TFD, RVB及び エンタングルメント

Quantum Fluctuation, Thermo Field Dynamics and Quantum Monte Carlo Methods

CHAPTER 10

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9. *Applications to the two-dimensional triangular antiferromagnetic quantum Heisenberg model*

As one of the most interesting applications of the thermo field dynamics, we consider Anderson's problem of the phase coherence of movable singlet pairs in the two-dimensional triangular antiferromagnetic quantum Heisenberg model (Anderson 1973, Fazekas and Anderson 1974). Quite recently Hirakawa et al. (1983, 1985) found an experimental candidate, namely $NaTiO_2$, to test Anderson's picture.

For the purpose of studying the quantum effect in this system at finite temperatures, the present formulation of thermo field dynamics in quantum spin systems may be most appropriate, because we know the explicit form of the thermal state

$$|O(\beta)\rangle = \mathcal{N}\exp(-\tfrac{1}{2}\beta\mathcal{H})\,|I\rangle; \quad |I\rangle \equiv \sum_n |n\rangle|\tilde{n}\rangle \text{ and} \tag{9.1}$$

where the Hamiltonian $\mathcal{H}$ is given by $\mathcal{H}|n\rangle = E_n|n\rangle$, $\tilde{\mathcal{H}}|\tilde{n}\rangle = E_n|\tilde{n}\rangle$

$$\mathcal{H} = \sum_{\langle ij\rangle}\mathcal{H}_{ij}; \quad \mathcal{H}_{ij} = -J\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j \quad (J<0). \tag{9.2}$$

double Hilbert space $(\mathcal{H}, \tilde{\mathcal{H}})$

$\overline{Q} = \mathrm{Tr}\,\rho Q = \langle O(\beta)|Q|O(\beta)\rangle$

9.1. *Pair-product and higher approximants*

As was first proposed by the present author (Suzuki 1966), the simplest variational thermal state is (J. Phys. Soc. Jpn. 21 (1966) 2274)

$$|O(\beta)\rangle_{\mathrm{PPA}} = \mathcal{N}_1\prod_{\langle ij\rangle}\exp\left(-\tfrac{1}{2}\beta\mathcal{H}_{ij}\right)|I\rangle, \tag{9.3}$$

where

$$\begin{aligned}\exp\left(-\tfrac{1}{2}\beta\mathcal{H}_{ij}\right) &= \exp\left(\tfrac{1}{2}K\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right)\\ &= \hat{a} + \hat{b}(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)\end{aligned} \tag{9.4}$$

with $K = \beta J$ and with

$$\hat{a} = \tfrac{1}{4}(3\,e^{K/2} + e^{-3K/2}) \quad \text{and} \quad \hat{b} = \tfrac{1}{4}(e^{K/2} - e^{-3K/2}). \tag{9.5}$$

The expression (6.16) will be useful in studying the property of $|O(\beta)\rangle_{\mathrm{PPA}}$ explicitly, which will be discussed in the near future. The partition function in this approximation might be obtained in a closed form.

In order to study the present system more systematically, we may use the following formulation 指数演算子分解公式

$$|O(\beta)\rangle^{(n)}_{\mathrm{PPA}} = \mathcal{N}_2\left[\prod_{\langle ij\rangle}\exp\left(-\frac{1}{2n}\beta\mathcal{H}_{ij}\right)\right]^n|I\rangle \tag{9.6}$$

This may be useful for studying our system in the thermo field transfer matrix and Monte Carlo methods proposed in sect. 7 and 8, respectively.

9.2. *Triangular cell approximant*

One of the remarkable features of the two-dimensional triangular antiferromagnetic Heisenberg model is that there exists the frustration effect first pointed out by Toulouse (1977). Another feature is that there is no phase transition with ordinary long-range order at any finite temperature when the interaction is isotropic (Mermin and Wagner 1966). Therefore, any phase transition, if it exists, must be of a new type. It might be transition into a "coherent phase" of movable singlet pairs, as was pointed out by Anderson (Anderson 1973, Fazekas and Anderson 1974).

