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Quantum Statistical Monte Carlo Methods and Applications to Spin Systems

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A short review is given concerning the quantum statistical Monte Carlo method based on the equivalence theorem[1] that d-dimensional quantum systems are mapped onto $(d+1)$-dimensional classical systems. The convergence property of this approximate tansformation is discussed in detail. Some applications of this geneal appoach to quantum spin systems are reviewed. A new Monte Carlo method, "thermo field Monte Carlo method," is presented, which is an extension of the projection Monte Carlo method at zero temperature to that at finite temperatures.

KEY WORDS: Quantum statistical Monte Carlo; equivalence theorem; decomposition formulas of exponential operators; thermo field Monte Carlo; quantum spin system; thermo field transfer-matrix method.

1. INTRODUCTION

Since Metropolis et al.[2] introduced the classical Monte Carlo method, many applications of it to cooperative phenomena have been published.[3–5] Numerical simulations of quantum systems at zero temperature were started in rather early days after quantum mechanics was established; see Kalos' paper, this volume, and Ref. 5. However, quantum Monte Carlo at finite temperatures had been believed to be quite difficult except for a special symmetric system of the isotropic Heisenberg model[7] until the present author[8–10] proposed a general approach of "quantum statistical Monte Carlo" in which d-dimensional quantum systems are mapped onto

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[2] Invited talk presented at "Frontiers of Quantum Monte Carlo," Los Alamos National Laboratory, September 3–6, 1985.

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$(d+1)$-dimensional classical systems using the following decomposition formula of exponential operators[8,11,12]

$$e^{A_1+A_2+\cdots+A_p}=\lim_{n\to\infty}(e^{(1/n)A_1}e^{(1/n)A_2}\cdots e^{(1/n)A_p})^n \tag{1}$$

This can be intuitively realized as follows

$$e^{A_1+\cdots+A_p}=(e^{(1/n)(A_1+\cdots+A_p)})^n\simeq(e^{(1/n)A_1}\cdots e^{(/n)A_p})^n \tag{2}$$

for large n, as was already discussed by the present author.[13] More mathematical arguments[8,11,12] will be given later. Then, the Metropolis Monte Carlo method can be applied to the transformed $(d+1)$-dimensional classical systems.

The above general approach was first applied to quantum spin systems by Suzuki, Miyashita, and Kuroda.[10] Soon after this method was reported by the present author[14] at the International Conference on Frontiers of Theoretical Physics to celebrate the 50th anniversary of bose statistics held at New Dehli in January, 1977, Barma and Shastry[15] applied this general idea to find equivalent classical models of one-dimensional fermi lattices. In 1981, Hirsch et al.[16] greatly implemented the above general approach[8–14] in one-dimensional fermi lattices and performed explicitly Monte Carlo simulations in fermi systems. On the other hand, De Raedt and Langendijk[17,18] studied extensively quantum spin, fermi and bose systems, and polaron problems, using the above general transformation method (1).

Many numerical investigations of the validity and convergence of the above general approach based on (1) have been reported by De Raedt-De Raedt,[19] Wiesler,[20] and Cullen–Landau.[21] Many other interesting applications have been reported of the above idea to $S=\frac{1}{2}$ spin systems by Satija–Wysin–Bishop,[22] Marcu–Müller–Schmatzer,[23] and Sakaguchi–Kubo–Takada,[24] to higher-spin systems by Takano[25] and Marcu–Wiesler,[26] and to fermi gas by Takahashi and Imada[27] although they have devised their own classical representations such as the coherent states[25] and path integral[27] representations in applying explicitly the above general approach.[8–13] Kolb[28] performed Monte Carlo renormalization group calculations in the two-dimensional quantum transverse Ising model by transforming it to the corresponding three-dimensional Ising model, as was suggested by the present author.[9] Betsuyaku[29,30] performed calculations of the linear quantum spin systems numerically by using the quantum transfer-matrix which was implicitly used by the present author[9] to obtain the solution of the quantum transverse Ising model on the basis of the above equivalence theorem without diagonalizing the Hamiltonian. Tsuzuki[31] extended this method to a cluster decomposition.

In Section 2, basic ideas of the quantum statistical Monte Carlo will be explained in more detail while in Section 3 improved decomposition formulas of exponential operators and their convergence properties will be summarized. Some useful inequalities concerning traces of decomposed exponential operators are given in Section 4 and in Section 5, random decomposition formulas of exponential operators are given with some possible applications to random quantum systems. In Section 6, the accuracy of cluster decomposition of exponential operators is discussed, and some explicit applications of the general quantum statistical Monte Carlo approach will be presented in Section 7. In Section 8, the quantum Monte Carlo renormalization approach will be discussed while in Section 9, the thermo field Monte Carlo method[32-37] will be explained, as well as the thermo field transfer-matrix method.[32-36] In Section 10, some possible applications of the equivalence theorem to analytic and numerical calculations of quantum systems, namely closed solutions of the nth approximant (4) and the quantum transfer-matrix method(9,29–31) are given. In Section 11, some possibilities of extension of the present general method to dynamics are discussed. Summary and discussion will be given in Section 12.

2. BASIC IDEAS OF QUANTUM STATISTICAL MONTE CARLO

In the present section, we explain a general basic idea of quantum Monte Carlo at finite temperatures, namely "quantum statistical Monte Carlo Method." It is based on the following equivalence theorem.

Equivalence Theorem.[9] The partition function of the relevant d-dimensional quantum system is transformed into that of the corresponding $(d+1)$-dimensional classical system by using the decomposition formula (1) of exponential operators

$$Z = \mathrm{tr} \exp(-\beta \mathscr{H}) = \mathrm{tr}^{(d+1)} \exp \mathscr{H}_{\mathrm{eff}}^{(d+1)} \tag{3}$$

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

$$\begin{aligned} Z &= \mathrm{tr} \exp(-\beta \mathscr{H}) \\ &= \mathrm{tr} \exp[-\beta(\mathscr{H}_1 + \mathscr{H}_2 + \cdots + \mathscr{H}_p)] \\ &= \mathrm{tr} \left\{ \exp\left[-\frac{\beta}{n} (\mathscr{H}_1 + \mathscr{H}_2 + \cdots + \mathscr{H}_p) \right] \right\}^n \end{aligned}$$

$$= \lim_{n\to\infty} \mathrm{tr}\left\{\exp\left(-\frac{\beta}{n}\mathscr{H}_1\right)\exp\left(-\frac{\beta}{n}\mathscr{H}_2\right)\cdots\exp\left(-\frac{\beta}{n}\mathscr{H}_p\right)\right\}^n$$

$$= \lim_{n\to\infty} \sum_{|\alpha_1\rangle}\cdots\sum_{|\alpha_{np}\rangle} \langle\alpha_1|\rho_1|\alpha_2\rangle\langle\alpha_2|\rho_2|\alpha_3\rangle$$

$$\cdots\langle\alpha_p|\rho_p|\alpha_{p+1}\rangle\langle\alpha_{p+1}|\rho_1|\alpha_{p+2}\rangle\cdots\langle\alpha_{np}|\rho_p|\alpha_1\rangle$$

$$\equiv \mathrm{tr}^{(d+1)}\exp\mathscr{H}_{\mathrm{eff}}^{(d+1)} \tag{4}$$

with $\rho_j=\exp(-\beta\mathscr{H}_j/n)$, where the states $\{|\alpha_j\rangle\}$ denote arbitrary orthogonal complete (or over-complete) sets.

As shown in Fig. 1, new many-body interactions appear in equivalent $(d+1)$-dimensional effective lattices. The additional $(d+1)$th dimension plays a role of quantum effect, namely, the noncommutativity of the relevant operators. Thus, the additional dimension may be called "quantal dimension" (or Trotter's direction). Quantum dynamics in equilibrium can be expressed by correlations in this quantal dimension, as will be discussed in more detail in Section 11. Therefore, the introduction of the quantal dimension in the present formulation is essential in studying the quantum effect of the relevant system.

