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Thermo Field Dynamics of Quantum Spin Systems

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Thermo field dynamics of quantum spin systems is formulated, which gives a new variational principle at finite temperatures. The KMS relation is reformulated as identities among thermal vacuum states. Path integral formulations of the thermal vacuum state are given, which yield a new "thermo field Monte Carlo method." Thermo field dynamics of finite-spin systems are studied in detail as simple examples of the present method. Pertubational expansion methods of the thermal state and time-dependent state are also given.

KEY WORDS: Thermo field dynamics; quantum spin system; Monte Carlo method; thermal vacuum; KMS relation; variational principle; path integral; triangular lattice; Heisenberg model.

1. INTRODUCTION

The purpose of the present paper is to extend the thermo field dynamics(1-3) to quantum spin systems and to give a formal expression of the thermal state. This is convenient for constructing a variational theory at finite temperatures and for numerical calculations. Thermo field Monte Carlo and transfer-matrix methods are proposed to study numerically the thermal vacuum state of quantum spin systems. Some useful formulas concerning the thermal vacuum state and projection operators are given in the Appendix. The thermal states of finite-spin systems are given explicitly. Perturbational expansions of the thermal state and nonequilibrium state are also given.

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2. GENERAL FORMULATION OF THERMO FIELD DYNAMICS IN QUANTUM SPIN SYSTEMS

As was generally formulated in Fermi and Bose systems,$^{(1-3)}$ the statistical average of any physical quantity Q at temperature T is expressed by the "thermal vacuum" expectation value of the form

$$\langle Q\rangle \equiv Z^{-1}(\beta)\operatorname{Tr} Qe^{-\beta\mathscr{H}} = \langle O(\beta)|\, Q\, |O(\beta)\rangle \tag{1}$$

and

$$Z(\beta) = \operatorname{Tr} e^{-\beta\mathscr{H}}, \qquad \beta = \frac{1}{k_B T} \tag{2}$$

where $\mathscr{H}$ is the Hamiltonian of the relevant quantum system. Here, the thermal vacuum state $|O(\beta)\rangle$ is constructed in a replicated space $|n, \tilde{n}\rangle \equiv |n\rangle\, |\tilde{n}\rangle$ as

$$\begin{aligned} |O(\beta)\rangle &= Z(\beta)^{-1/2} \sum_n e^{-\beta E_n/2}\, |n, \tilde{n}\rangle \\ &= Z(\beta)^{-1/2}\, e^{-(1/2)\beta\mathscr{H}} \sum_n |n, \tilde{n}\rangle \end{aligned} \tag{3}$$

where $|n\rangle$ is an eigenstate of $\mathscr{H}$ with an eigenvalue E_n, namely,

$$\mathscr{H}\, |n\rangle = E_n\, |n\rangle \tag{4}$$

and $|\tilde{n}>$ is the corresponding eigenstate in the fictitious dynamical system $\tilde{\mathscr{H}}$ which is identical to the original system $\mathscr{H}$ through the following mapping:

(1) The tilde spin operator $\tilde{S}$ is, in general, defined$^{(1-3)}$ by

$$\langle \tilde{n}|\, \tilde{S}\, |\tilde{m}\rangle = \langle m|\, S^\dagger\, |n\rangle = \langle n|\, S\, |m\rangle^* \tag{5}$$

(2) The commutation rule is given by

$$[S, \tilde{Q}] = 0 \tag{6}$$

Then, we obtain the following conjugation rules$^{(1-3)}$:

$$\begin{gathered} \widetilde{AB} = \tilde{A}\tilde{B}, \qquad \widetilde{c_1 A + c_2 B} = c_1^* \tilde{A} + c_2^* \tilde{B} \\ \widetilde{A^\dagger} = \tilde{A}^\dagger, \qquad \tilde{\tilde{A}} = A, \qquad \text{and} \qquad \widetilde{|O(\beta)\rangle} = |O(\beta)\rangle \end{gathered} \tag{7}$$

Here c_1 and c_2 are c numbers and c^* denotes the complex conjugate of c.

For spin operators S^x, S^y, and S^z, we have explicitly

$$\widetilde{S^x}=\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \widetilde{S^y}=\frac{1}{2}\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix},\quad \widetilde{S^z}=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$
$$\widetilde{S^+}=\widetilde{S^x}-i\widetilde{S^y}=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad \widetilde{S^-}=\widetilde{S^x}+i\widetilde{S^y}=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} \tag{8}$$
$$[\widetilde{S^x},\widetilde{S^y}]=-i\widetilde{S^z}$$

More conveniently, the above thermal vacuum state is also expressed$^{(4)}$ by

$$|O(\beta)\rangle=Z(\beta)^{-1/2}\exp(-\tfrac{1}{2}\beta\mathscr{H})\,|I\rangle \tag{9}$$

where

$$|I\rangle=\sum_s |s,\tilde{s}\rangle \tag{10}$$

Here $|s\rangle$ is a microstate as a direct product of N spinors

$$\alpha_i=\begin{pmatrix}1\\0\end{pmatrix}_i,\qquad \beta_i=\begin{pmatrix}0\\1\end{pmatrix}_i,\qquad S_i^z\alpha_i=\tfrac{1}{2}\alpha_i,\qquad \text{and}\quad S_i^z\beta_i=-\tfrac{1}{2}\beta_i$$

namely,

$$|s\rangle=|s_1,s_2,\ldots,s_N\rangle,\qquad |s_i\rangle=\alpha_i\quad\text{or}\quad\beta_i \tag{12}$$

The space $|\tilde{s}\rangle$ is the tilde spin space defined by (5) and (6).

It is easy to prove$^{(4)}$ that

$$\sum_n |n,\tilde{n}\rangle=\sum_s |s,\tilde{s}\rangle=|I\rangle \tag{13}$$

using the unitarity of the transformation

$$\{|n\rangle\}=U\{|s\rangle\}$$

i.e.,

$$|n\rangle=\sum_s U_{ns}\,|s\rangle \tag{14}$$

namely,

$$\sum_n U_{ns}U_{nr}^*=\delta_{s,r} \tag{15}$$

This yields the equivalence of the two expressions (3) and (9). This equivalence is very useful from a practical point of view, because the state $|s, \tilde{s}\rangle$ is immediately obtained, while the state $|n, \tilde{n}\rangle$ is generally difficult to obtain.(5)

More generally, the time-dependent state $|\Psi(t)\rangle$ is expressed by

$$|\Psi(t)\rangle = \rho(t)^{1/2}\,|I\rangle = \rho(t)^{1/2} \sum_s |s, \tilde{s}\rangle \tag{16}$$

where the density matrix $\rho(t)$ is given by the solution of the equation

$$i\hbar \frac{\partial}{\partial t}\rho(t) = [\mathscr{H}(t), \rho(t)] \tag{17}$$

for a time-dependent Hamiltonian $\mathscr{H}(t)$. Therefore, we have

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \widehat{\mathscr{H}(t)}\,|\Psi(t)\rangle \tag{18}$$

when $[\mathscr{H}(t), \tilde{\mathscr{H}}(t)] = 0$ as is usually the case, and

$$\widehat{\mathscr{H}(t)} = \mathscr{H}(t) - \widetilde{\mathscr{H}(t)} \tag{19}$$

An equation similar to (18) was obtained(6,7) for a time-independent Hamiltonian $\mathscr{H}$.