We introduce here the following triangular cell approximant

$$|O(\beta)\rangle^{(n)}_{\mathrm{TCA}} = \mathcal{N}_3\left[\prod_{\langle ijk\rangle}\exp\left(-\frac{1}{2n}\beta\mathcal{H}_{ijk}\right)\right]^n|I\rangle, \tag{9.7}$$

where $\mathcal{H}_{ijk}$ is the local Hamiltonian of the triangular cell shown in fig. 4, that is,

$$\mathcal{H}_{ijk} = -J(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_i). \tag{9.8}$$

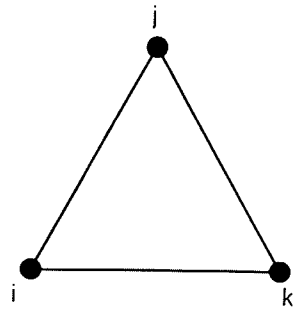


Fig. 4. Triangular cell.

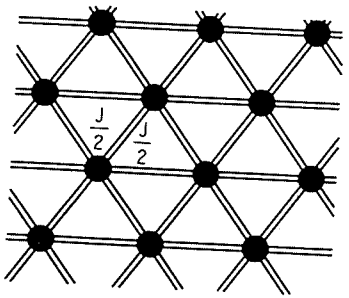


Fig. 5. Triangular lattice and its decomposition into triangular cells with interaction $J/2$.

The whole lattice is decomposed (Suzuki 1986) into overlapping triangular cells with the "half interaction",

J. Stat. Phys. 42 (1986) 1047.

$$\tilde{\mathscr{H}}_{ijk} = -\tfrac{1}{2}J(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_i), \tag{9.9}$$

as shown in fig. 5. This is one of our important "computationics", namely strategies of computation.

Then, the partition function of this system is expressed by

$$Z(\beta) = \mathrm{Tr}\exp\Big(-\beta\sum_{\langle ij\rangle}\mathscr{H}_{ij}\Big) = \mathrm{Tr}\exp\Big(-\beta\sum_{\langle ijk\rangle}\tilde{\mathscr{H}}_{ijk}\Big)$$

$$= \lim_{n\to\infty}\mathrm{Tr}\Big\{\prod_{\langle ijk\rangle}\exp\Big(-\frac{\beta}{n}\tilde{\mathscr{H}}_{ijk}\Big)\Big\}^n. \tag{9.10}$$

等価な3次元 Ising model (6体力)

Thus, we obtain an equivalent three-dimensional Ising system with six-spin interaction, having the partial Boltzmann factor

$$q(\sigma_i, \sigma_j, \sigma_k; \sigma_i', \sigma_j', \sigma_k') = \langle\sigma_i, \sigma_j, \sigma_k|\mathrm{e}^{-(\beta/n)\tilde{\mathscr{H}}_{ijk}}|\sigma_i', \sigma_j', \sigma_k'\rangle, \tag{9.11}$$

where $|\sigma_1, \sigma_2, \ldots, \sigma_N\rangle$ diagonalizes $\{\sigma_j^z\}$. This factor is easily found to be

$$\begin{aligned} &q(\sigma_i, \sigma_j, \sigma_k; \sigma_i', \sigma_j', \sigma_k') \\ &= \delta(\sigma_i, \sigma_i')\,\delta(\sigma_j, \sigma_j')\,\delta(\sigma_k, \sigma_k')\cosh(3K_n) \\ &\quad + \tfrac{1}{3}\sinh(3K_n)\Big[\Big\{\sigma_i\sigma_j\delta(\sigma_i, \sigma_i')\,\delta(\sigma_j, \sigma_j') \\ &\quad + \frac{(1-\sigma_i\sigma_i')(1-\sigma_j\sigma_j') - (\sigma_i-\sigma_i')(\sigma_j-\sigma_j')}{4}\Big\}\delta(\sigma_k, \sigma_k') + (\text{cyclic})\Big], \end{aligned} \tag{9.12}$$

with $K_n = \beta J/n$. Here, we have used the identity

$$\boxed{\mathrm{e}^{K\mathscr{H}_3} = \cosh(3K) + \tfrac{1}{3}\sinh(3K)\cdot\mathscr{H}_3,} \tag{9.13}$$

for

$$\mathscr{H}_3 \equiv (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j) + (\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k) + (\boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_i). \tag{9.14}$$