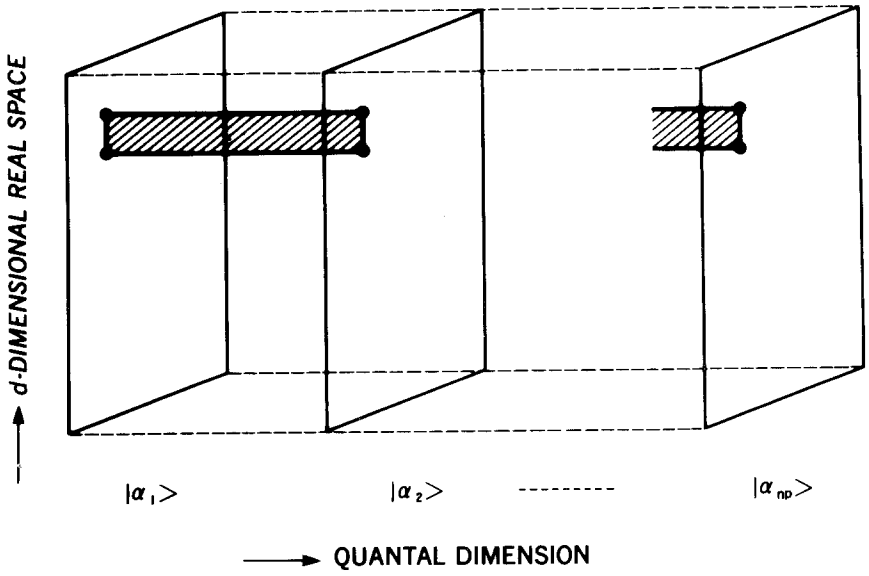

Fig. 1. Transformed effective $(d+1)$-dimensional lattice with many-body interactions denoted by shading.

Decomposing the relevant Hamiltonian $\mathscr{H}$ into p kinds of the sub-Hamiltonians is not unique as

$$\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2 + \cdots + \mathscr{H}_p \tag{5}$$

This nonuniqueness of the decomposition is useful in finding a more precise classical representation convenient for practical Monte Carlo simulations.

The principle of the decomposition (5) is that any matrix element $\langle \alpha_k | \rho_j | \alpha_{k+1} \rangle$ can be calculated explicitly and that it is "local," namely, of finite range, in the effective $(d+1)$-dimensional lattice shown in Fig. 1. The above second condition on the decomposition is very important from a practical point of view of Monte Carlo simulations. The success of quantum statistical Monte Carlo proposed in Ref. 9 is that some explicit representations which satisfy the above two conditions were found, as shown in Figs. 2 and 3 for quantum spin systems with nearest-neighbor interactions. In order to find such representations, it is sufficient to decompose[9] the original Hamiltonian into sub-Hamiltonians $\mathscr{H}_1, \mathscr{H}_2, \ldots, \mathscr{H}_p$ which are composed of single local operators $\{\mathscr{H}(r)\}$ or a sum of "local" commutable operators $\{\mathscr{H}_{jk}\}$ as

$$\mathscr{H}_j = \sum_k \mathscr{H}_{jk} \qquad [\mathscr{H}_{jk}, \mathscr{H}_{jl}] = 0 \tag{6}$$

Here, by "local," we mean[9] a finite-range cluster interaction. There may be two different formulations of decomposition, as was classified by the present author[9]:

(i) The first formulation is to decompose into a small finite number of sub-Hamiltonians, namely $p =$ finite. For example, the transverse Ising model is decomposed conveniently into the following two parts

$$\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2; \quad \mathscr{H}_1 = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \quad \text{and} \quad \mathscr{H}_2 = -\Gamma \sum_j \sigma_j^x \tag{7}$$

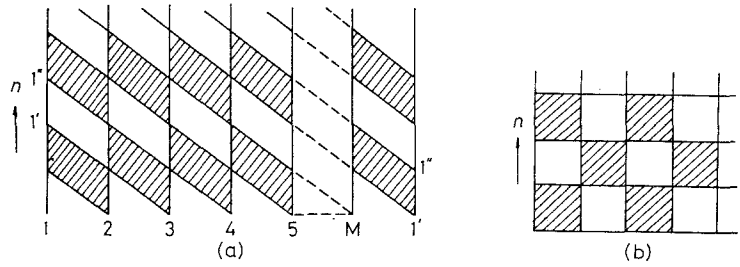

Fig. 2. Two effective lattices[9] (a) and (b) for the linear chain. Each shaded region denotes a four-spin interaction.

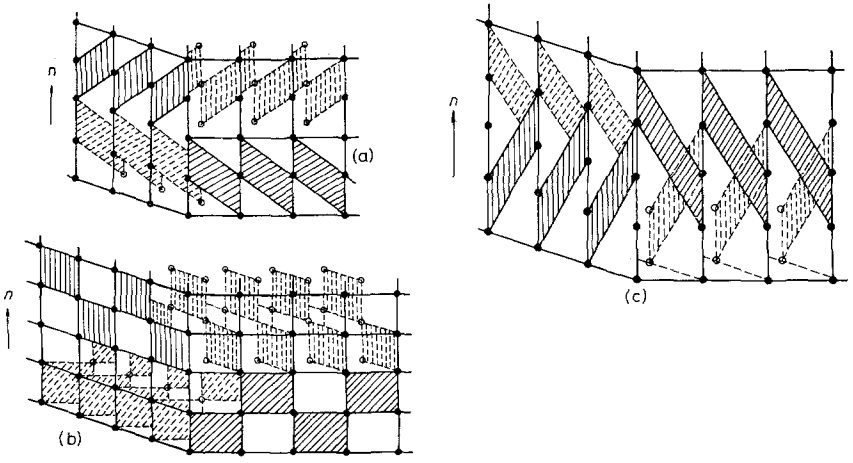

Fig. 3. Effective three-dimensional lattices[9] (a), (b), and (c). Each shaded region denotes a four-spin interaction plus pair interactions.

where σ_j^x, σ_j^y and σ_j^z are Pauli operators defined by

$$\sigma_j^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j \qquad \sigma_j^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j \qquad \text{and} \qquad \sigma_j^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \tag{8}$$

Clearly each sub-Hamiltonian is a sum of local commutable operators and consequently this satisfies the above two conditions, as was discussed explicitly already in one dimension[9]. Another example of the first formulation is to decompose the Heisenberg chain into the following two sub-Hamiltonians

$$\mathscr{H} = \mathscr{H}_e + \mathscr{H}_o \tag{9}$$

$$\mathscr{H}_e = -J \sum_j \boldsymbol{\sigma}_{2j} \cdot \boldsymbol{\sigma}_{2j+1} \qquad \text{and} \qquad \mathscr{H}_o = -J \sum_j \boldsymbol{\sigma}_{2j-1} \cdot \boldsymbol{\sigma}_{2j} \tag{10}$$

This was proposed by the present author[9] as a possible way of decomposition, as is shown[9] in Fig. 2(b). This checkerboard decomposition was first used explicitly by Barma and Shartry[15] to find an equivalent classical system and was used successfully by Hirsch et al.[16] in fermi systems.