The formal solution of (18) is given by

$$|\Psi(t)\rangle = \exp_+\left(\frac{1}{i\hbar}\int_0^t \hat{\mathscr{H}}(s)\,ds\right)|\Psi(0)\rangle \tag{20}$$

using Kubo's generalized ordered exponential.(8) The above expressions (13) and (20) hold in general quantum systems as well as in quantum spin systems.

3. KUBO–MARTIN–SCHWINGER RELATION

As in Bose and Fermi systems,(2) it is easy to express the Kubo–Martin–Schwinger (KMS) relation(9,10) in terms of the thermo field dynamics.

The Heisenberg representations of spin operator S and $\tilde{S}$ are given by

$$S(t) = e^{(it/\hbar)\hat{\mathscr{H}}}\, S e^{(-it/\hbar)\hat{\mathscr{H}}} = e^{(it/\hbar)\mathscr{H}}\, S e^{(-it/\hbar)\mathscr{H}} \tag{21}$$

and

$$\widetilde{S(t)} = e^{(it/\hbar)\hat{\mathscr{H}}}\, \tilde{S} e^{(-it/\hbar)\hat{\mathscr{H}}} = e^{(-it/\hbar)\tilde{\mathscr{H}}}\, \tilde{S} e^{(it/\hbar)\mathscr{H}} \tag{22}$$

Then we have$^{(2-4)}$ the following relations:

$$\widetilde{S(t)}\,|O(\beta)\rangle = S^{\dagger}(t-\tfrac{1}{2}i\hbar\beta)\,|O(\beta)\rangle \tag{23}$$

and

$$\langle O(\beta)|\,S(t) = \langle O(\beta)|\,\widetilde{S}^{\dagger}(t+\tfrac{1}{2}i\hbar\beta) \tag{24}$$

These are called thermal state conditions.$^{(2,3)}$ The above relations are proven$^{(4)}$ even in the spin representation $|s, \tilde{r}\rangle$. The above thermal state (KMSTU$^{(4)}$) conditions (23) and (24) yield$^{(2-4)}$ the ordinary KMS relation:

$$\begin{aligned}
&\langle O(\beta)|\,S(t)\,Q(t')\,|O(\beta)\rangle \\
&\quad = \langle O(\beta)|\,\widetilde{S}^{\dagger}(t+\tfrac{1}{2}i\hbar\beta)\,\widetilde{Q}^{\dagger}(t'-\tfrac{1}{2}i\hbar\beta)\,|O(\beta)\rangle \\
&\quad = \langle O(\beta)|\,Q(t')\,S(t+i\hbar\beta)\,|O(\beta)\rangle
\end{aligned} \tag{25}$$

The above relations (23) and (24) will be useful in C^*-algebraic formulations of statistical mechanics in terms of thermo field dynamics.

4. TILDE-CONJUGATION INVARIANT UNITARY SPIN TRANSFORMATION

It is convenient to find here a tilde-conjugation invariant unitary spin transformation U such that

$$S_j^{\pm}(\beta) = U S_j^{\pm} U^{-1}, \qquad \widetilde{S^{\pm}(\beta)} = U \widetilde{S_j^{\pm}} U^{-1} \tag{26}$$

where

$$U^{\dagger} = U \qquad \text{and} \quad \tilde{U} = U \tag{27}$$

Then, the transformed "thermal operators" $S_j^{\pm}(\beta)$, $\widetilde{S_j^{\pm}(\beta)}$,... satisfy the spin and antispin commutation relations

$$\begin{aligned}
&[S_j^x(\beta), S_j^y(\beta)] = iS_j^z(\beta), &&\widetilde{[S_j^x(\beta)}, \widetilde{S_j^y(\beta)}] = -i\widetilde{S_v^z} \\
&[S_j^x(\beta), S_j^y(\beta)] = 0, &&[S_j^y(\beta), \widetilde{S_j^z(\beta)}] = 0
\end{aligned} \tag{28}$$

and

$$[S_j^z(\beta), \widetilde{S_j^x(\beta)}] = 0$$

and the Hermiticity relations

$$(S_j^x(\beta))^{\dagger} = S_j^x(\beta), \ (S_j^{\pm}(\beta))^{\dagger} = S_j^{\mp}(\beta) \tag{29}$$

The simplest and nontrivial example may be given by the following transformation:

$$S_j^{\pm}(\beta) = uS_j^{\pm} + 2vS_j^z\widetilde{S_j^{\mp}}$$
$$\widetilde{S_j^{\pm}}(\beta) = u\widetilde{S_j^{\pm}} + 2v\widetilde{S_j^z}S_j^{\mp}$$
$$S_j^z(\beta) = u^2S_j^z - v^2\widetilde{S_j^z} - uv(S_j^+\widetilde{S_j^+} + S_j^-\widetilde{S_j^-})$$

and

$$\widetilde{S_j^z}(\beta) = u^2\widetilde{S_j^z} - v^2S_j^z - uv(S_j^+\widetilde{S_j^+} + S_j^-\widetilde{S_j^-}) \tag{30}$$

where the coefficients u and v are real parameters satisfying the relation

$$u^2 + v^2 = 1 \tag{31}$$

namely, they are functions of a single variable β as

$$u = u(\beta) \qquad \text{and} \qquad v = v(\beta) \tag{32}$$

It is easily shown[4] that the above new spin variables $S_j^{\pm}(\beta)$, $\widetilde{S_j^{\pm}(\beta)}$, $S_j^z(\beta)$ and $\widetilde{S_j^z(\beta)}$ are generated by the following unitary transformation:

$$U = \exp[\theta(\beta)(S_j^+\widetilde{S_j^+} - S_j^-\widetilde{S_j^-})] \tag{33}$$

through (26) with $u(\beta) = \cos\theta(\beta)$.

Now we define a thermal state $|O(\beta)\rangle^{(0)}$ by

$$|O(\beta)\rangle^{(0)} = \prod_j (u + vS_j^+\widetilde{S_j^+})\,|0\rangle \tag{34}$$

where

$$|0\rangle = \beta_1\beta_2\cdots\beta_N \equiv \begin{pmatrix}0\\1\end{pmatrix}_1 \times \begin{pmatrix}0\\1\end{pmatrix}_2 \times \cdots \times \begin{pmatrix}0\\1\end{pmatrix}_N \tag{35}$$

and N denotes the number of spins. Then, we can confirm easily that

$$\begin{gathered}
S_j^z(\beta)\,|O(\beta)\rangle^{(0)} = \widetilde{S_j^z(\beta)}\,|O(\beta)\rangle^{(0)} = -\tfrac{1}{2}\,|O(\beta)\rangle^{(0)} \\
S_j^-(\beta)S_j^+(\beta)\,|O(\beta)\rangle^{(0)} = |O(\beta)\rangle^{(0)}, \qquad \widetilde{S_j^-(\beta)}\widetilde{S_j^+(\beta)}\,|O(\beta)\rangle^{(0)} = |O(\beta)\rangle^{(0)} \\
S_j^-(\beta)\,|O(\beta)\rangle^{(0)} = 0, \qquad \widetilde{S_j^-}(\beta)\,|O(\beta)\rangle^{(0)} = 0 \\
S_j^-(\beta)\,|1(\beta)\rangle_j^{(0)} = |O(\beta)\rangle^{(0)}, \qquad \widetilde{S_j^-(\beta)}\,|\widetilde{1(\beta)}\rangle_j^{(0)} = |O(\beta)\rangle^{(0)}
\end{gathered} \tag{36}$$

where

$$|1(\beta)\rangle_j^{(0)} \equiv S_j^+(\beta)\,|O(\beta)\rangle^{(0)} = S_j^+\,|0\rangle, \quad |1(\beta)\rangle_j \equiv \widetilde{S_j^+(\beta)}\,|O(\beta)\rangle^{(0)} = \widetilde{S_j^+}\,|0\rangle \tag{37}$$

That is, the "thermal state" $|O(\beta)\rangle^{(0)}$ is the "eigenstate" of the "thermal operators" $S_j^z(\beta)$ and $\widetilde{S_j^z(\beta)}$.