The above identity (9.13) is easily derived by noting that the operator

$$P_3 \equiv \tfrac{1}{6}(\mathscr{H}_3 + 3) \tag{9.15}$$

Projection operator

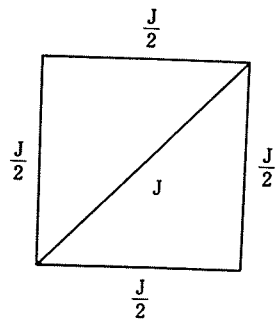
is the projection operator into the quartet state ($S = \frac{3}{2}$), namely

$$P_3^2 = P_3; \quad \mathscr{H}_3^2 = 9, \tag{9.16}$$

and that $(1 - P_3)$ is the projection operator into the doublet state ($S = \frac{1}{2}$).

9.3. Square cell and larger cluster approximants

Larger clusters with an even number of spins such as square cells shown in fig. 6 may be much more effective in Anderson's problem, because such clusters them-



Entanglement of two pairs!

Fig. 6. Four-spin cluster.

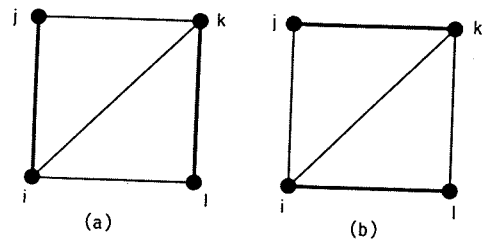


Fig. 7. Two singlet pairs. Two different kinds of decomposition: (a) and (b).

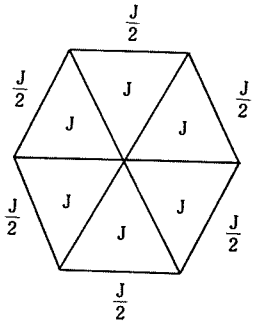


Fig. 8. Seven-spin cluster.

selves can be decomposed into products of singlet pairs, as is shown in fig. 7. This decoupling method has been used by Takasu, Miyashita and Suzuki (1985) in performing the quantum Monte Carlo simulation based on the equivalence theorem discussed in sect. 8.

ST変換

The seven-spin cluster decoupling (fig. 8) may be more effective than the four-spin cluster decoupling (fig. 7), though the former is composed of an odd number of spins. However, it is rather complicated to calculate the matrix elements of such large clusters—even numerically.

As was discussed in sect. 8 (see fig. 2), it is very effective to increase both the cluster size m and Trotter's number n.

変分理論（反強磁性三角格子）

9.4. Variational theory of Anderson's problem

Variational calculations have been made for quantum spin systems at zero temperature (Anderson 1952, Suzuki and Miyashita 1978, Miyashita 1984, Oguchi et al. 1985, Fujiki and Betts 1985).

It will be essential to study the present system at finite temperatures in order to see whether a new type of coherent phase appears or not. For this purpose, the thermo field variational method will be very convenient. It is difficult, however, to find an appropriate variational thermal state in Anderson's problem.

We give here only some preliminary considerations, Anderson (Anderson 1973, Fazekas and Anderson 1974) 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. 9. This state is given as

変分状態

$$|\Psi\rangle_A = \mathcal{N}_A\left[\sum\prod_{\langle ij\rangle}(\theta_i\theta_j P_{ij})\right]|I,\theta\rangle,\quad |I,\theta\rangle = |I\rangle|\theta\rangle, \tag{9.17}$$

RVB state

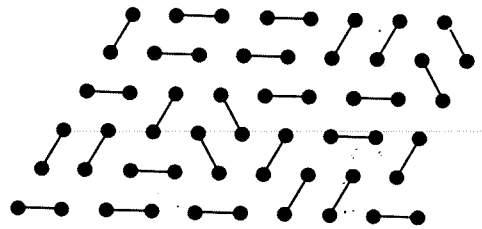


Fig. 9. Anderson's variational ground state (Anderson 1973).