(ii) The second formulation is to decompose[9] directly into a "local" cluster of interactions as

$$\mathscr{H} = \sum_r \mathscr{H}(\boldsymbol{r}) \qquad \mathscr{H}(\boldsymbol{r}) = \text{local} \tag{11}$$

This is sometimes called "real-space decomposition," (RSD). For example, the Heisenberg chain is decomposed as

$$\mathscr{H} = \sum_{j=1}^{N} \mathscr{H}_j \qquad \mathscr{H}_j = -J\boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1} \tag{12}$$

More generally it is decomposed into a sum of clusters of interactions as

$$\mathscr{H} = \sum_{j=1}^{N/m} \mathscr{H}_j^{(m)} \qquad \mathscr{H}_j^{(m)} = -J \sum_{k=1}^{m} \boldsymbol{\sigma}_{mj+k-1} \cdot \boldsymbol{\sigma}_{mj+k} \tag{13}$$

The convergence properties of these cluster decompositions will be discussed in the succeeding section.

3. DECOMPOSITION FORMULAS OF EXPONENTIAL OPERATORS AND THEIR CONVERGENCE PROPERTIES

It will be instructive to summarize here some useful decomposition formulas

Theorem 1.[11] For any set of operators $\{A_j\}$ in a Banach algebra (i.e., normed space)

$$\left\| \exp\left(\sum_{j=1}^{p} A_j\right) - \left(\prod_{j=1}^{p} e^{(1/n)A_j}\right)^n \right\| \leqslant \frac{1}{2n}\left(\sum_{j>k} \|[A_j, A_k]\| \exp\left(\sum_{j=1}^{p} \|A_j\|\right)\right) \tag{14}$$

with an arbitrary positive integer p. Therefore, we have (1).

In particular, for $p=2$, we obtain so-called Trotter's formula[39,40]

$$e^{A+B} = \lim_{n\to\infty} (e^{(1/n)A}\, e^{(1/n)B})^n \tag{15}$$

Theorem 2.[11] For any operators A and B in a Banach algebra,

$$\|e^{A+B} - (e^{(1/2n)A}\, e^{(1/n)B}\, e^{(1/2n)A})^n\| \leqslant \frac{1}{n^2} \Delta_2(A, B) \tag{16}$$

where

$$\Delta_2(A, B) = \frac{1}{12}\left\{ \|[[A, B], B]\| + \frac{1}{2}\|[[A, B]A]\| \right\} \times \exp(\|A\| + \|B\|) \tag{17}$$

Theorem 3.[12] For any operators A and B in a Banach algebra, the trace $f(n) \equiv \mathrm{tr}(e^{A/n} e^{B/n})^n$ is an even function of n. Therefore, the correc-

tion of this approximant $f(n)$ to the trace $f(\infty) \equiv \operatorname{tr} \exp(A+B)$ is of the order of $1/n^2$.

This $1/n^2$ correction law for two operators A and B was pointed out by Hirsch et al.[16] and De Raedt et al.[38] in a simple perturbational expansion as

$$e^{\tau(A+B)} = e^{(\tau/2)A}\, e^{\tau B}\, e^{(\tau/2)A} + O(\tau^3) \tag{18}$$

Now we discuss the decomposition of the general exponential operator $\exp(A_1 + A_2 + \cdots + A_p)$. We have the following theorem.

Theorem 4. If we define the following approximant $f_m(\{A_j\})$

$$\exp\left(\frac{1}{n}\sum_{j=1}^{p} A_j\right) = f_m\left(\left\{\frac{1}{n} A_j\right\}\right) + O\left(\frac{1}{n^m}\right) \tag{19}$$

then we have

$$\exp\left(\sum_{j=1}^{p} A_j\right) = \left[f_m\left(\left\{\frac{1}{n} A_j\right\}\right)\right]^n + O\left(\frac{1}{n^{m-1}}\right) \tag{20}$$

For example, the approximant defined by

$$f_{m+1}\left(\frac{A}{n}, \frac{B}{n}\right) = e^{(1/n)A}\, e^{(1/n)B}\, e^{(1/n^2)C_2} \cdots e^{n^{-m}C_m} \tag{21}$$

satisfies the condition (19), if the coefficients $\{C_j\}$ are given by[8,42-44]

$$C_2 = \tfrac{1}{2}[B, A] \qquad C_3 = \tfrac{1}{3}[C_2, A + 2B] \tag{22}$$

and in general

$$C_n = \frac{1}{n!}\left[\frac{\partial^n}{\partial \lambda^n}\left(e^{-\lambda^{n-1}C_{n-1}} \cdots e^{-\lambda^2 C_2}\, e^{-\lambda B}\, e^{-\lambda A}\, e^{\lambda(A+B)}\right)\right]_{\lambda=0} \tag{23}$$

The correction of (20) is lower than that of (19) by the order of $1/n$. However, in the case of $\exp(A+B)$ we have the $1/n^2$ correction law, although the operator $\exp(A/n)\exp(B/n)$ itself has a $1/n^2$ correction. This is because

$$\operatorname{tr}(e^{(1/n)A}\, e^{(1/n)B})^n = \operatorname{tr}(e^{(1/2n)A}\, e^{(1/n)B}\, e^{(1/2n)A})^n \tag{24}$$

Then, how about a more general case of $\exp(A_1 + A_2 + \cdots + A_p)$? Clearly the trace of the product $\{\exp(A_1/n) \cdots \exp(A_p/n)\}^n$ is not equal to the trace of $[f_n^{(s)}(\{(1/n)A_j\})]^n$ for the symmetrized decomposition[10]

$$f^{(s)}\left(\left\{\frac{1}{n} A_j\right\}\right) = e^{(1/2n)A_1} \cdots e^{(1/2n)A_{p-1}}\, e^{(1/n)A_p}\, e^{(/2n)A_{p-1}} \cdots e^{(1/2n)A_1} \tag{25}$$

Here, if we impose some restriction to the operators $\{A_j\}$, then we have the evenness law

Theorem 5.[44] If $f_m(\{A_j\})$ satisfies the condition

$$f_m(\{-A_j\})^{-1} = f_m(\{A_j\})^t \tag{26}$$

then the approximant

$$Z_m(n) \equiv \mathrm{tr}\left[f_m\left(\left\{\frac{1}{n}A_j\right\}\right)\right]^n \tag{27}$$

is an even function of n, namely

$$Z_m(-n) = Z_m(n) \tag{28}$$

This theorem yields the following result

Theorem 6. (Corollary of Theorem 5):[44] With the conditions (19) and (26), we have

$$Z_{2m}(n) = Z_{\mathrm{exact}} + O\left(\frac{1}{n^{2m}}\right) \tag{29}$$

In particular, if we put

$$f_2(\{A_j\}) = e^{A_1} e^{A_2} \cdots e^{A_p} \tag{30}$$

for symmetric $\{A_j\}$ (namely, $A_j^t = A_j$), then we have the following theorem

Theorem 7.[44] If $\{A_j\}$ are symmetric operators (i.e., $A_j^t = A_j$), then we have

$$Z_2(n) \equiv \mathrm{tr}(e^{(1/n)A_1} e^{(1/n)A_2} \cdots e^{(1/n)A_p})^n = Z_2(-n) \tag{31}$$

Consequently we have

$$Z_2(n) = Z_2(\infty) + O(1/n^2) \tag{32}$$

This was first obtained by Fye[45] for a general integer p in a different condition.

Theorem 7 suggests[44] the following new extrapolation method

$$Z_2(n) \simeq Z_2(\infty) + a/(n^2 + b) \tag{33}$$

Theorem 8.[44] If $Q^t = Q$ with the condition (26), the average of any quantum operator Q defined by

$$\langle Q \rangle_m(n) \equiv \mathrm{tr}\, Q[f_{2m}(\{(1/n)A_j\})]^n / Z_{2m}(n) \tag{34}$$

is an even function of n, namely

$$\langle Q \rangle_m(-n) = \langle Q \rangle_m(n) \tag{35}$$

In particular, we have

$$\langle Q \rangle_1(n) = \langle Q \rangle_{\text{exact}} + O(1/n^2) \tag{36}$$

Theorems 5 and 8 suggest the following extrapolation methods

$$Z_{2m}(n)(\text{or } \langle Q \rangle_m(n)) \simeq \frac{1}{n^{2m-2}} \frac{a}{n^2+b} + c \tag{37}$$

The coefficients a, b, and c are determined by the least-square method from Monte Carlo data.