The inverse transformations of (30) are given by

$$\begin{aligned}
S_j^{\pm} &= uS_j^{\pm}(\beta) - 2vS_j^z(\beta)\,\widetilde{S_j^{\mp}(\beta)} \\
S_j^{\pm} &= u\widetilde{S_j^{\pm}(\beta)} - 2v\widetilde{S_j^z(\beta)}\,S_j^{\mp}(\beta) \\
S_j^z &= u^2 S_j^z(\beta) - v^2\widetilde{S_j^z(\beta)} + uv(S_j^{+}(\beta)\,\widetilde{S_j^{+}(\beta)} + S_j^{-}(\beta)\,\widetilde{S_j^{-}(\beta)}) \\
S_j^z &= u^2\widetilde{S_j^z(\beta)} - v^2 S_j^z(\beta) + uv(S_j^{+}(\beta)\,\widetilde{S_j^{+}(\beta)} + S_j^{-}(\beta)\,\widetilde{S_j^{-}(\beta)})
\end{aligned} \tag{38}$$

This inverse transformation will be useful in expressing spin Hamiltonians in terms of thermal operators. Such Hamiltonians expressed by thermal operators can be used to derive temperature-dependent spin waves, as will be published elsewhere.

The above state $|O(\beta)\rangle^{(0)}$ is shown easily to be the thermal vacuum state of the following noninteracting spin system:

$$\mathscr{H}_0 = -\mu_B H \sum_{j=1}^{N} S_j^z \tag{39}$$

under the relations that

$$u(\beta) = (1 + e^{-2\beta\omega})^{-1/2}, \qquad v(\beta) = e^{-\beta\omega}(1 + e^{-2\omega})^{-1/2} \tag{40}$$

with $\omega = \frac{1}{2}\mu_B H$.

In practical applications of the above transformation, the transformation coefficients u and v (or $\beta\omega \equiv \frac{1}{2}\beta\mu_B H$) may have more general and physical meaning such as an effective field, as will be discussed later in more detail.

5. PATH INTEGRAL FORMULATION OF THE THERMAL STATE AND TRIAL THERMAL VACUUM

According to the present general formulation of the thermo field dynamics of quantum spin systems, the thermal vacuum of a spin system with Hamiltonian $\mathscr{H}$ is formally given by

$$|O(\beta)\rangle = (Z(\beta)/2^N)^{-1/2}\, e^{-(1/2)\beta\mathscr{H}}\,|O(0)\rangle \tag{41}$$

where the state $|O(0)\rangle$ is the thermal vacuum in the high-temperature limit and it is given explicitly by

$$|O(0)\rangle = \prod_j \frac{1}{\sqrt{2}}\,(1+S_j^+\widetilde{S_j^+})\,|0\rangle = 2^{-N/2}\,|I\rangle \tag{42}$$

with (10) in our spin representation.

It is convenient to make use of the generalized Trotter formula$^{(11-14)}$

$$e^{A_1+A_2+\cdots+A_p} = \lim_{n\to\infty}\,(e^{(1/n)A_1}e^{(1/n)A_2}\cdots e^{(1/n)A_p})^n \tag{43}$$

The convergence of the limit (43) is assured by the following inequality$^{(11-14)}$:

$$\left\|\exp\left(\sum_{j=1}^{p} A_j\right) - \left(\prod_{j=1}^{p} e^{(1/n)A_j}\right)^n\right\| \leqslant \frac{1}{n}\left(\sum_{j=1}^{p}\|A_j\|\right)^2 \exp\left(\sum_{j=1}^{p}\|A_j\|\right) \tag{44}$$

With the use of the above formula (43), we obtain the following path integral formulation of the thermal state:

$$\begin{aligned}|O(\beta)\rangle = Z(\beta)^{-1/2} \lim_{n\to\infty} &\{e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_1)}\times\cdots\times e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_N)}\}^{(1\text{st})}\\ \times &\{e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_1)}\times\cdots\times e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_N)}\}^{(2\text{nd})}\\ &\vdots\\ \times &\{e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_1)}\cdots e^{-(1/2n)\beta\mathscr{H}(\mathbb{r}_N)}\}^{(n\text{th})}\,|I\rangle\end{aligned} \tag{45}$$

where the Hamiltonian $\mathscr{H}$ is decomposed into local operators as

$$\mathscr{H} = \sum_{\mathbb{r}} \mathscr{H}(\mathbb{r}) \tag{46}$$

There are many other representations$^{(4)}$ of path integrals of the thermal state.

Some useful formulas to calculate (45) explicitly are given in the Appendix.

6. THERMO FIELD VARIATIONAL PRINCIPLE

The path integral formulation (45) in the preceding section suggests a "thermo field variational theory." That is, we consider a trial thermal state of the form

$$|\Psi(\theta)\rangle = \prod_{\langle ij\cdots k\rangle} U_{ij\cdots k}(\theta)\,|O(0)\rangle \tag{47}$$

with some appropriate local operators $U_{ij\cdots k}(\theta)$. The variational parameter θ (or many parameters $\theta_{ij\cdots k}$) can be determined by the variational principle of minimization of the free energy $F(\theta)$ given by

$$F(\theta) = E(\theta) - TS(\theta) \tag{48}$$

where the variational energy

$$E(\theta) = \langle \Psi(\theta) | \, \mathscr{H} \, | \Psi(\theta) \rangle / \langle \Psi(\theta) | \, \Psi(\theta) \rangle \tag{49}$$

and the variational entropy $S(\theta)$ may be calculated as

$$S(\theta) = -k_B \sum_{\alpha} p_\alpha \log p_\alpha \tag{50}$$

with the probability p_α to find the trial vacuum $|\Psi(\theta)\rangle$ in a state $|\alpha\rangle$ specified by the spin representation.

From this point of view, the nth approximant of the path integral formula (or decomposition formula) (45) may be regarded as a systematic variational state, namely,

$$|\Psi_n\rangle = (Z_n(\beta)/2^N)^{-1/2} (e^{-(\beta/2n)\mathscr{H}_1} \cdots e^{-(\beta/2n)\mathscr{H}_N})^n \, |O(0)\rangle \tag{51}$$

where $\mathscr{H}_j = \mathscr{H}(\mathbb{r}_j)$, and

$$Z_n(\beta) = \mathrm{Tr}(e^{-(\beta/2n)\mathscr{H}_1} \cdots e^{-(\beta/2n)\mathscr{H}_N})^{2n} \tag{52}$$

This is very important from a practical point of view, as will be shown later.

