian (2.1) of short-range interaction, the three limits (2.18) and (2.19) exist and they are all equal, namely $f = \tilde{f} = \hat{f}$.

Proof: We divide the proof in the following three steps.

Step 1: First we prove the uniform convergence of $f_{m,n}$ for $m \to \infty$. Similarly to Griffith's arguments[21] on the ordinary thermodynamic limit, we separate the whole system into 2^d parts as shown in Fig. 3, where d denotes the dimensionality of the system. It is easily shown that

$$| f_{m',n} - f_{m,n} | \le \frac{d}{m'} \frac{|J|}{n} n = \frac{d\,|J|}{m'} \ , \qquad (2.20)$$

where $m' = 2m$ and J denotes a typical strength of interaction. Consequently, we have

$$| f_{m'',n} - f_{m,n} | \le \frac{d}{m} |J| \ , \ \ m'' = 2^p m \qquad (2.21)$$

for any positive integers m, n, and p. Thus we arrive at the inequality

$$| f_{m,n} - f_{m',n} | < \epsilon \qquad (2.22)$$

for any $m, m' > N_1 = d\,|J|/\epsilon$, irrespectively of n. This is Cauchy's condition on uniform convergence. That is, we have

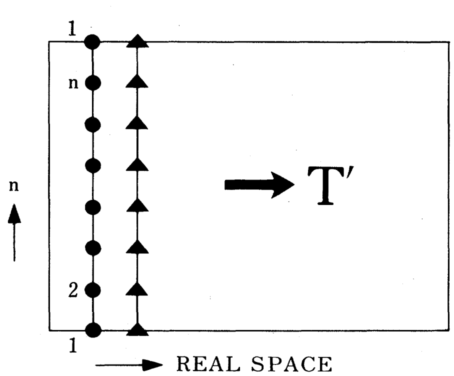

FIG. 2. Transfer matrix T' in virtual space and $(d-1)$-dimensional real space.

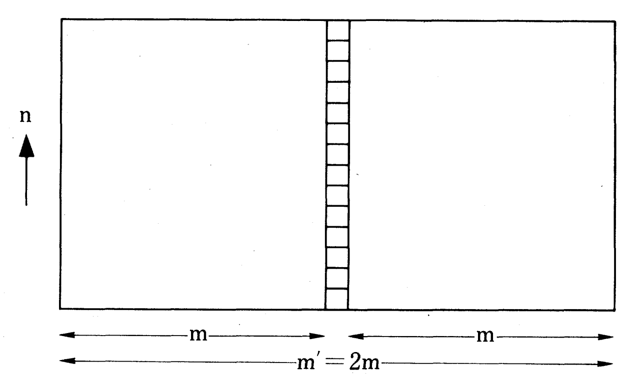

FIG. 3. Separation of the $(d+1)$-dimensional system into 2^d subregions; $m' = 2m$.

$$\lim_{m\to\infty} f_{m,n} = \tilde{f}_n(\text{uniformly}) . \tag{2.23}$$

Step 2: First, we prove the following lemma on the double series $\{a_{m,n}\}$. *Lemma*: If the limits

$$\lim_{n\to\infty} a_{m,n} = \alpha_m \quad \text{for all } m \quad \text{and} \quad \lim_{m\to\infty} \alpha_n = \alpha \tag{2.24}$$

exist and the limit

$$\lim_{m\to\infty} a_{m,n} = \beta_n \tag{2.25}$$

converges uniformly, namely irrespectively of n, then the limit of β_n exists and it is equal to α, namely

$$\lim_{n\to\infty} \beta_n = \alpha . \tag{2.26}$$

Proof of Lemma: From (2.24), for m fixed, we have

$$| a_{m,n} - \alpha_m | < (\epsilon/3) \quad \text{for } n > N_1 . \tag{2.27}$$

From the second condition in (2.24), we also have

$$| \alpha_m - \alpha | < (\epsilon/3) \quad \text{for } m > N_2 . \tag{2.28}$$

The condition of uniform convergence yields

$$| a_{m,n} - \beta_n | < (\epsilon/3) \quad \text{for } m > N_3 . \tag{2.29}$$

Thus we obtain

$$| \beta_n - \alpha | < | \beta_n - a_{m,n} | + | a_{m,n} - \alpha_m | + | \alpha_m - \alpha | < \epsilon \tag{2.30}$$

for $n > N_1$ [and for $m > \max(N_2, N_3)$]. This completes the proof. If we apply this lemma to our problem, we obtain $\tilde{f} = f$ from (2.10) and (2.11).