It is easy to confirm that $f_m(A, B)$ in (21) and $f^{(s)}(\{A_j\})$ in (25) satisfy condition (26), when $\{A_j\}$ are symmetric, namely $A_j^t = A_j$, which is valid in ordinary quantum spin systems.

The above $1/n^2$ correction law explains well the numerical results by Betsuyaku[29] and by Marcu and Wiesler[26].

4. SOME USEFUL INEQUALITIES CONCERNING TRACES OF DECOMPOSED EXPONENTIALS

It will be worthwhile to study the lower and upper bounds of the approximants of the partition function given in the preceding section.

Golden,[46] Symanzik,[47] and Thompson[48] proved the following inequality

$$\text{tr } e^{A+B} \leqslant \text{tr } e^A e^B \tag{38}$$

for finite hermitian matrices A and B.

Here we generalize as follows

Theorem 9. If A and B are hermitian matrices, we have

$$\text{tr } e^{A+B} \leqslant \text{tr}(e^{(1/n)A} e^{(1/n)B})^n \tag{39}$$

for any nonzero integer n.

Proof. Note Thompson's lemma

Lemma 1.[48] If X and Y are finite hermitian matrices, we have

$$\text{tr}(XY)^{2m} \leqslant \text{tr}(X^2 Y^2)^m \tag{40}$$

for any positive integer m.

Now, we put

$$Z_n^{(m)} = \mathrm{tr}\left[\exp\left(\frac{A}{2^m \cdot n}\right)\exp\left(\frac{B}{2^m \cdot n}\right)\right]^{2^m \cdot n} \tag{41}$$

for $m = 0, 1, 2,...$, and for any nonzero integer n. Then, Thompson's lemma (40) yields

$$Z_n^{(m)} \geqslant Z_n^{(m+1)} \geqslant \cdots \geqslant Z_n^{(\infty)} = Z \tag{42}$$

Here, the equality that $Z_n^{(\infty)} = Z$ is assured by Theorem 1.

In particular, we obtain

$$Z_n \equiv Z_n^{(0)} \geqslant Z \tag{43}$$

for $m = 0$. This gives Theorem 9. The case $n = 1$ in (39) is the Golden–Thompson–Symanzik inequality.

Furthermore, we obtain the following theorem

Theorem 10. If we define the following higher-order approximants

$$\hat{Z}_n^{(2)} \equiv \mathrm{tr}(e^{(1/n)A_1} e^{(1/n)A_2} \cdots e^{(1/n)A_p} e^{(1/n^2)C_2})^n \tag{44}$$

for finite hermitian matrices $\{A_j\}$ with C_2 defined by[8]

$$\begin{aligned} C_2 &= \frac{1}{2}\left[\frac{\partial^2}{\partial\lambda^2}(e^{-\lambda A_p}\cdots e^{\lambda A_2} e^{\lambda A_1} e^{\lambda(A_1+\cdots+A_p)})\right]_{\lambda=0} \\ &= -\frac{1}{2}\{[A_1, A_2+\cdots+A_p]+[A_2, A_3+\cdots+A_p] \\ &\quad +\cdots+[A_{p-1}, A_p]\} \end{aligned} \tag{45}$$

then we have

$$\hat{Z}_{2n}^{(2)} \leqslant Z_n^{(s)} \tag{46}$$

where

$$Z_n^{(s)} \equiv \mathrm{tr}(e^{(1/2n)A_1}\cdots e^{(1/2n)A_p} e^{(1/2n)A_p}\cdots e^{(1/2n)A_1})^n \tag{47}$$

The proof of Theorem 10 is given with the use of the following inequality[48]

$$|\mathrm{tr}\, X^{2n}| \leqslant \mathrm{tr}(XX^\dagger)^n \tag{48}$$

for a positive integer n. If we put

$$X = e^{(1/2n)A_1} e^{(1/2n)A_2} \cdots e^{(1/2n)A_p} e^{(1/4n^2)C_2} \tag{49}$$

then we have $\mathrm{tr}(XX^\dagger)^n = Z_n^{(s)}$ using $C_2^\dagger = -C_2$ and we have also $|\mathrm{tr}\, X^{2n}| = \hat{Z}_{2n}^{(2)}$ for hermitian matrices $\{A_j\}$. Thus we obtain Theorem 10.

In particular, for $p = 2$ we have

$$\hat{Z}_n^{(1)} \equiv \mathrm{tr}(e^{A/n} e^{B/n})^n \geqslant |\mathrm{tr}(e^{A/2n} e^{B/2n} e^{(1/4n^2)C_2})| \equiv \hat{Z}_{2n}^{(2)} \tag{50}$$

where $C_2 = -\frac{1}{2}[A, B]$. It is interesting to note that the numerical results by De Raedt et al.[38] satisfy these inequalities, and that $Z_{-n}^{(s)} = Z_n^{(s)}$ and $\hat{Z}_{-n}^{(2)} = \hat{Z}_n^{(2)}$.

The above result (46) can easily be extended to the following general operator X

$$X = e^{(1/2n)A_1} e^{(1/2n)A_2} \cdots e^{(1/2n)A_p} e^{[1/(2n)^2]C_2} e^{[1/(2n)^3]C_3} \cdots e^{[1/(2n)^m]C_m} \tag{51}$$

with[8] $\{C_m\}$ satisfying the relations $C_{2m}^\dagger = -C_{2m}$ and $C_{2m+1}^\dagger = C_{2m+1}$. Details are omitted here.

5. RANDOM DECOMPOSITION FORMULAS OF EXPONENTIAL OPERATORS

It will be useful to extend the decomposition formulas (1) to the following random case

Theorem 11. If we put $E(j) = \exp(A_j/n)$, we have

$$\exp(A_1 + \cdots + A_p) = \lim_{n \to \infty} \prod_{i=1}^{np} E(k_i) \tag{52}$$

where k_i takes one of the values 1, 2,..., p with equal probability.

The convergence of (52) can be proved in a way[8,11] similar to that of (1).

There are many other extensions similar to (52), which will be published elsewhere.

6. ACCURACY OF CLUSTER DECOMPOSITION OF EXPONENTIAL OPERATORS

As discussed already,[9,35] how to decompose the Hamiltonian $\mathscr{H}$ into local sub-Hamiltonians $\{\mathscr{H}(r)\}$ is arbitrary. It is intuitively clear that

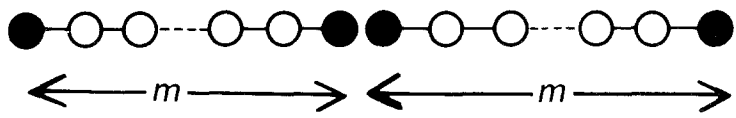

Fig. 4. Decomposition of the linear chain into m clusters.

larger-cluster decomposition is better than smaller one, for the same value of the Trotter number n in our general equivalence Theorem 4.

The purpose of the present section is to discuss the accuracy of cluster decomposition as a function of the cluster size m. For example, the one-dimensional quantum system may be decomposed as in Fig. 4. The two-dimensional triangular lattice may be decomposed as in Fig. 5, in which three-spin clusters are used as unit cells. Four-spin and seven-spin clusters, shown in Fig. 6 may also be used as unit cells. These will be used in explicit quantum Monte Carlo simulations.[37]

In order to obtain better approximations based on equivalence Theorem 4, i.e., generalized decomposition formula, there are three ways shown in Fig. 7, namely (a) to increase the cluster size m for a fixed value of the Trotter number n, (b) to increase the value of n for m fixed, and (c) to increase both m and n.