As a simple example of the "thermo field variational method," we discuss here the well-known molecular field theory in the Heisenberg model

$$\mathscr{H} = -J \sum_{\langle ij \rangle} \mathbb{S}_i \cdot \mathbb{S}_j \tag{53}$$

The molecular field thermal state of this system is given in the form

$$|O(\beta)\rangle^{(mf)} = \prod_j \, (u_m + v_m S_j^+(\beta) \, \widetilde{S_j^+}(\beta)) \, |0\rangle \tag{54}$$

where the coefficients u_m and v_m are determined self-consistently by minimizing the free energy $F = E - TS$. Here the energy E is expressed by

$$E = -\frac{NzJ}{2} \langle O(\beta) | \, \mathbb{S}_i \cdot \mathbb{S}_j \, | O(\beta) \rangle^{(mf)} = -\tfrac{1}{2} NzJm^2 \tag{55}$$

in terms of the magnetization $m \equiv \langle S_j^z \rangle$, in our approximation for the relevant spin system with interaction J, where z denotes the number of nearest neighbors. The entropy S is also given by the expression

$$\begin{aligned} S &= -Nk_B(u_m^2 \log u_m^2 + v_m^2 \log v_m^2) \\ &= -Nk_B\{(\tfrac{1}{2}+m)\log(\tfrac{1}{2}+m) \\ &\quad + (\tfrac{1}{2}-m)\log(\tfrac{1}{2}-m)\} \end{aligned} \tag{56}$$

from the molecular field thermal state (54), because the magnetization m takes the form

$$\begin{aligned} m &= \langle S_j^z \rangle = \langle O(\beta)|\, S_j^z \,|O(\beta)\rangle^{(mf)} \\ &= \tfrac{1}{2}(v_m^2 - u_m^2) = \tfrac{1}{2} - u_m^2 = v_m^2 - \tfrac{1}{2} \end{aligned} \tag{57}$$

with the normalization condition $u_m^2 + v_m^2 = 1$. Now, the minimization of the free energy $F = E - TS$ yields the molecular field equation of state

$$m = \tfrac{1}{2}\tanh(\tfrac{1}{2}\beta zJm) \tag{58}$$

A more practical application will be given later.

7. THERMO FIELD TRANSFER-MATRIX METHOD

As one of important applications of the path integral formulation of the thermal state, we propose here "thermo field transfer-matrix method." From the general formulation on the thermo field dynamics given in the preceding sections, the thermal vacuum is also written

$$|O(\beta)\rangle = \mathcal{N} \lim_{n\to\infty} \mathcal{T}^n \,|O(0)\rangle \tag{59}$$

where $\mathcal{N}$ denotes the normalization and

$$\mathcal{T} = \mathcal{T}_1 \cdots \mathcal{T}_j \cdots \mathcal{T}_N; \qquad \mathcal{T}_j = \exp\left(-\frac{1}{2n}\beta\mathcal{H}_j\right) \tag{60}$$

as was given in (45). This formulation has the great merit that the transfer-matrix $\mathcal{T}$ can be obtained explicitly for finite systems without diagonalizing the Hamiltonian. The product $\mathcal{T}^n$ is also easily calculated by a high-speed computer through the formula

$$\mathcal{T}^n = (\cdots((\mathcal{T}^2)^2)\cdots)^2 \tag{61}$$

for $n = 2^p$.

The transfer-matrix method for the partition function in quantum spin systems was already discussed by the present author(12,14) and by Betsuyaku.(16)

8. THERMO FIELD MONTE CARLO METHODS

Owing to the path integral formulation of the thermal state given in Section 5, we can now extend the Kuti–Blankenbecler–Suger (KBS) Monte Carlo method at zero temperature(16) to finite temperatures. Blankenbecler and Sugar(17) applied Kuti's stochastic method with important sampling(16) to their formula

$$\langle Q \rangle_{T=0} = \langle \Psi_0 | \, Q \, | \Psi_0 \rangle = \lim_{B \to \infty} \frac{\langle \chi | \, e^{-\beta \mathscr{H}} Q e^{-\beta \mathscr{H}} \, | \phi \rangle}{\langle \chi | \, e^{-2\beta \mathscr{H}} \, | \phi \rangle} \tag{62}$$

for the ground state $|\Psi_0\rangle$, using Trotter's formula (43), as was applied to quantum Monte Carlo simulations first by Suzuki, Miyashita, and Kuroda.(18)

Now we can extend their method(17) to the thermal vacuum state $|O(\beta)\rangle$ which is expressed by the path summation (45). This may be called(19) "thermo field Monte Carlo method." For more details, see Ref. 19.

There are two new aspects in the present thermo field MC methods. The first one is that the thermal state $|O(\beta)\rangle$ contains the replicated tilde states $\{|\tilde{0}\rangle_j, |\tilde{1}\rangle_j\}$. The second point is that Trotter's number n and temperature T are related to each other in our formulation, as shown in Fig. 1. Namely, if we put $\beta/(2n) = \Delta\tau$ and fix it for a specific simulation, then we have $n = \beta/(2\Delta\tau) = 1/(2k_B T \Delta\tau)$. That is, if we increase the number of Monte Carlo steps, i.e., n, for $\Delta\tau$ fixed, then the system moves to lower temperatures. The state $|O(\beta_n)\rangle$ thus obtained becomes now the initial state of the MC simulation of the state $|O(\beta_{n+1})\rangle$ at lower temperature β_{n+1}, as shown in Fig. 1. Therefore we can perform successively MC simulations for a wide range of temperatures very efficiently. This is one of the great merits of the present new methods.

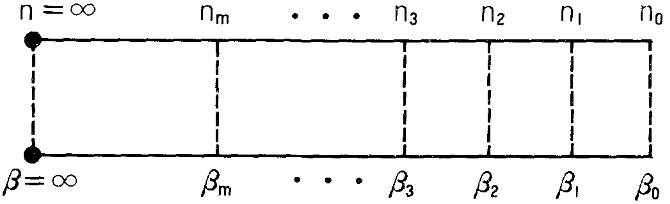

Fig. 1. Illustration of continuous change of inverse temperatures $\{B\}$ by increasing Trotter's number n in the thermo field Monte Carlo simulation.

9. APPLICATIONS TO THE TWO-DIMENSIONAL TRIANGULAR ANTIFERROMAGNETIC QUANTUM HEISENBERG MODEL

One of the most interesting applications of the thermo field dynamics will be Anderson's problem on the phase coherence of movable singlet pairs in the two-dimensional triangular antiferromagnetic quantum Heisenberg model.(21) Quite recently Hirakawa *et al.*(22) found an experimental candidate such as $\mathrm{NaTiO_2}$ to test Anderson's picture.

In order to study the quantum effect of this system at finite temperatures, the present formulation of thermo field dynamics in quantum spin systems is very appropriate, because we can discuss the thermal state explicitly in the form

$$|O(\beta)\rangle = \mathcal{N} \exp(-\tfrac{1}{2}\beta\mathcal{H})\,|I\rangle \tag{63}$$

where the Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H} = \sum_{\langle ij\rangle} \mathcal{H}_{ij}; \qquad \mathcal{H}_{ij} = -J\sigma_i \cdot \sigma_j \qquad (J<0) \tag{64}$$

9.1. Cell Approximants

A practical method to study the thermal vacuum state of this system will be to decompose the exponential operator in (41), as was discussed already. A new aspect is, however, how a large cell should be used in the decomposition of (41). The simplest one is given by the following pair-product approximant(23):

$$|O(\beta)\rangle_{\mathrm{PPA}} = \mathcal{N}_1 \prod_{\langle ij\rangle} \exp(-\tfrac{1}{2}\beta\mathcal{H}_{ij})\,|I\rangle \tag{65}$$

Here, the partial exponential operator in (65) is given by

$$\begin{aligned}\exp(-\tfrac{1}{2}\beta\mathcal{H}_{ij}) &= \exp(\tfrac{1}{2}K\sigma_i \cdot \sigma_j)\\ &= aQ_{ij} + bP_{ij}\end{aligned} \tag{66}$$

where $K = J/k_B T < 0$, and

$$a = e^{(1/2)K} \qquad \text{and} \qquad b = e^{-(3/2)K} \tag{67}$$

Here P_{ij} and Q_{ij} are projection operators defined by

$$\begin{aligned}&P_{ij} = \tfrac{1}{4}(1 - \sigma_i\sigma_j), \qquad Q_{ij} = \tfrac{1}{4}(3 + \sigma_i \cdot \sigma_j)\\ &P_{ij}^2 = P_{ij},\ Q_{ij}^2 = Q_{ij} \qquad \text{and} \qquad P_{ij} + Q_{ij} = 1\end{aligned} \tag{68}$$

The partition function in this approximation might be obtained in a closed form. It will be reported in future.