Step 3: From (2.30), with $a_{m,n} = f_{m,n}$, $\beta_n = \tilde{f}_n$, $\alpha = f = \tilde{f}$, we obtain

$$| f_{m,n} - \tilde{f} | \le | f_{m,n} - \tilde{f}_n | + | \tilde{f}_n - \tilde{f} | < \epsilon/3 + \epsilon < \tfrac{4}{3}\epsilon \tag{2.31}$$

for $m,n > N$. Therefore, we arrive at the conclusion that the double limit $\hat{f}$ exists and that $\hat{f} = \tilde{f} = f$. Theorem 2 is the basis for the virtual-space transfer-matrix method for quantum spin systems.

III. DEMONSTRATION OF THE TRANSFER-MATRIX METHOD IN AN EXACTLY SOLUBLE TRANSVERSE ISING MODEL

In the present section we study the following one-dimensional transverse Ising model:

$$\mathcal{H} = -J \sum_{j=1}^{m} \sigma_j^z \sigma_{j+1}^z - \Gamma \sum_{j=1}^{m} \sigma_j^x, \quad \sigma_{m+1} \equiv \sigma_1 \tag{3.1}$$

where σ_j^x and σ_j^z denote Pauli matrices

$$\sigma_j^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_j \quad \text{and} \quad \sigma_j^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_j \tag{3.2}$$

being located at the jth lattice point. Equivalence theorem (1.1) yields the following classical expression[3] of the partition function:

$$Z = \operatorname{Tr} e^{-\beta\mathcal{H}} = \operatorname{Tr} \exp \left[K \sum_{j=1}^{m} \sigma_j^z \sigma_{j+1}^z + \gamma \sum_{j=1}^{m} \sigma_j^x \right]$$
$$= \lim_{n\to\infty} A_n^{mn} \operatorname{Tr} \exp \left[\sum_{j=1}^{m} \sum_{k=1}^{n} \left[\frac{K}{n} \sigma_{j,k} \sigma_{j+1,k} + K_n \sigma_{j,k} \sigma_{j,k+1} \right] \right] , \tag{3.3}$$

where $\sigma_{j,n} = \pm 1$, $K = J/k_B T$, $\gamma = \Gamma/k_B T$, and

$$A_n = \left[\frac{1}{2} \sinh \left[\frac{2\gamma}{n} \right] \right]^{1/2} \quad \text{and} \quad K_n = \tfrac{1}{2} \ln \coth(\gamma/n) . \tag{3.4}$$

We apply here the two kinds of transfer matrices, $T(m)$ and $T'(n)$, introduced in Sec. II.

A. Real-space transfer-matrix method

This was discussed in the previous paper.[3] For convenience, we review briefly our previous result. Since the above classical representation (3.3) is nothing but the two-dimensional ordinary Ising model, the transfer matrix $T(m)$ corresponding to (3.3) has been already diagonalized by Onsager[19] and Kaufman,[20] and consequently we obtain[3]

$$Z_m = \lim_{n\to\infty} A_n^{mn} \tfrac{1}{2} [2\sinh(2K_n)]^{mn/2} \left\{ \prod_{k=1}^{m} \left[2\cosh \left[\frac{n}{2} \gamma_{2k} \right] \right] + \prod_{k=1}^{m} \left[2\sinh \left[\frac{n}{2} \gamma_{2k} \right] \right] \right.$$
$$\left. + \prod_{k=1}^{m} \left[2\cosh \left[\frac{n}{2} \gamma_{2k-1} \right] \right] + \prod_{k=1}^{m} \left[2\sinh \left[\frac{n}{2} \gamma_{2k-1} \right] \right] \right\} , \tag{3.5}$$