The approximate partition function $Z_{m,n}$ for the cluster size m and the Trotter number n is shown[35] to satisfy

$$|Z - Z_{m,n}| \leqslant \frac{C(T)}{(m+a)(n^2+b)} \tag{53}$$

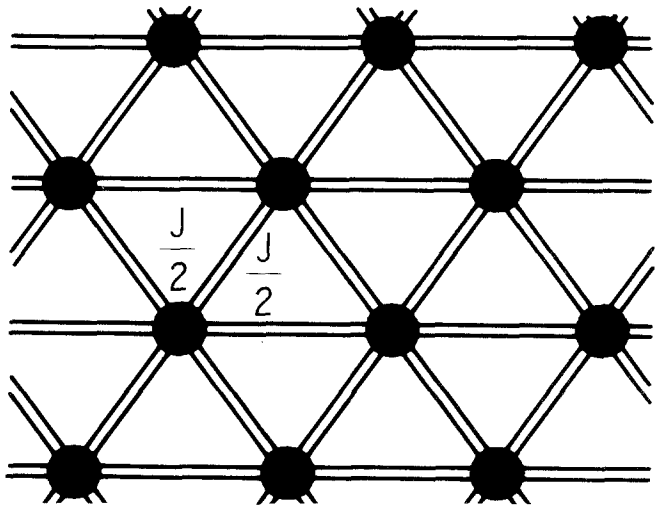

Fig. 5. Decomposition[34–36] of the triangular lattice into triangular cells.

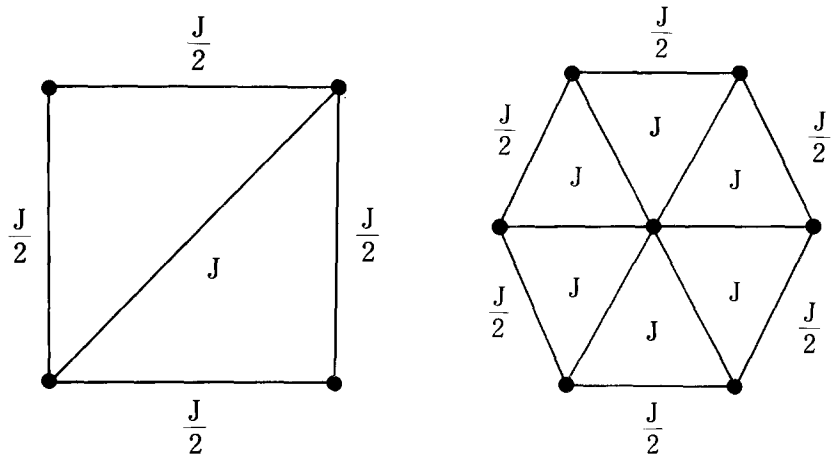

Fig. 6. Larger cells: (a) four-spin cluster and (b) seven-spin cluster.

with some appropriate constants a and b under the condition that $\{\mathscr{H}(\boldsymbol{r})\}$ are symmetric, i.e., $\mathscr{H}'(\boldsymbol{r}) = \mathscr{H}(\boldsymbol{r})$. The coefficient $C(T)$ is a function of temperature independent of m and n. For more details of the m-dependence of $Z_{m,n}$, see the paper by Fye.[45]

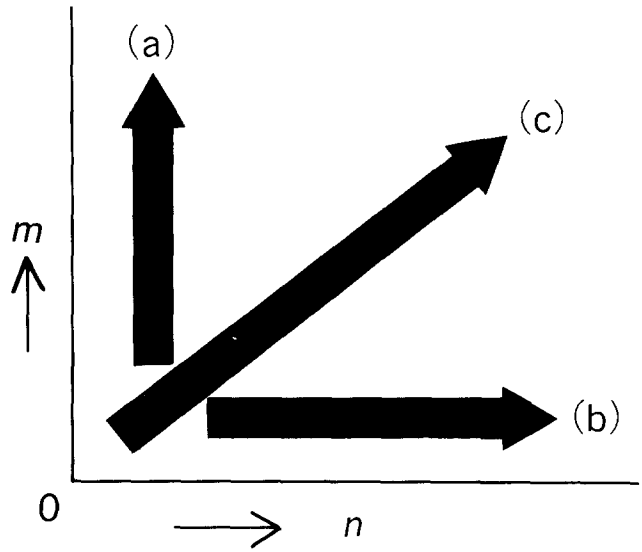

Fig. 7. Three approximate methods: (a) to enlarge the cluster size m, to enlarge Trotter's number n, and (c) both.[35]

The above result suggests the following extrapolation formula

$$Z \simeq \frac{C}{(m+a)(n^2+b)} + Z_\infty \tag{54}$$

That is, all the approximants $\{Z_{m,n}\}$ which satisfy the condition $(m+a)(n^2+b) = \text{constant}$ for some appropriate constants a and b give the same result with almost the same precision. The least-square method yields the values of the parameters a, b, c, and Z_∞, which give the desired quantity of Z.

7. APPLICATIONS TO QUANTUM SPIN SYSTEMS

It will be instructive to review first some applications of the general quantum statistical Monte Carlo approach to spin systems.

The first application of it was given[10] to the following anisotropic Heisenberg model

$$\mathscr{H} = \sum_{\langle ij \rangle} \mathscr{H}_{ij} = -\sum_{\langle ij \rangle} (J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z) \tag{55}$$

with Pauli matrices σ_i^x, σ_j^y, and σ_j^z. The "local density matrix" $\rho_{ij} = \exp(-\beta \mathscr{H}_{ij})$ is given by[9,10]

$$\rho_{ij} = (\langle \sigma_i, \sigma_j | \rho_{ij} | \sigma_i', \sigma_j' \rangle) = \tilde{a} \begin{pmatrix} 1+X_3 & 0 & 0 & X_1 - X_2 \\ 0 & 1-X_3 & X_1+X_2 & 0 \\ 0 & X_1+X_2 & 1-X_3 & 0 \\ X_1-X_2 & 0 & 0 & 1+X_3 \end{pmatrix} \tag{56}$$

in the subspace representation $|\sigma_i, \sigma_j\rangle$ with $\sigma_j = \pm 1$, where

$$\tilde{a} = \cosh K_x \cosh K_y \cosh K_z - \sinh K_x \sinh K_y \sinh K_z$$

$$X_1 = \frac{\tanh K_x - \tanh K_y \tanh K_z}{1 - \tanh K_x \tanh K_y \tanh K_z} \qquad K_x = \frac{J_x}{k_B T}, \ldots \tag{57}$$

and X_2 and X_3 are cyclic with respect to x, y, and z.

Monte Carlo simulations were performed[10] on the basis of the classical representation (4).