In order to study the present system more systematically, we may use the following formulation:

$$|O(\beta)\rangle_{\mathrm{PPA}}^{(n)} = \mathcal{N}_2 \left[\prod_{\langle ij \rangle} \exp\left(-\frac{1}{2n} \beta \mathcal{H}_{ij} \right) \right]^n |I\rangle \tag{69}$$

in some appropriate order of partial exponential operators. This may be useful in studying our system in the thermo field transfer-matrix and Monte Carlo methods proposed in Sections 7 and 8, respectively.

There are many other larger cell approximants.(4)

9.2. Variational Theory of Anderson's Problem

The previous pair-product approximant (65), namely,

$$|O(\beta)\rangle_{\mathrm{PPA}} = \mathcal{N} \prod_{\langle ij \rangle} (aQ_{ij} + bP_{ij})\, |I\rangle \tag{70}$$

suggests a variational treatment of the present problem *at finite temperatures*, though there have been published many papers(24–27) concerning variational calculations on quantum spin systems *at zero temperature.*

It will be essential to study the present system at finite temperatures to see whether a new type of coherent phase appears or not. For this purpose, the thermo field variational method will be very convenient. We give here only some preliminary considerations concerning the above problem.

P. W. Anderson(21) proposed that random arrangements of singlet pair bonds on a triangular lattice would give a trial ground state with an energy lower than that in the Néel state at zero temperature, as shown in Fig. 2. This state is represented as

$$|\Psi\rangle_A = \mathcal{N}_A \left[\sum \prod_{\langle ij \rangle} (\theta_i \theta_j P_{ij}) \right] |I\rangle\, |\theta\rangle \tag{71}$$

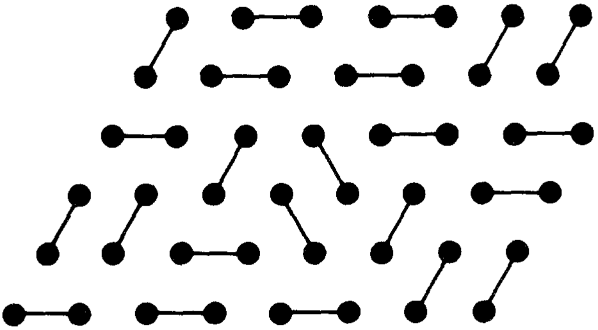

Fig. 2. Anderson's variational ground state.(21)

in our representation, where P_{ij} is the projection operator into the singlet state, being given by (68), and $\{\theta_j\}$ are an algebra defined by

$$[\theta_j, \theta_k]=0, \qquad \theta_j^2=0, \qquad \text{and} \qquad \langle\theta|\,\theta_j^\dagger\theta_j\,|\theta\rangle=1 \tag{72}$$

which are quite analogous to the Grassmann algebra.[28]

Now we extend Anderson's state (71) at zero temperature to the case at finite temperatures. The simplest extension of it may be

$$|\Psi\rangle_T=\mathcal{N}_T\sum\prod_{\langle ij\rangle}[\theta_i\theta_j(uQ_{ij}+vP_{ij})]\,|I\rangle\,|\theta\rangle \tag{73}$$

in our formulation, where Q_{ij} is the projection operator into the triplet state, being given by (68). Then, the total energy of this trial thermal state is given by

$$\begin{aligned} E&=\langle\Psi|\,\mathscr{H}\,|\Psi\rangle_T=-\tfrac{1}{2}NJ\,\langle\Psi|\,\sigma_i\cdot\sigma_j\,|\Psi\rangle_T\\ &=-\tfrac{1}{2}NJ\,\langle\Psi|\,1-4P_{ij}\,|\Psi\rangle_T\simeq-\tfrac{3}{2}NJ(u^2-v^2) \end{aligned}\tag{74}$$

in the pair-bond approximation.

The total entropy may be given by

$$S=-\tfrac{1}{2}Nk_B(3u^2\log u^2+v^2\log v^2) \tag{75}$$

On the other hand, the normalization of the thermal vacuum state gives the relation

$$3u^2+v^2=1 \tag{76}$$

where we have used the properties

$$\langle 1|\,P_{ij}\,|1\rangle_{ij}=1 \qquad \text{and} \qquad \langle 1|\,Q_{ij}\,|1\rangle_{ij}=3 \tag{77}$$

with the notation $|1\rangle_{ij}$ given in the Appendix. Therefore, our free energy is expressed by

$$\begin{aligned} F&=E-TS\\ &=\frac{1}{2}N\left\{-J(1-4x)+k_BT\left[(1-x)\log\frac{1-x}{3}+x\log x\right]\right\} \end{aligned}\tag{78}$$

with $x=v^2$. By minimizing this free energy with respect to x, we obtain

$$u^2=\frac{1}{e^{-4K}+3} \qquad \text{and} \qquad v^2=\frac{e^{-4K}}{e^{-4K}+3} \tag{79}$$

where $K = J/k_B T$. Thus, the thermal state coefficients u and v behave as in Fig. 3. A crossover effect occurs around the temperature $T^\times$ given by $v^2(T_c) \simeq 1/2$, namely

$$T^\times \simeq \left(\frac{|J|}{k_B}\right) \frac{4}{\log 3} \simeq 3.6\, |J|/k_B \tag{80}$$

Below this crossover temperature, singlet pairs are dominant. Above $T^\times$, the thermal vacuum state becomes disordered. This quantum crossover effect(29) might be relevant to the experimental result by Hirakawa *et al.*(22)

The above treatment may be too simple, because it is equivalent to the independent pair approximation. In order to take into account the correlation effect among singlet pairs, we have to include the interaction among singlet pairs. For this purpose, the larger-cell approximants discussed in Section 9.1 will be useful. The research in this direction is promising.

There is another possibility that there might occur a phase transition below which the long-range order (LRO) does not exist but only the phase coherence among singlet pairs exists, in the two-dimensional triangular antiferromagnetic quantum Heisenberg model, as was pointed out by P. W. Anderson.(21) It will be a quite interesting problem to study which possibility is realized in the above system, by extending the present thermo field variational theory. This investigation is now in progress.