where γ_k is given by

$$\cosh\gamma_k = \cosh\left[\frac{2\gamma}{n}\right]\cosh\left[\frac{2K}{n}\right] - \sinh\left[\frac{2\gamma}{n}\right]\sinh\left[\frac{2K}{n}\right]\cos\left[\frac{\pi k}{m}\right] . \tag{3.6}$$

Therefore, we obtain

$$\lim_{n\to\infty}\frac{n}{2}\gamma_k = \beta\epsilon_k \equiv \left[(\Gamma^2+J^2) - 2\Gamma J\cos\left[\frac{\pi k}{m}\right]\right]^{1/2} . \tag{3.7}$$

Thus the partition function of the quantum system (3.1) for m spins is expressed[3] by the sum of the following products:

$$Z_m = \frac{1}{2}\left[\prod_{k=1}^{m}[2\cosh(\beta\epsilon_{2k})] + \prod_{k=1}^{m}[2\sinh(\beta\epsilon_{2k})] + \prod_{k=1}^{m}[2\cosh(\beta\epsilon_{2k-1})] + \prod_{k=1}^{m}[2\sinh(\beta\epsilon_{2k-1})]\right] . \tag{3.8}$$

In the thermodynamic limit $m\to\infty$, we obtain[3]

$$f \equiv \lim_{m\to\infty} f_m \equiv \lim_{m\to\infty}\frac{-k_BT}{m}\ln Z_m = \frac{-k_BT}{2\pi}\int_0^{2\pi}\ln\{2\cos[\beta\epsilon(q)]\}dq , \tag{3.9}$$

where

$$\epsilon(q) = (J^2+\Gamma^2-2J\Gamma\cos q)^{1/2} . \tag{3.10}$$

This is a well-known result.[16,17]

It will be instructive to discuss here the other limit $\tilde{f}_n \equiv \lim_{m\to\infty} f_{m,n}$ by using (3.5) in order to exemplify theorem 2. By taking the limit $m\to\infty$ in (3.5), we obtain

$$\tilde{f}_n = -\frac{k_BT}{2\pi}\int_0^{2\pi}\ln\left[2\cosh\left[\frac{n}{2}\gamma_n(q)\right]\right]dq , \tag{3.11}$$

where

$$\cosh\gamma_n(q) = \cosh\left[\frac{2\gamma}{n}\right]\cosh\left[\frac{2K}{n}\right] - \sinh\left[\frac{2\gamma}{n}\right]\sinh\left[\frac{2K}{n}\right]\cos q . \tag{3.12}$$

Consequently, we arrive at

$$\lim_{n\to\infty}\tilde{f}_n = \tilde{f} = f . \tag{3.13}$$

Therefore, theorem 2 yields the relation $f = \tilde{f} = \hat{f}$, which can be also confirmed directly from (3.5).

B. Virtual-space transfer-matrix method

The transfer-matrix T' of the present method is easily obtained and it has the same structure as T with different parameters. From the exact solution by Onsager[19] and Kaufman,[20] we obtain again

$$\begin{aligned}-\beta f_{m,n} &= \frac{1}{m}\ln Z_m = \frac{1}{m}\ln \mathrm{Tr}[T'(n)]^m \\ &= \frac{1}{m}\ln\left[\frac{1}{2}\left[\sinh\left[\frac{2\gamma}{n}\right]\sinh\left[\frac{2K}{n}\right]\right]^{mn/2}\left\{\prod_{k=1}^{n}\left[2\cosh\left[\frac{m}{2}\hat{\gamma}_{2k-1}\right]\right] + \prod_{k=1}^{n}\left[2\sinh\left[\frac{m}{2}\hat{\gamma}_{2k-1}\right]\right]\right.\right. \\ &\qquad \left.\left. + \prod_{k=1}^{n}\left[2\cosh\left[\frac{m}{2}\hat{\gamma}_{2k}\right]\right] + \prod_{k=1}^{n}\left[2\sinh\left[\frac{m}{2}\hat{\gamma}_{2k}\right]\right]\right\}\right] ,\end{aligned} \tag{3.14}$$