7.1. One-Dimensional Quantum Spin Systems

In the one-dimensional case, we used[10] the equivalent lattice shown in Fig. 2(a). The temperature dependence of the perpendicular suscep-

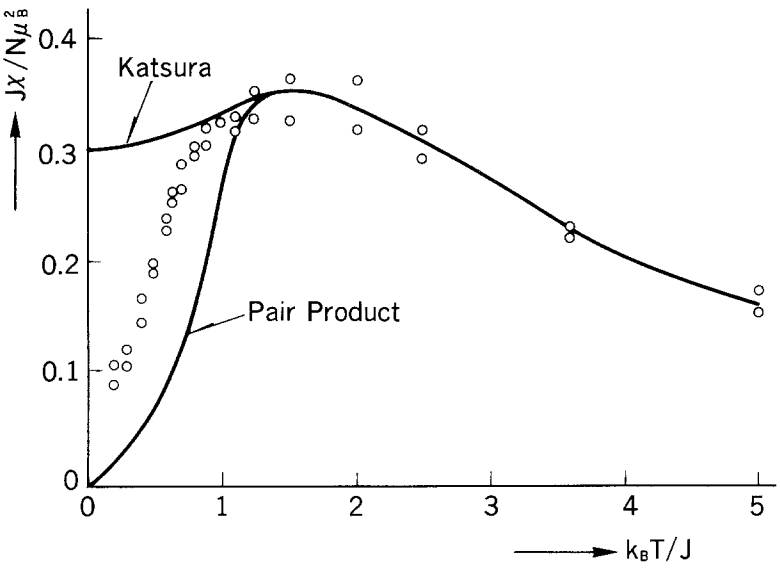

Fig. 8. Temperature dependence of the perpendicular susceptibility for the one-dimensional quantum XY model ($N=33$, $n=2$).[10]

tibility of the XY chain is shown in Fig. 8 together with Katsura's exact result[49] and that obtained[50] in the first approximant $n=1$. The $n=2$ result is between the $n=1$ and exact results in the low temperature region, as it should be.

7.2. Two-Dimensional *XY* Model

The two-dimensional classical planar model shows the Kosterlitz–Thouless transition[51]; it is also quite interesting to study the two-dimensional XY model[52] with the help of Monte Carlo simulations.[10] The unit cell of the transformed effective lattice is shown in Fig. 9. The specific heat calculated for the $n=1$ case is shown in Fig. 10, which seems to show no divergence of the specific heat in this precision. More elaborate calculations have been reported[53,54] but they are not yet conclusive. It is certain that the susceptibility in the XY plane diverges at low temperatures, as shown[10] in Fig. 11.

7.3. Two-Dimensional Triangular Antiferromagnetic Quantum Heisenberg Model–Anderson Problem

Anderson[55] proposed a new coherent phase in two-dimensional frustrated quantum spin systems, namely antiferromagnetic triangular lat-

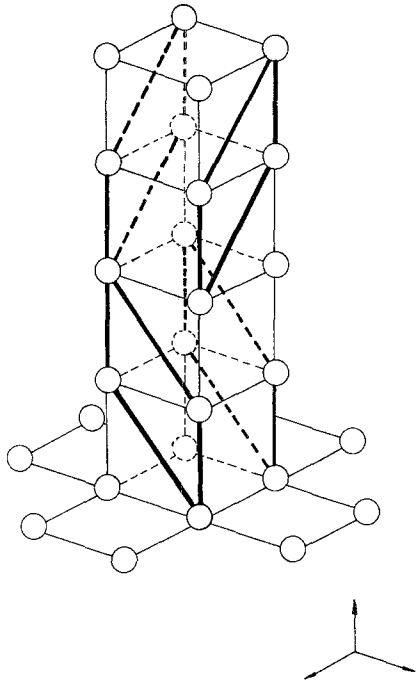

Fig. 9. Unit cell of the effective lattice: effective four-spin interactions are denoted by boldfaced solid of dotted lines.[10]

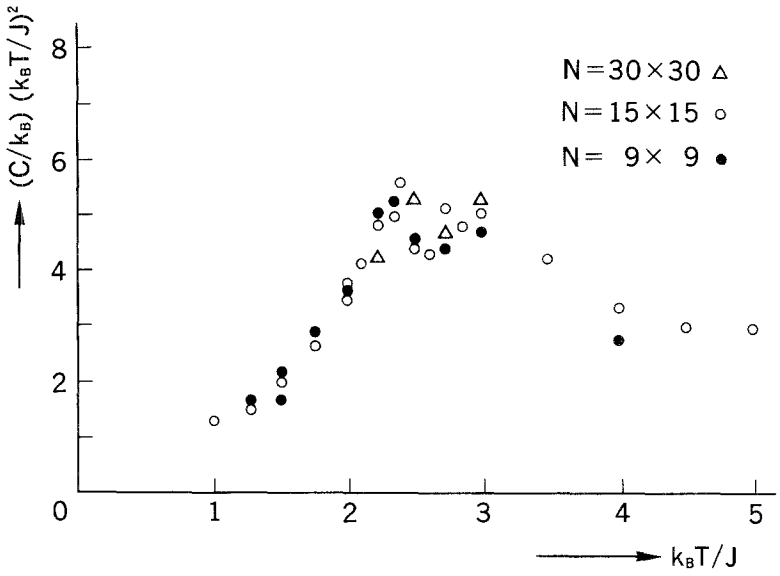

Fig. 10. Size dependence of the specific heat for the two-dimensional XY model.[10]

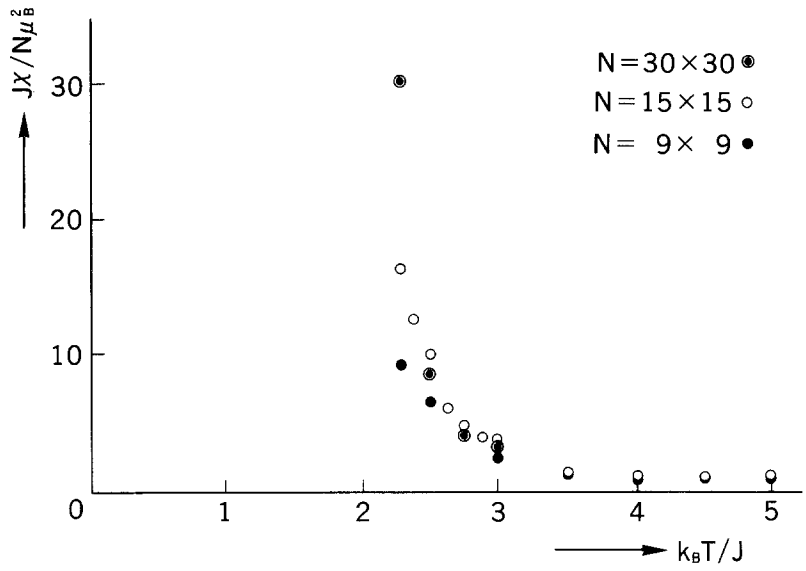

Fig. 11. Temperature and size dependence of susceptibility in the XY plane for the two-dimensional XY model.[10]

tices. Hirakawa et al.[56] have found a candidate of such materials, namely $NaTiO_2$.

Thus, it will be quite interesting to perform quantum Monte Carlo simulations to study the thermodynamic properties of the triangular antiferromagnetic Heisenberg model shown in Fig. 5. The ground state has been studied numerically already by Marland and Betts[57] and by Oguchi, Nishimori, and Taguchi[58] for finite lattices. Details of the Monte Carlo simulations of this system at finite temperatures will be published elsewhere.[59]

8. QUANTUM MONTE CARLO RENORMALIZATION GROUP APPROACH

Since Wilson[60] proposed the renormalization group approach to critical phenomena, many investigations on it have been reported. In particular, the Monte Carlo renormalization group approach has been applied successfully to the three-dimensional Ising model.[61–63] Quite recently Kikuchi and Okabe[64] performed Monte Carlo renormalization group calculations of the Ising model by devising a powerful algorithm.