"entanglement of many pairs"

in our representation, where P_{ij} is the projection operator into the singlet state given by

P_{ij} は singlet state への 射影演算子

$$P_{ij} = \tfrac{1}{4}(1-\sigma_i\cdot\sigma_j),\quad P_{ij}^2 = P_{ij}, \tag{9.18}$$

and $\{\theta_j\}$ are an algebra defined by

$$[\theta_j,\theta_k]=0,\quad \theta_j^2=0,\quad \text{and}\quad \langle\theta|\theta_j^\dagger\theta_j|\theta\rangle = 1, \tag{9.19}$$

analogously to the Grassmann algebra (Brezin 1966).

Now we extend Anderson's state (9.17) of zero temperature to the case of finite temperatures. The simplest extension may be

有限温度の

$$|\Psi\rangle_T = \mathcal{N}_T\sum\prod_{\langle ij\rangle}\left[\theta_i\theta_j(u_{ij}Q_{ij}+v_{ij}P_{ij})\right]|I\rangle, \tag{9.20}$$

◎ Thermo Field Dynamics → 変分状態

in our formulation, where Q_{ij} is the projection operator into the triplet state, namely

Q_{ij} は triplet state への 射影演算子

$$Q_{ij} = 1-P_{ij}\quad\text{and}\quad P_{ij}Q_{ij} = Q_{ij}P_{ij} = 0. \tag{9.21}$$

Then, the total energy of this trial thermal state is given by

エネルギー E

$$E = \langle\Psi|\mathcal{H}|\Psi\rangle = -\tfrac{1}{2}NJ\langle\Psi|\sigma_i\cdot\sigma_j|\Psi\rangle_T$$

$$= -\tfrac{1}{2}NJ\langle\Psi|1-4P_{ij}|\Psi\rangle_T \simeq -\tfrac{3}{2}NJ(u^2-v^2), \tag{9.22}$$

in the "pair-approximation", where we have assumed that $u_{ij}=u$ and $v_{ij}=v$. The total entropy may be given by

エントロピー S

$$S = -\tfrac{1}{2}Nk_B(3u^2\log u^2 + v^2\log v^2). \tag{9.23}$$

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

$$3u^2+v^2 = 1, \tag{9.24}$$

変分理論による物理的描象

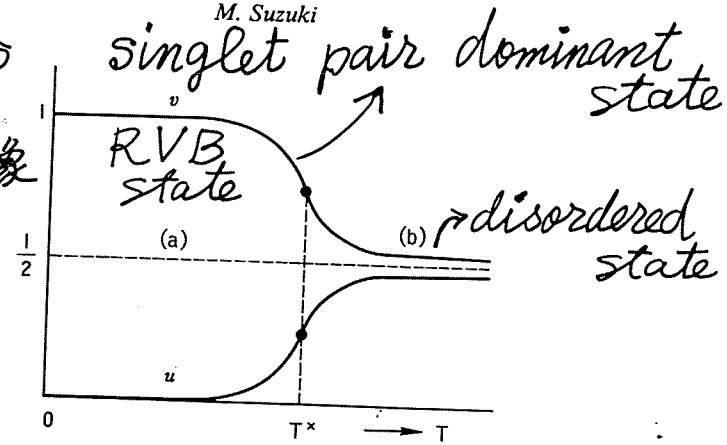


Fig. 10. Schematic temperature dependence of u and v, where $T^{\times}$ denotes the crossover temperature: (a) singlet pairs dominant thermal state, and (b) disordered state.

because $T^{\times}$ クロスオーバー温度

$$\langle 1|P_{ij}|1\rangle_{ij}=1 \quad \text{and} \quad \langle 1|Q_{ij}|1\rangle_{ij}=3. \tag{9.25}$$

Therefore, our free energy is expressed by

$$F=E-TS$$ 自由エネルギー $F=E-TS$

$$=\tfrac{1}{2}N\left[-J(1-4x)+k_{\mathrm{B}}T\left\{(1-x)\log\frac{1-x}{3}+x\log x\right\}\right], \tag{9.26}$$