where

$$\cosh\hat{\gamma}_k = \coth\left[\frac{2\gamma}{n}\right]\coth\left[\frac{2K}{n}\right] - \mathrm{csch}\left[\frac{2\gamma}{n}\right]\mathrm{csch}\left[\frac{2K}{n}\right]\cos\left[\frac{\pi k}{n}\right] . \tag{3.15}$$

We have to be careful in taking the limit $m\to\infty$ before the limit $n\to\infty$. It is a key point for our purpose to note the following formula:

$$\cosh(nx)=2^{n-1}\prod_{j=1}^{n}\left[\cosh x-\cos\left[\frac{(2j-1)\pi}{2n}\right]\right] . \tag{3.16}$$

With the help of this formula, we have

$$\cosh\left[\frac{m}{2}\hat{\gamma}_k\right]=2^{m/2-1}\prod_{j=1}^{m/2}\left[\cosh\hat{\gamma}_k-\cos\left[\frac{(2j-1)\pi}{m}\right]\right] . \tag{3.17}$$

The first product in (3.14) can be expressed by a double product

$$\begin{aligned}\prod_{k=1}^{n}\left[2\cosh\left[\frac{m}{2}\hat{\gamma}_{2k-1}\right]\right]&=2^{mn/2}\prod_{k=1}^{n}\prod_{j=1}^{m/2}\left[\cosh\hat{\gamma}_{2k-1}-\cos\left[\frac{(2j-1)\pi}{m}\right]\right]\\&=\left[2\,\mathrm{csch}\left[\frac{2\gamma}{n}\right]\mathrm{csch}\left[\frac{2K}{n}\right]\right]^{mn/2}\prod_{k=1}^{n}\prod_{j=1}^{m/2}\left[\cosh\gamma_{2j-1}-\cos\left[\frac{(2k-1)\pi}{n}\right]\right] .\end{aligned} \tag{3.18}$$

This form of double product was obtained first by Fisher[23] and later by many authors.[24,26] Thus we arrive at

$$\begin{aligned}&\left[\sinh\left[\frac{2\gamma}{n}\right]\sinh\left[\frac{2K}{n}\right]\right]^{mn/2}\prod_{k=1}^{n}\left[2\cosh\left[\frac{m}{2}\hat{\gamma}_{2k-1}\right]\right]\\&\qquad=\prod_{j=1}^{m/2}\left\{2^n\prod_{k=1}^{n}\left[\cosh\gamma_{2j-1}-\cos\left[\frac{(2k-1)\pi}{n}\right]\right]\right\}=\prod_{j=1}^{m/2}\left[4\cosh^2\left[\frac{n}{2}\gamma_{2j-1}\right]\right] ,\end{aligned} \tag{3.19}$$

where we have assumed here, for simplicity, that m and n are both even. The above argument can be easily extended to the case of odd m or n, but it is a little more complicated.

Thus we obtain, from (3.14) and (3.19),

$$\tilde{f}_n=\lim_{m\to\infty}f_{m,n}=\frac{-k_BT}{2\pi}\int_0^{2\pi}\ln\left[2\cosh\left[\frac{n}{2}\gamma_n(q)\right]\right]dq , \tag{3.20}$$

which is an even function of n and satisfies the n^{-2}-correction law. This agrees with (3.11), though it is logically trivial if we start from a symmetric double product[23–26] of the partition function. Therefore, we arrive again at the desired result

$$\lim_{n\to\infty}\tilde{f}_n=\tilde{f}=f . \tag{3.21}$$

The above calculation gives a typical example of theorem 2.