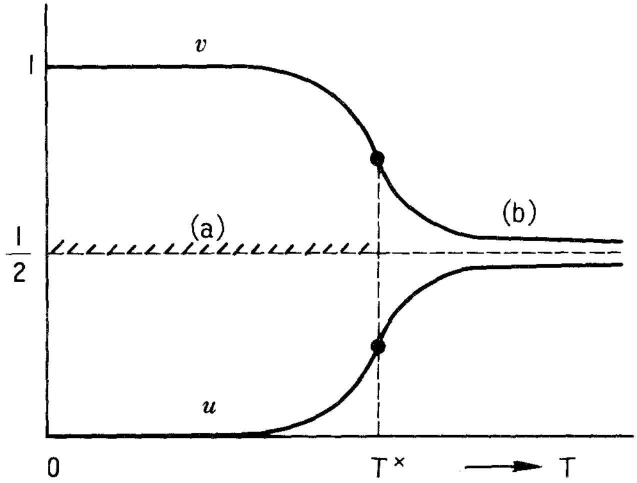

Fig. 3. Schematic temperature dependence of u and v, where $T^\times$ denotes the crossover temperature: (a) Singlet pairs dominant thermal state, and (b) disordered state.

10. THERMO FIELD DYNAMICS OF FINITE-SPIN SYSTEMS

As an illustrative example of the thermo field dynamics, we consider here finite-spin systems. The simplest example is a single-spin system, or equivalently a noninteracting spin system as was discussed in Section 4 to obtain the generalized Bogoliubov transformation.

10.1. Two-Spin System

The next simple example is a two-spin system of the form

$$\mathscr{H}_2 = -J_\perp(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) - J_\parallel \sigma_i^z\sigma_j^z - \mu_B H \sum_j \sigma_j^z \tag{81}$$

The thermal vacuum of this system is given by

$$\begin{aligned} |O(\beta)\rangle_h &= \mathscr{N}_h e^{-(1/2)\beta\mathscr{H}_2}\,|I\rangle \\ &= \mathscr{N}_h e^{(1/2)K_\perp \sigma_i\cdot\sigma_j} e^{(1/2)(K_\parallel - K_\perp)\sigma_i^z\sigma_j^z + (1/2)h(\sigma_i^z+\sigma_j^z)}\,|I\rangle \end{aligned} \tag{82}$$

where

$$K_\perp = \beta J_\perp, \qquad K_\parallel = \beta J_\parallel, \qquad \text{and} \qquad h = \beta\mu_B H \tag{83}$$

It is easy to show that

$$\begin{aligned} |O(\beta)\rangle_h = \mathscr{N}_h\{&(b_0 - a_0)(c-s)\,\hat{s}_{ij} \\ &+ a_0(c+s)(c_h^2 + s_h^2)\,|\hat{1}\rangle_{ij} - 2a_0(cs_h^2 + sc_h^2)(\hat{\alpha}_i\hat{\beta}_j + \hat{\beta}_i\hat{\alpha}_j) \\ &+ 2a_0(c+s)\,c_h s_h(\hat{\alpha}_i\hat{\alpha}_j - \hat{\beta}_i\hat{\beta}_j)\}, \qquad \hat{\alpha} = \alpha\tilde{\alpha} \end{aligned} \tag{84}$$

where we have used the formulas in the Appendix and also used the following abbreviations:

$$\begin{aligned} &c = \cosh\tfrac{1}{2}(K_\parallel - K_\perp), \qquad s = \sinh\tfrac{1}{2}(K_\parallel - K_\perp) \\ &c_h = \cosh(\tfrac{1}{2}h), \qquad s_h = \sinh(\tfrac{1}{2}h) \\ &a_0 = \exp(\tfrac{1}{2}K_\perp), \qquad b_0 = \exp(-\tfrac{3}{2}K_\perp) \end{aligned} \tag{85}$$

and

$$|\hat{1}\rangle_{ij} = \hat{\alpha}_i\hat{\alpha}_j + \hat{\alpha}_i\hat{\beta}_j + \hat{\beta}_i\hat{\alpha}_j + \hat{\beta}_i\hat{\beta}_j \tag{86}$$

Now the thermal state can be expanded as

$$|O(\beta)\rangle_h = |O(\beta)\rangle_0 + h\,|O(\beta)\rangle_{(1)} + O(h^2) \tag{87}$$

where

$$|O(\beta)\rangle_0 = \mathcal{N}_0\{[(b_0 - a_0)(c-s)\,\hat{s}_{ij} + a_0(c+s)\,|\hat{1}\rangle_{ij} - 2a_0 s(\hat{\alpha}_i\hat{\beta}_j + \hat{\beta}_i\hat{\alpha}_j)\}]$$

and

$$|O(\beta)\rangle_{(1)} = \mathcal{N}_{(1)} a_0(c+s)(\hat{\alpha}_i\hat{\alpha}_j - \hat{\beta}_i\hat{\beta}_j) \tag{88}$$

In particular, for the isotropic case, the zeroth thermal state is reduced to

$$\begin{aligned}|O(\beta)\rangle_2^{(\mathrm{iso})} &= \mathcal{N}_0(a\,|\hat{1}\rangle_{ij} + (b-a)\,\hat{s}_{ij}) \\ &= \mathcal{N}_0(aQ_{ij} + bP_{ij})\,|\hat{1}\rangle_{ij}\end{aligned} \tag{89}$$

with $a = \exp(K/2)$ and $b = \exp(-3K/2)$, in agreement with (65).

10.2. Three-Spin System

Next we consider a three-spin system shown in Fig. 4, whose Hamiltonian is given by

$$\mathscr{H}_{ijk} = -J(\sigma_i \cdot \sigma_j + \sigma_j \cdot \sigma_k + \sigma_k \cdot \sigma_i) \tag{90}$$

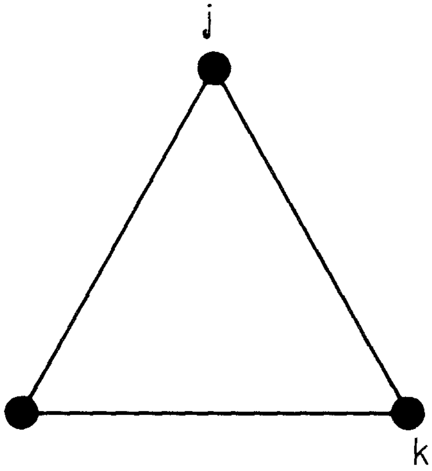

Fig. 4. Three-spin system.

The thermal state of this system is expressed by

$$\begin{aligned}|O(\beta)\rangle_3 &= \mathcal{N}_3 \exp(-\tfrac{1}{2}\beta\mathcal{H}_{ijk})\,|I\rangle \\ &= \mathcal{N}_3 \exp[-\tfrac{1}{2}\beta(\mathcal{H}_{ij}+\mathcal{H}_{jk}+\mathcal{H}_{ki})]\,|I\rangle \\ &= \mathcal{N}_3[\cosh(\tfrac{3}{2}K)+\tfrac{1}{3}\sinh(\tfrac{3}{2}K)(\sigma_i\cdot\sigma_j+\sigma_j\cdot\sigma_k+\sigma_k\cdot\sigma_i)]\,|I\rangle \end{aligned} \tag{91}$$

where we have used the identity

$$e^{K\mathcal{H}_3} = \cosh(3K) + \tfrac{1}{3}\sinh(3K)\,\mathcal{H}_3 \tag{92}$$

with

$$\mathcal{H}_3 = \sigma_i\cdot\sigma_j + \sigma_j\cdot\sigma_k + \sigma_k\cdot\sigma_i \tag{93}$$

Equivalently the thermal state (91) is written

$$|O(\beta)\rangle_3 = \mathcal{N}_3\{e^{(3/2)K} - \tfrac{4}{3}\sinh(\tfrac{3}{2}K)(P_{ij}+P_{jk}+P_{ki})\}\,|I\rangle \tag{94}$$