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

xに関して変分をとる

$$u^2=\frac{1}{\mathrm{e}^{-4k}+3} \quad \text{and} \quad v^2=\frac{\mathrm{e}^{-4K}}{\mathrm{e}^{-4K}+3}, \tag{9.27}$$

where $K=J/k_{\mathrm{B}}T$. Thus, the thermal state coefficients u and v behave as in fig. 10. A crossover effect occurs around the temperature $T^{\times}$ given by

$$T^{\times}\simeq\frac{|J|}{k_{\mathrm{B}}}\frac{4}{\log 3}\simeq 3.6|J|/k_{\mathrm{B}}. \tag{9.28}$$

クロスオーバー温度

Below this crossover temperature, singlet pairs are dominant. Above $T^{\times}$, the thermal vacuum state becomes disordered (i.e. $u\cong v\cong\frac{1}{2}$, namely $|\Psi\rangle_T\cong|I\rangle$).

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 cluster (or larger cell) method discussed in sect. 9.2 and 9.3 will be useful. The research in this direction is now in progress.

This quantum crossover effect (Suzuki 1977b) might be relevant to the experimental result by Hirakawa et al. (1983, 1985). ↓ Prog. Theor. Phys. 58 775.

As was mentioned in the beginning of sect. 9.2, there is another possibility that there might occur a phase transition below the critical point of which the long-range order does not exist but only the phase coherence among singlet pairs exists in the two-dimensional triangular antiferromagnetic quantum Heisenberg model (Anderson 1973, Fazekas and Anderson 1974). It will be an interesting problem to study which possibility is realized in the above system, by extending the present thermo field variational theory.

*) M. S. Prog. Theor. Phys. 56 (1976) 1454.

10. Summary and concluding remarks

◎ TFDの一般表現定理 (by M.S. 1985年)

Thermo field dynamics of quantum spin systems has been formulated, which yields the KMS relation as identities among thermal vacuum states. Path integral formulations of the thermal state have been presented, which give trial thermal states. Thermo field variational method has also been proposed. The present thermo field dynamics in quantum spin systems yields a new proposal of "thermo field Monte Carlo method". The relation between this new method and the quantum Monte Carlo method proposed by the present author (Suzuki 1976b)*) have been discussed.

The above formulations have been presented in terms of quantum spin systems. Almost all the fundamental formulations in the present paper are similarly valid in general quantum systems such as Fermi and Bose systems, as was mentioned already at the end of sect. 2. In particular, it should be remarked that our *general formulation for the thermal state*, 有限温度の状態ベクトル

$$|\mathrm{O}(\beta)\rangle=Z(\beta)^{-1/2}\exp(-\tfrac{1}{2}\beta\mathscr{H})|I\rangle, \tag{10.1}$$

for any interacting quantum system $\mathscr{H}$ is a very useful one from a practical point of view, as has been explained in the present paper, where the identity state $|I\rangle$ is expressed by

一般表現定理 ($|I\rangle$は表示に依らない)

$$\boxed{|I\rangle=\sum_{\alpha}|\alpha,\tilde{\alpha}\rangle,} \tag{10.2}$$

M.S. J. Phys. Soc. Jpn. 54 (1985) 4483.

for any representation $\{|\alpha\rangle\}$. $|\psi\rangle=a|m\rangle+b|n\rangle\to|\psi\rangle^{\sim}=a^*|\tilde{m}\rangle+b^*|\tilde{n}\rangle$

The second new general result is that the time-dependent state $|\psi(t)\rangle$ is described by the equation

⊙この定理は「トレースが表示に依らない」ことは違って、TFDで最重要な概念的定理であり、応用上も極めて重要である。

基礎方程式

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle=\hat{\mathscr{H}}(t)|\Psi(t)\rangle \tag{10.3}$$

for any quantum system, when $[\mathscr{H}(t),\tilde{\mathscr{H}}(t)]=0$ as is the case. Here,

$$\hat{\mathscr{H}}(t)=\mathscr{H}(t)-\tilde{\mathscr{H}}(t) \tag{10.4}$$

ディラックの電子論と類似性がある。⊛

⊛ tilde particle ↔ 反粒子

and $\mathscr{H}(t)$ is an *arbitrary time-dependent Hamiltonian*. It is easy to derive the Kubo formula (Kubo 1957) from the above general equation (10.3) with (10.4). For more details, see the paper by the present author (Suzuki 1985b). J. Math. Phys. 26