IV. MONTE CARLO METHOD FOR THE TWO-DIMENSIONAL TRIANGULAR ANTIFERROMAGNETIC HEISENBERG MODEL

Our classical representation[3] of quantum spin systems is not unique and the separation of the Hamiltonian is rather arbitrary, as in (2.1). By making use of this property, it may be possible to optimize the separation of the Hamiltonian. That is, we separate now the Hamiltonian into the following local operators:

$$\mathcal{H}=\sum_{\underset{\sim}{r}}\mathcal{H}(\underset{\sim}{r}) . \tag{4.1}$$

By applying formula (1.3), the partition function of the system is expressed as[3]

$$Z=\mathrm{Tr}\,e^{-\beta\mathcal{H}}=\lim_{n\to\infty}\mathrm{Tr}\left[\prod_{\underset{\sim}{r}}\exp\left[-\frac{\beta}{n}\mathcal{H}(\underset{\sim}{r})\right]\right]^n=\lim_{n\to\infty}\sum_{\{\alpha_j\}}\exp\mathcal{H}_{\mathrm{eff}} , \tag{4.2}$$

where

$$\mathcal{H}_{\mathrm{eff}}=\sum_{\underset{\sim}{r}}\sum_{j=1}^{n}\ln\left\langle\alpha_{\underset{\sim}{r},j}\left|\exp\left[-\frac{\beta}{n}\mathcal{H}(\underset{\sim}{r})\right]\right|\alpha_{\underset{\sim}{r},j+1}\right\rangle . \tag{4.3}$$

Here it should be remarked that the above local operator $\mathscr{H}(\underset{\sim}{r})$ is not necessarily the original local interaction itself, but it may be some cluster[3,11] of local Hamiltonians. If we take a larger cluster as $\mathscr{H}(\underset{\sim}{r})$, then the noncommutativity (or quantum) effect can be taken into account more appropriately for a smaller value of n. It becomes, however, more difficult to calculate the equivalent classical interaction (4.3), because the diagonalization of $\mathscr{H}(\underset{\sim}{r})$ becomes more complicated as the cluster size increases. Thus some optimization between the cluster size and the value n will be necessary. First we discuss a quite interesting example of the two-dimensional triangular antiferromagnetic quantum Heisenberg model[27–29]

$$\mathscr{H}_A = -J\sum_{\langle ij\rangle} \tilde{\sigma}_i\cdot\tilde{\sigma}_j = -J\sum_{\langle ij\rangle}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y+\sigma_i^z\sigma_j^z)\ , \tag{4.4}$$

where $\tilde{\sigma}_j$ denotes a vector of Pauli matrices σ_j^x, σ_j^y, and σ_j^z located at the jth lattice. If we are interested in the quantum frustration in the triangular lattice, then it seems to be essential to take, at least, three-spin clusters as the local operator $\mathscr{H}(\underset{\sim}{r})$, namely

$$\mathscr{H}(\underset{\sim}{r})\to\mathscr{H}_{ijk} = -J(\tilde{\sigma}_i\cdot\tilde{\sigma}_j+\tilde{\sigma}_j\cdot\tilde{\sigma}_k+\tilde{\sigma}_k\cdot\tilde{\sigma}_i)\ , \tag{4.5}$$

as shown in Fig. 4.

In order to study such dynamical coherence of the phase of singlet pairs as was suggested by Anderson,[27] we separate the whole lattice as in Fig. 5, namely we consider the following elementary local operator

$$\tilde{\mathscr{H}}_{ijk} = -\tfrac{1}{2}J(\tilde{\sigma}_i\cdot\tilde{\sigma}_j+\tilde{\sigma}_j\cdot\tilde{\sigma}_k+\tilde{\sigma}_k\cdot\tilde{\sigma}_i)\ . \tag{4.6}$$

