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Monte Carlo Simulation of Quantum Spin Systems. I

Masuo SUZUKI, Seiji MIYASHITA and Akira KURODA

Department of Physics, University of Tokyo, Tokyo 113

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A general explicit formulation of Monte Carlo simulation for quantum systems is given in this paper on the basis of the previous fundamental proposal by Suzuki. This paper also demonstrates explicitly the possibility of it and gives new interesting physical results on the two-dimensional XY-model. That is, the present preliminary simulation seems to indicate a phase transition with a divergent susceptibility, and a very weak singularity of specific heat if it exists, and without long-range order.

§ 1. Introduction

A possible phase transition of two-dimensional spin systems such as the Heisenberg model and XY-model has been investigated by many authors,[1)~11)] since Stanley and Kaplan[12)] proposed a new type of phase transition without ordinary long-range order. The mechanism of this phase transition, however, is not well understood. In this situation, it is very useful to perform Monte Carlo simulations for quantum systems, which have been proposed by one[13),14)] of the present authors, and whose applications to the two-dimensional XY-model have been reported already briefly.[15),16)]

The purpose of our paper is to show explicitly the possibility of Monte Carlo simulation in quantum spin systems and to present interesting results on the one- and two-dimensional spin systems in detail. The present paper is the first one of a series of papers concerning Monte Carlo simulation on quantum systems, so that the method itself is also described in detail.

In § 2 a general formulation[14)] of Monte Carlo simulation is presented. As a simple application of it, the one-dimensional Heisenberg model and XY-model are studied in § 3. The two-dimensional case is presented in § 4. Some considerations are given in § 5.

§ 2. Monte Carlo method for quantum systems

The key point of our method is to make use of classical representations of quantum systems[14),17),18)] based on the *generalized Trotter formula*:[13)] *For any set of operators* $\{A_j\}$ *in a Banach algebra*

$$\left\| \exp\left(\sum_{j=1}^{p} A_j\right) - \{e^{A_1/n}e^{A_2/n}\cdots e^{A_p/n}\}^n \right\| \leq \frac{2}{n}\left(\sum_{j=1}^{p}\|A_j\|\right)^2 \exp\left(\frac{n+2}{n}\sum_{j=1}^{p}\|A_j\|\right), \tag{2·1}$$

where p is an arbitrary positive integer.
For bounded operators $\{A_j\}$,

$$\exp\left(\sum_{j=1}^{p} A_j\right) = \lim_{n\to\infty} \left(e^{A_1/n} e^{A_2/n} \cdots e^{A_p/n}\right)^n. \tag{2·2}$$

It should be remarked that the operators $\{A_j\}$ do not necessarily commute with one another, and that the above formula (2·2) can be used effectively as an approximation for finite n.

Now let the Hamiltonian of a quantum system be given by a sum of local Hamiltonians $\mathcal{H}(\boldsymbol{r})$ as $\mathcal{H} = \sum_{\boldsymbol{r}} \mathcal{H}(\boldsymbol{r})$, which do not necessarily commute with one another. Then, we apply the generalized Trotter formula (2·2) as follows: The partition function Z is given by

$$Z = \mathrm{Tr} \exp(-\beta\mathcal{H}) = \lim_{n\to\infty} Z_n \tag{2·3}$$

and

$$Z_n = T_r \left\{ \prod_{\boldsymbol{r}} \exp\left[-\frac{1}{n} \beta\mathcal{H}(\boldsymbol{r}) \right] \right\}^n = \sum_{\{\alpha_j\}} \exp \mathcal{H}_{\mathrm{eff}}, \tag{2·4}$$

where

$$\mathcal{H}_{\mathrm{eff}} = \sum_{\boldsymbol{r}} \sum_{j=1}^{n} \hat{\mathcal{H}}(\alpha_{\boldsymbol{r},j}, \alpha_{\boldsymbol{r},j+1}) \tag{2·5}$$

and

$$\exp \hat{\mathcal{H}}(\alpha, \alpha') = \langle \alpha | \exp\left[-\frac{1}{n} \beta\mathcal{H}(\boldsymbol{r}) \right] | \alpha' \rangle, \tag{2·6}$$

with an appropriate diagonal representation $|\alpha\rangle$. For more details, see Ref. 14). Thus, the relevant quantum system is transformed to a $(d+1)$-dimensional classical system. The additional dimension plays a role of path integrals in a discrete space or it expresses the non-commutative effect of local Hamiltonians. Owing to this equivalence relation, the Monte Carlo method can be now applied to quantum systems, as in ordinary classical systems.[19)~22)] A small value of n in the formula (2·2) may be sufficient for practical calculations, except at low temperatures. As the temperature is decreased, the approximant (2·2) with a larger value of n should be used to keep an approximation of the same order. Furthermore, an asymptotic evaluation for a large n will be possible by calculating Z_n successively for gradually increasing values of n.