Kolb[28] first performed the quantum Monte Carlo renormalization calculation by using equivalence Theorem 4 by Suzuki.[9] That is, our starting point is the following decomposition[13]

$$\exp(-\beta\mathscr{H}) = \lim_{n\to\infty}\left(\exp\left(-\frac{1}{n}\hat{\mathscr{H}}_1\right)\exp\left(-\frac{1}{n}\hat{\mathscr{H}}_2\right)\right)^{Kn} \tag{58}$$

where $K=\beta J$ and $\mathscr{H}=J(\hat{\mathscr{H}}_1+\hat{\mathscr{H}}_2)$. As was discussed by the present author[13] and by Kolb,[28] the accuracy of the above decomposition (58) is independent of temperature T (or $\beta=1/k_BT$). This remark is substantial in applying the RG method to quantum systems, because the RG transformation makes the temperature T move to another one T'. Thus, our equivalent lattice has a $(d+1)$-dimensional structure as is shown[13] in Fig. 12. The temperature dependence comes[13] only through the thickness L (or Kn) in the $(d+1)$th quantal direction of the equivalent lattice.

There are two situations to apply to the above scheme.

(i) The case that $T=0$ is the critical point. This was discussed in detail[13] concerning the one-dimensional transverse Ising model[13,28] and the Kondo problem.[13] In this case, the RG transformation is expressed as

$$\log Z(K, h) = b^{-d}\log Z(b^y K, b^x h) \qquad h=\mu_B H/k_B T \tag{59}$$

for the scale factor b, where $Z(K, h)$ denotes the partition function per particle, and d is the dimensionality of the system. Here Trotter's number n

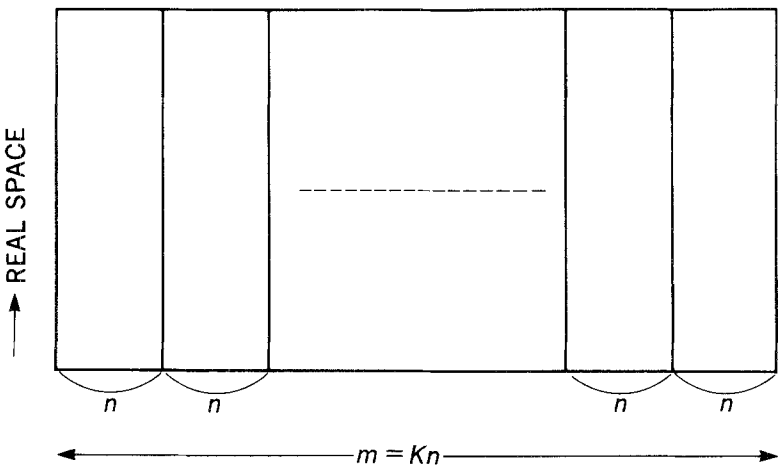

Fig. 12. Temperature dependent effective $(d+1)$-dimensional lattice[13]: $K=J/k_BT$, and n denotes Trotter's number.

should be fixed for the above Monte Carlo RG. Consequently the susceptibility, for example, satisfies the following scaling relation[64–66]

$$\chi(K, h) = b^{2x-d}\chi(b^y K, b^x h) \tag{60}$$

This yields the exponents of x and y.

(ii) The case $T_c \neq 0$. In this case, we can fix $m = Kn$ in (58), because K is very close to the critical point K_c. This is reduced to the previous formulation in classical systems[61–66]

9. THERMO FIELD MONTE CARLO METHOD

9.1. General Formulation

The statistical average of a physical quantity Q at temperature T is expressed by the expectation value of the form

$$\begin{aligned} \langle Q \rangle &\equiv \operatorname{tr} Q e^{-\beta \mathscr{H}}/Z(\beta) = \langle O(\beta)| Q |O(\beta)\rangle \\ Z(\beta) &= \operatorname{tr} e^{-\beta \mathscr{H}} \end{aligned} \tag{61}$$

where $\mathscr{H}$ is the Hamiltonian of the relevant quantum system. The thermal quantum state $|O(\beta)\rangle$ is defined by[67–69]

$$\begin{aligned} |O(\beta)\rangle &= Z(\beta)^{-1/2} \sum_n e^{-\beta E_n/2} |n, \tilde{n}\rangle \\ &= Z(\beta)^{-1/2} e^{-(1/2)\beta \mathscr{H}} |I\rangle \\ |I\rangle &\equiv \sum_n |n, \tilde{n}\rangle \end{aligned} \tag{62}$$

with an eigenvalue E_n and $|\tilde{n}\rangle$ the corresponding eigenstate in the fictitious dynamical system $\tilde{\mathscr{H}}$ identical to the original system together with the conjugation rules[67–69]

$$\begin{aligned} \widetilde{AB} &= \tilde{A}\tilde{B} \\ (c_1 A + c_2 B)^{\sim} &= c_1^* \tilde{A} + c_2^* \tilde{B} \\ (c_1 |m\rangle + c_2 |n\rangle)^{\sim} &= c_1^* |\tilde{m}\rangle + c_2^* |\tilde{n}\rangle \end{aligned} \tag{63}$$

Here c_1 and c_2 are c number and c^* denotes the complex conjugate of c. Owing to these conjugation rules, the state $|I\rangle$ is independent of representations, namely[32–36]

$$|I\rangle = \sum_n |n, \tilde{n}\rangle = \sum_\alpha |\alpha, \tilde{\alpha}\rangle \tag{64}$$

It is convenient from our point of view to take the number representation[33] for fermi and bose systems and the spin representation[32-36] for spin systems, because the state $|I\rangle$ can be esily given explicitly in these representations.

Our starting point is the following path-sum formulation[32-36] of the thermal quantum state

$$|O(\beta)\rangle = \lim_{n\to\infty} (Z_n(\beta)/Z(0))^{-1/2}(e^{-(\beta/2n)\mathscr{H}_1}\cdots e^{-(\beta/2n)\mathscr{H}_p})^n|O(0)\rangle \quad (65)$$

where $|O(0)> = Z(0)^{-1/2}|I\rangle$, $\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2 + \cdots + \mathscr{H}_p$, and

$$Z_n(\beta) = \mathrm{tr}(e^{-(\beta/2n)\mathscr{H}_1}\cdots e^{-(\beta/2n)\mathscr{H}_p})^{2n} \quad (66)$$

Here we have used the generalized Totter formula (1).

We decompose the Hamiltonian $\mathscr{H}$ into $\mathscr{H}_1 + \mathscr{H}_2 + \cdots + \mathscr{H}_p$ so that the matrix elements $\langle\alpha|\exp(-\beta\mathscr{H}_j)|\alpha'\rangle$ may be obtained explicitly with the use of effective local interactions, as was discussed before.

From a practical point of view, it is more convenient to use the following "symmetric" expression of the thermal quantum state

$$|O(\beta)\rangle = Z(\beta)^{-1/2}\exp(-\tfrac{1}{2}\beta\mathscr{H}^s)|I\rangle \qquad \mathscr{H}^s = \tfrac{1}{2}(\mathscr{H} + \tilde{\mathscr{H}}) \quad (67)$$

when $[\mathscr{H}, \tilde{\mathscr{H}}] = 0$ as is usually the case. Correspondingly we have the following "symmetric" path-sum formulation

$$|O(\beta)\rangle = \lim_{n\to\infty} |\Psi_n\rangle \quad (68)$$

where $|\Psi_n\rangle$ is given by

$$|\Psi_n\rangle = Z_n(\beta)^{-1/2}(e^{-(\beta/2n)\mathscr{H}_1^s}\cdots e^{-(\beta/2n)\mathscr{H}_p^s})^n|I\rangle \quad (69)$$

9.2. Basic Ideas of the Thermo Field Monte Carlo

Our basic idea of the thermo field Monte Carlo[32] is to calculate the thermal state $|\Psi_n\rangle$ as a diffusion process by extending the Kuti–Blanckenbecler–Sugar (KBS) Monte Carlo method at zero temperature[70-72] to that of finite temperatures, with important sampling.[70]

First we select the initial thermal state $|I\rangle_i$ randomly, as a subspace of $|I\rangle$. Then, we apply the partial "canonical thermal operator" $\exp[-\beta\mathscr{H}_j^s/(2n)]$ successively to the thermal state already obtained, namely

$$|O(\beta_j)\rangle \propto \exp[-\tfrac{1}{2}(\beta_j - \beta_{j-1})\mathscr{H}]|O(\beta_{j-1})\rangle \quad (70)$$

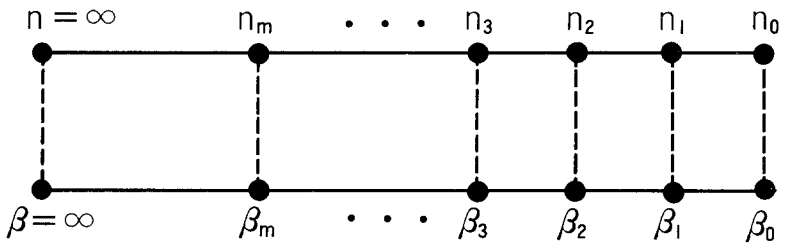

Fig. 13. The thermal quantum state $|O(\beta_j)\rangle$ is constructed successively from each previous higher-temperature thermal quantum state $|O(\beta_{j-1})\rangle$.