Thus the partition function of this system is expressed by

$$Z = \mathrm{Tr}\, e^{-\beta\mathscr{H}_A} = \mathrm{Tr}\exp\left[-\beta\sum_{\langle ijk\rangle}\mathscr{H}_{ijk}\right]$$

$$= \lim_{n\to\infty}\mathrm{Tr}\left[\prod_{\langle ijk\rangle}\exp\left[-\frac{\beta}{n}\tilde{\mathscr{H}}_{ijk}\right]\right]^n . \tag{4.7}$$

According to our general procedure[3] or the equivalence theorem (1.1), the partition function Z is expressed by that of the corresponding three-dimensional Ising model with the following six-spin partial Boltzmann factor:

$$q(\sigma_i,\sigma_j,\sigma_k;\sigma_i',\sigma_j',\sigma_k') = \left\langle \sigma_i,\sigma_j,\sigma_k \left| \exp\left[-\frac{\beta}{n}\tilde{\mathscr{H}}_{ijk}\right]\right| \sigma_i',\sigma_j',\sigma_k' \right\rangle \tag{4.8}$$

in terms of the representation $|\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$ which diagonalizes $\{\sigma_j^z\}$, where

$$\begin{aligned} q(\sigma_i,\sigma_j,\sigma_k;\sigma_i',\sigma_j',\sigma_k') &= \delta(\sigma_i,\sigma_i')\delta(\sigma_j,\sigma_j')\delta(\sigma_k,\sigma_k')\cosh(3K) \\ &\quad + \tfrac{1}{3}\sinh(3K)\left[\left[\sigma_i\sigma_j\delta(\sigma_i,\sigma_i')\delta(\sigma_j,\sigma_j')\right.\right. \\ &\quad \left.\left. + \frac{(1-\sigma_i\sigma_i')(1-\sigma_j\sigma_j')-(\sigma_i-\sigma_i')(\sigma_j-\sigma_j')}{4}\right]\delta(\sigma_k,\sigma_k')+(\text{cyclic})\right] \end{aligned} \tag{4.9}$$

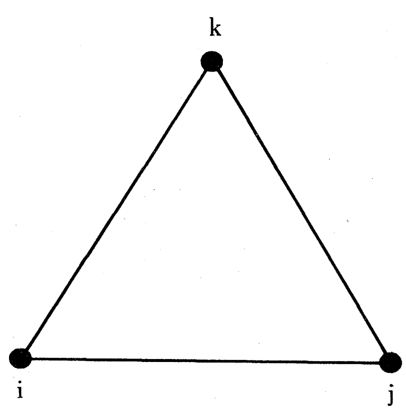

FIG. 4. Elementary triangular cluster.

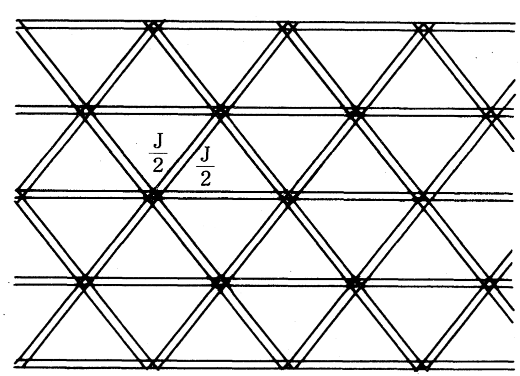

FIG. 5. Separation of the two-dimensional triangular lattice into each elementary triangular cluster.

with the Kronecker delta $\delta(x,y)$, where $K=\beta J/n$. Applications of this method are planned to be published elsewhere.

V. SUMMARY AND DISCUSSION

We have discussed the transfer-matrix method in quantum spin system and studied the relation among the three different limits of the partition function. This method has been applied to the exactly soluble one-dimensional transverse Ising model in order to show how our formulation works.

The real-space renormalization-group method[30] can be also applied[31,32] to quantum spin systems by transforming them into equivalent Ising systems. This is also planned to be discussed somewhere else.

Computational implementation of the triangular antiferromagnetic quantum Heisenberg model is also proposed. The present arguments on the transfer-matrix method will be also extended to boson and fermion systems in the future.

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