In the low-temperature limit $T \to 0$, we have

$$\begin{aligned}|O(\infty)\rangle_3 &= \mathcal{N}'_3(P_{ij}+P_{jk}+P_{ki})\,|I\rangle \\ &= \mathcal{N}'_3(\hat{s}_{ij}\,|\hat{1}\rangle_k + \hat{s}_{jk}\,|\hat{1}\rangle_i + \hat{s}_{ki}\,|\hat{1}\rangle_j)\end{aligned} \tag{95}$$

for $J < 0$. The physical picture of this state is clear, where

$$|\hat{1}\rangle_k = \hat{\alpha}_k + \hat{\beta}_k = \alpha_k\tilde{\alpha}_k + \beta_k\tilde{\beta}_k \tag{96}$$

Namely, *the singlet pair is moving around coherently in the triangular cell.* This picture holds still at finite temperatures low enough, as is seen from the expression (94). More explicitly, we have

$$|O(\beta)\rangle_3 = \mathcal{N}_3\left[e^{(3/2)K}\,|I\rangle - \frac{4}{3}\sinh\left(\frac{3}{2}K\right)(\hat{s}_{ij}\,|\hat{1}\rangle_k + \hat{s}_{jk}\,|\hat{1}\rangle_i + \hat{s}_{ki}\,|\hat{1}\rangle_j)\right] \tag{97}$$

By the way, the pair-product approximant of the thermal state of this system is given by

$$\begin{aligned}|O(\beta)\rangle_{\mathrm{PPA}} = \mathcal{N}_{\mathrm{PPA}} &\exp\left(-\frac{\beta}{2}\mathcal{H}_{ij}\right)\exp\left(-\frac{\beta}{2}\mathcal{H}_{jk}\right) \\ &\times \exp\left(-\frac{\beta}{2}\mathcal{H}_{ki}\right)|\hat{1}\rangle_{ijk}\end{aligned}$$

$$
\begin{aligned}
&= \mathcal{N}_{\mathrm{PPA}}\{a^3\,|\hat{1}\rangle_{ijk} - a^2 c(\hat{s}_{ij}\,|\hat{1}\rangle_k + \hat{s}_{jk}\,|\hat{1}\rangle_i + \hat{s}_{ki}\,|\hat{1}\rangle_j) \\
&\quad + \frac{1}{2}ac^2[s_{ij}\widetilde{s_{kj}}(\tilde{\alpha}_i\alpha_k + \tilde{\beta}_i\beta_k) + s_{jk}\widetilde{s_{ik}}(\tilde{\alpha}_j\alpha_i + \tilde{\beta}_i\beta_j) \\
&\quad + s_{ki}\widetilde{s_{ji}}(\tilde{\alpha}_k\alpha_j + \tilde{\beta}_k\beta_j)] \\
&\quad + \frac{1}{4}c^3 s_{ji}\widetilde{s_{ik}}(\tilde{\alpha}_j\alpha_k + \tilde{\beta}_j\beta_k)\}, \qquad c \equiv b - a
\end{aligned}
\tag{98}
$$

where we have used the formula in the Appendix. In the low-temperature limit $T \to 0$, the above pair-product thermal state becomes

$$
|O(\beta)\rangle^{(T=0)}_{\mathrm{PPA}} = \mathcal{N}'_{\mathrm{PPA}} s_{ij}\widetilde{s_{ij}}(\tilde{\alpha}_j\alpha_k + \tilde{\beta}_j\beta_k)
\tag{99}
$$

for $J < 0$. It should be remarked that this state is rather different from the true ground state (95), namely, our pair-product approximant is not so good at very low temperatures, as it should be.

Next we discuss the variational thermal state $|\Psi\rangle_T$ in (73) for our comparison. It is expressed by

$$
\begin{aligned}
|\Psi\rangle_T &= \mathcal{N}_T \sum \prod_{\langle ij\rangle} [\theta_i\theta_j(uQ_{ij} + vP_{ij})]\,|I\rangle \\
&= \mathcal{N}_T[3u + (v-u)(P_{ij} + P_{jk} + P_{ki})]\,|I\rangle \\
&= \mathcal{N}_T\left[\tfrac{3}{4}(v+3u) - \frac{v-u}{4}(\sigma_i\cdot\sigma_j + \sigma_j\cdot\sigma_k + \sigma_k\cdot\sigma_i)\right]|I\rangle
\end{aligned}
\tag{100}
$$

in our three-spin system, where u and v are given by (79) or are shown in Fig. 3. In the low-temperature limit, we have

$$
\begin{aligned}
|\Psi\rangle_{T=0} &= \mathcal{N}_0(P_{ij} + P_{jk} + P_{ki})\,|I\rangle \\
&= \mathcal{N}_0(\hat{s}_{ij}\,|\hat{1}\rangle^k + \hat{s}_{jk}\,|\hat{1}\rangle_i + \hat{s}_{ki}\,|\hat{1}\rangle_j)
\end{aligned}
\tag{101}
$$

for $J < 0$.

Thus, the variational thermal state agrees with the true ground state (95) in the low-temperature limit. Even at finite temperatures, the variational thermal state of this three-spin system is rather good. Compare the coefficients $(v-u)$ and $3u$ with $-\frac{4}{3}\sinh(3K/2)$ and $e^{(3/2)K}$, respectively. Thus, we find that the variational thermal state (100) is much better than the pair-product thermal state (98) in the whole region of temperature. The reason why the above variational thermal state (100) is improved compared with the pair-product thermal state (84) is that the both states are quite similar in form, but that there is no overlap of singlet pairs in (100), whose restriction in the variational thermal state may compensate the noncommutativity of pair interactions $\{\mathscr{H}_{ij}\}$ in the thermal state (91).

11. PERTURBATIONAL EXPANSION OF THE THERMAL STATE AND TIME-DEPENDENT STATE

We consider here a system $\mathscr{H}_0$ with a perturbation $\mathscr{H}_1$ as

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1 \tag{102}$$

The corresponding thermal vacuum state can be expanded as

$$\begin{aligned} |O(\beta)\rangle &= \mathscr{N} \exp(-\tfrac{1}{2}\beta\mathscr{H}_0 - \tfrac{1}{2}\beta\mathscr{H}_1)\,|I\rangle \\ &= \mathscr{N}' \left\{ 1 + \sum_{n=1}^{\infty} \left(-\tfrac{1}{2}\right)^n \int_0^{\beta} d\beta_1 \cdots \int_0^{\beta_{n-1}} d\beta_n \mathscr{H}_1(\beta_n) \cdots \mathscr{H}_1(\beta_1) \right\} O(\beta)\rangle_0 \end{aligned} \tag{103}$$

where

$$|O(\beta)\rangle_0 = \mathscr{N}_0 \exp(-\tfrac{1}{2}\beta\mathscr{H}_0)\,|I\rangle \tag{104}$$

and

$$\mathscr{H}_1(\beta) = e^{-(1/2)\beta\mathscr{H}_0} \mathscr{H}_1 e^{(1/2)\beta\mathscr{H}_0} \tag{105}$$

Here the normalization constant $\mathscr{N}'$ should be expanded as

$$\begin{aligned} (\mathscr{N}')^{-2} &= \langle I|\exp(-\beta\mathscr{H}_0 - \beta\mathscr{H}_1)\,|I\rangle \\ &= \langle I|\, e^{-\beta\mathscr{H}_0} \left[1 + \sum_{n=1}^{\infty} (-1)^n \int_0^{\beta} d\beta_1 \cdots \int_0^{\beta_{n-1}} \right. \\ &\quad \left. \times\ d\beta_n\, \mathscr{H}_1(2\beta_n) \cdots \mathscr{H}_1(2\beta_1) \right] |I\rangle \end{aligned} \tag{106}$$

These results will be useful in discussing the response function for the perturbation $\mathscr{H}_1$.