Thus, the thermal states can be calculated successively from each previous thermal states at a higher temperature, as shown in Fig. 13. This procedure makes a diffusion process in the double Hilbert space $(\mathscr{H}, \tilde{\mathscr{H}})$. That is, the thermal state can be obtained as a "sample ensemble" of the form

$$|O(\beta)\rangle \simeq \sum_{p,q \in S} W_{p,q}(\beta)\,|p, \tilde{q}\rangle \tag{71}$$

where the weight $W_{p,q}(\beta)$ is given by

$$W_{p,q}(\beta) = \mathscr{N}(\beta) \sum_{r \in S_0} \langle \tilde{q}, p|\, (e^{-(\beta/2n)\mathscr{H}^s_1} \cdots e^{-(\beta/2n)\mathscr{H}^s_p})^n\, |r, \tilde{r}\rangle \tag{72}$$

with some appropriate normalization $\mathscr{N}(\beta)$. Here, S_0 denotes the initial sample set in which all the states $|r, \tilde{r}\rangle$ have an equal probability, and S denotes a final ensemble produced by the Monte Carlo method. Consequently, the average of a physical quantity Q is given by

$$\begin{aligned} \langle Q\rangle_{\text{eq}} &= \langle O(\beta)|\, Q\, |O(\beta)\rangle \\ &\simeq \sum_{p,s \in S} \langle p|\, Q\, |s\rangle \sum_{q \in S} W^*_{p,q}(\beta)\, W_{s,q}(\beta)\, \mathscr{N}^2(\beta) \end{aligned} \tag{73}$$

9.3. Folding Monte Carlo Method

The above arguments suggest the following expression[32–36]

$$\begin{aligned} \langle Q\rangle_{\text{eq}} &= \text{tr}\, \exp(-\tfrac{1}{2}\beta\mathscr{H})\, Q\, \exp(-\tfrac{1}{2}\beta\mathscr{H})/Z(\beta) \\ &= \sum_{m,n,s} \langle m|\, Q\, |n\rangle\, \langle n|\, e^{-(1/2)\beta\mathscr{H}}\, |s\rangle\, \langle s|\, e^{-(1/2)\beta\mathscr{H}}\, |m\rangle / Z(\beta) \end{aligned} \tag{74}$$

where

$$Z(\beta) = \sum_{m,n} |\langle n|\, \exp(-\tfrac{1}{2}\beta\mathscr{H})\, |m\rangle|^2 \tag{75}$$

This simple reinterpretation of the average $\langle Q \rangle$ is very useful; namely no periodic boundary condition in Trotter's direction is necessary (which makes MC simulations very efficient), and each element in (75) is always positive.

10. POSSIBLE APPLICATIONS OF THE EQUIVALENCE THEOREM TO ANALYTIC AND NUMERICAL CALCULATIONS OF QUANTUM SYSTEMS—CLOSED-FORM SOLUTIONS OF THE *n*TH APPROXIMANT AND QUANTUM TRANSFER-MATRIX METHODS

10.1. Closed Solutions of the $n=1$ (Pair-Product) Approximants

It will be useful to study analytically even the $n=1$ approximant in equivalence Theorem 4.

10.1.1. Closed Solution of the $n=1$ Approximant of the Anisotropic Heisenberg Chain. As was given by the present author,[50] the partition function Z_1 for $n=1$ is given by

$$Z_1 = 2^N(\cosh K_x \cosh K_y \cosh K_z - \sinh K_x \sinh K_y \sinh K_z)^N \quad (76)$$

with K_x, K_y, and K_z defined by (57) for the Hamiltonian (55) in one dimension.

10.1.2. Closed-form Solution of the Two-Dimensional Spin Systems. The first nontrivial closed-form solution of the two-dimensional XY model was given by Lagendijk and De Raedt[73] for the $n=1$ approximant, which shows a phase transition with the logarithmic divergence of specific heat at a finite critical temperature.

The critical line of the anisotropic Heisenberg model was found by Onogi et al.[74] for the $n=1$ approximant in two dimensions. It is expected that closed-form solutions of many other "*n*th approximants" will be obtained in the near future.

10.2. Quantum Transfer-Matrix Methods

Equivalence Theorem 4 yields the idea to apply the classical transfer-matrix methods to quantum systems. This idea was first performed analytically by the present author[9] implicitly, and numerically first by Betsuyaku.[29,30] Recently the present author proposed the thermo field transfer-matrix method.[32,34–36] One of the merits of this method is that the

thermal states can be calculated successively from the high temperature limit to the low temperature limit ($T=0$), as shown in Fig. 13. Some applications of this method will be reported elsewhere.

11. QUANTUM MONTE CARLO METHOD OF DYNAMICS

It is also of great interest to study dynamical problems with the use of Monte Carlo simulations. According to Kubo's linear response theory,[75] we need the time correlation function of the form

$$\langle A(t)\, A(0)\rangle = Z(\beta)^{-1}\, \mathrm{tr}(e^{-\beta\mathscr{H}}\, e^{it\mathscr{H}/\hbar}\, A e^{-it\mathscr{H}/\hbar} A) \tag{77}$$

in order to calculate transport coefficients.[75] Recently Hirsch et al.[16] and Wolynes[76] tried to calculate (77) using the quantum Monte Carlo method based on equivalence Theorem 4, by separating the real and imaginary parts of the temporal evolution operator $\exp(it\mathscr{H}/\hbar)$. For more details, see Refs. 16 and 76.

There may be another method to evaluate (77) numerically by calculating first the imaginary time correlation function

$$C(z) = \langle e^{z\mathscr{H}}\, A e^{-z\mathscr{H}} A\rangle \tag{78}$$

for real z and then by a numerical analytic continuation of $C(z)$ to the real time axis. This requires a very long computing time, because a large value of Trotter's number n has to be used to calculate explicitly the canonical operator $\exp(z\mathscr{H})$ on the basis of equivalence Theorem 4. This will remain a future problem.

12. SUMMARY AND DISCUSSION

In the present paper we have reviewed some basic ideas of the quantum statistical Monte Carlo method, namely quantum Monte Carlo at finite temperatures, based on the equivalence theorem proposed by the present author. Some useful techniques for this method, namely "computationics," are discussed in detail. As a new method, the thermo field Monte Carlo method has been explained briefly. A thermo field real-space renormalization group approach will be also useful in the near future.

Many other people[77–83] have also started to work in this field of quantum statistical Monte Carlo.

In frustrated quantum spin systems and higher-dimensional fermi systems, the so-called "negative sign problem" appears, and the accuracy of calculations becomes worse for larger systems. Hopefully, this problem will be solved in the near future.

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