Similarly, we can discuss the perturbational expansion of the time-dependent perturbation $\mathscr{H}_1(t)$. Our starting point is Eqs. (18) with (19), namely,

$$i\hbar \frac{\partial}{\partial t}\,|\Psi(t)\rangle = (\hat{\mathscr{H}}_0 + \hat{\mathscr{H}}_1(t))\,|\Psi(t)\rangle \tag{107}$$

where

$$\hat{\mathscr{H}}_0 = \mathscr{H}_0 - \tilde{\mathscr{H}}_0 \qquad \text{and} \qquad \hat{\mathscr{H}}_1(t) = \mathscr{H}_1(t) - \tilde{\mathscr{H}}_1(t) \tag{108}$$

The formal solution of (129) is given by

$$|\Psi(t)\rangle = \mathscr{N} \exp_+ \left(\frac{1}{i\hbar} \int_{t_0}^{t} (\hat{\mathscr{H}}_0 + \hat{\mathscr{H}}_1(s))\, ds \right) |\Psi(t_0)\rangle \tag{109}$$

This can be expanded as

$$\begin{aligned} |\Psi(t)\rangle = \mathscr{N} &\left[1 + \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar} \right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n\, \hat{\hat{\mathscr{H}}}_1(t_n) \cdots \hat{\hat{\mathscr{H}}}_1(t_1) \right] \\ &\times \exp\left[\frac{(t-t_0)}{i\hbar} \hat{\mathscr{H}}_0 \right] |\Psi(t_0)\rangle \end{aligned} \tag{110}$$

where

$$\hat{\hat{\mathscr{H}}}_1(t) = V_0(t)\, \hat{\mathscr{H}}_1(t)\, V_0^{\dagger}(t) \tag{111}$$

with

$$V_0(t) = \exp\left(\frac{t-t_0}{i\hbar} \hat{\mathscr{H}}_0 \right) \tag{112}$$

Some applications of this perturbational method will be given elsewhere.

CONCLUDING REMARKS

In the present paper, the thermo field dynamics for interacting quantum systems is formulated. However, the present formulation is quite general and holds in general quantum systems such as Fermi and Bose systems. In particular, it should be remarked that the thermal vacuum state is given by

$$|O(\beta)\rangle = Z(\beta)^{-1/2} \exp(-\tfrac{1}{2}\beta\mathscr{H})\, |I\rangle \tag{113}$$

for any interacting Hamiltonian $\mathscr{H}$ and for the identity state $|I\rangle$ which is expressed as

$$|I\rangle = \sum_{\alpha} |\alpha, \tilde{\alpha}\rangle \tag{114}$$

for any representation $|\alpha\rangle$. This property is essential in performing quantum Monte Carlo simulations in the present formulation.

The temporal evolution of the time-dependent state $|\Psi(t)\rangle$ is described by the equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{\mathscr{H}}(t) \, |\Psi(t)\rangle \tag{115}$$

where $\hat{\mathscr{H}}(t)$ is given by

$$\hat{\mathscr{H}}(t) = \mathscr{H}(t) - \tilde{\mathscr{H}}(t) \tag{116}$$

We can derive Kubo's linear response theory[9] from the above fundamental temporal evolution (115).

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APPENDIX: SOME USEFUL FORMULAS CONCERNING THE THERMAL VACUUM STATE AND PROJECTION OPERATORS

The present formulations of the variational theory and quantum Monte Carlo simulation are quite different from the previous ones,[24–27,12,15,18,20,30–48] in that we are treating here replicated systems, namely real spins $\{S_j\}$ and tilde spins $\{\tilde{S}_j\}$. Thus, we need some new formulas concerning the above new operators and states.

First we define the sates, α_i, β_i, $\tilde{\alpha}_i$, $\tilde{\beta}_i$, $\hat{\alpha}_i$, $\hat{\beta}_i$, $|\hat{1}\rangle_{ij}$, singlet state s_{ij} by

$$\alpha_i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i, \quad \beta_i = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i, \quad S_i^z \alpha_i = \frac{1}{2} \alpha_i, \quad S_i^z \beta_i = -\frac{1}{2} \beta_i$$

$$\widetilde{S_i^z} \tilde{\alpha}_i = \tfrac{1}{2} \tilde{\alpha}_i, \quad \widetilde{S_i^z} \tilde{\beta}_i = -\tfrac{1}{2} \tilde{\beta}_i, \quad \hat{\alpha}_i = \alpha_i \tilde{\alpha}_i, \quad \text{and} \quad \hat{\beta}_i = \beta_i \tilde{\beta}_i \tag{A1}$$

$$s_{ij} = 2^{-1/2} (\alpha_i \beta_j - \beta_i \alpha_j) \tag{A2}$$

and

$$|\hat{1}\rangle_{ij} = \hat{\alpha}_i \hat{\alpha}_j + \hat{\alpha}_i \hat{\beta}_j + \hat{\beta}_i \hat{\alpha}_j + \hat{\beta}_i \hat{\beta}_j \tag{A3}$$

Then, we have the following formulas:

$$\text{(a)}\quad P_{ij}\,|\hat{1}\rangle_{ij}=s_{ij}\widetilde{s_{ij}}\equiv\widehat{s_{ij}} \tag{A4}$$

where P_{ij} is the projection operator defined by (90).

$$\text{(b)}\quad P_{ij}(\alpha_i\beta_j)=2^{-1/2}s_{ij},\qquad P_{ij}(\beta_i\alpha_j)=-2^{-1/2}s_{ij} \tag{A5}$$

$$\text{(c)}\quad P_{ij}P_{kl}\,|\hat{1}\rangle_{ijkl}=\widehat{s_{ij}}s_{kl} \tag{A6}$$

$$\text{(d)}\quad P_{ij}(s_{ik}\alpha_j)=\tfrac{1}{2}s_{ij}\alpha_k,\qquad P_{ij}(s_{ik}\beta_j)=\tfrac{1}{2}s_{ij}\beta_k \tag{A7}$$

$$\text{(e)}\quad P_{ik}P_{jk}\,|\hat{1}\rangle_{ijk}=s_{ij}\widetilde{s_{jk}}(\tilde{\alpha}_i\alpha_j+\tilde{\beta}_i\beta_j)/2 \tag{A8}$$

$$\text{(f)}\quad P_{ij}P_{ik}P_{jk}\,|\hat{1}\rangle_{ijk}=s_{ij}\widetilde{s_{jk}}(\tilde{\alpha}_i\alpha_k+\tilde{\beta}_i\beta_k)/4 \tag{A9}$$

$$\text{(g)}\quad P_{jl}P_{ij}P_{kl}\,|\hat{1}\rangle_{ijkl}=\tfrac{1}{2}s_{ik}s_{jl}\widetilde{s_{ij}}\widetilde{s_{kl}} \tag{A10}$$

$$\text{(h)}\quad P_{ik}P_{jl}P_{ij}P_{kl}\,|\hat{1}\rangle_{ijkl}=\tfrac{1}{2}s_{ik}s_{jl}\widetilde{s_{ij}}\widetilde{s_{kl}} \tag{A11}$$

Here $i\neq j\neq k\neq 1$. Many other formulas can be obtained easily.

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