In order to carry out the above scheme of Monte Carlo calculations for quantum systems, it is necessary to formulate more explicitly the Monte Carlo procedure by taking into consideration conservation laws and some other restrictions due to quantum effects. In general, the ensemble average of a certain physical quantity is given by[19)]

$$\langle X \rangle = \frac{1}{M} \sum_{j=1}^{M} \langle \alpha_j | X | \alpha_j \rangle \tag{2·7}$$

in the Monte Carlo simulation, where $|\alpha_j\rangle$ denotes the j-th Monte Carlo state which is generated with the probability proportional to $\langle\alpha_j|\exp(-\beta\mathcal{H})|\alpha_j\rangle$. When $\mathcal{H}$ is classical or is diagonalized from the beginning as usual,[19] this probability is easily calculated. It is difficult, however, to evaluate the matrix element $\langle\alpha|\exp(-\beta\mathcal{H})|\alpha\rangle$ for quantum systems. The generalized Trotter formula (2·2) provides an approximate method to calculate it. That is, the n-th approximant of the matrix element is expressed as

$$\langle\alpha|\exp(-\beta\mathcal{H})|\alpha\rangle_n=\sum_{\substack{|\beta_{ij}\rangle,\ i=1,\cdots,n-1\\ j=1,\cdots,p}}\langle\alpha|\exp(-\hat{\mathcal{H}}_1)|\beta_{11}\rangle\langle\beta_{11}|\cdots$$

$$\cdots\langle\beta_{n-1,p-1}|\exp(-\hat{\mathcal{H}}_p)|\alpha\rangle\equiv\mathrm{Tr}\exp_n(\alpha;\{\beta_{ij}\}) \tag{2·8}$$

with $\hat{\mathcal{H}}_i=n^{-1}\beta\mathcal{H}_i$, for $\mathcal{H}=\mathcal{H}_1+\cdots+\mathcal{H}_p$. If the interaction $\mathcal{H}_i$ is of finite range, it is quite easy to calculate the matrix element $\langle\alpha|\exp(-\hat{\mathcal{H}}_i)|\beta\rangle$ explicitly, for example, by diagonalizing $\hat{\mathcal{H}}_i$.

One of the key-point of our method is to treat a set $\{|\alpha\rangle, |\beta_{ij}\rangle; i=1, 2, \cdots, n-1$ and $j=1, 2, \cdots, p-1\}$ as a state in the Monte Carlo simulation and to denote it by $|\alpha;\{\beta_{ij}\}\rangle$. At first sight, this seems intractable, because there exist $(n-1)\cdot(p-1)$ states $|\beta_{ij}\rangle$ even for a specified state $|\alpha\rangle$, where p is of order N (the system-size). For finite range interactions, the matrix element $\langle\beta_{ij}|\exp(-\hat{\mathcal{H}}_j)|\beta_{ij+1}\rangle$ is non-vanishing only when the microscopic states of $|\beta_{ij}\rangle$ and $|\beta_{ij+1}\rangle$ are identical except for the interaction range of $\mathcal{H}_j$, as was generally discussed in Ref. 14). Thus, the state $|\alpha,\{\beta_{ij}\}\rangle$ for a specific α has only $r(n-1)$ degrees of freedom, where r is the atom (or spin) number of the relevant lattice region of $\mathcal{H}_j$. It should be remarked again that the state $|\alpha;\{\beta_{ij}\}\rangle$ is not generated by the probability of the associated energy of the state, but is generated by the partial Boltzmann factor.

Now the energy of the system is expressed by

$$\langle E\rangle=-\frac{\partial}{\partial\beta}\log Z=-\frac{\partial}{\partial\beta}\log\sum_{|\alpha\rangle}\langle\alpha|e^{-\beta\mathcal{H}}|\alpha\rangle$$

$$=\lim_{n\to\infty}\sum_{|\alpha,\{\beta_{ij}\}\rangle}\mathrm{Prob}_n(\alpha,\{\beta_{ij}\})E_n(\alpha,\{\beta_{ij}\}), \tag{2·9}$$

by using the formulae (2·3) and (2·8). Here $\mathrm{Prob}_n(\alpha,\{\beta_{ij}\})$ denotes the probability to find the state $|\alpha,\{\beta_{ij}\}\rangle$, which is given by

$$\mathrm{Prob}_n(\alpha,\{\beta_{ij}\})=Z^{-1}\exp_n(\alpha;\{\beta_{ij}\}), \tag{2·10}$$

and $E_n(\alpha,\{\beta_{ij}\})$ is the energy function defined by

$$E_n(\alpha,\{\beta_{ij}\})=-\sum_{i,j}\langle\beta_{ij}|\frac{\partial}{\partial\beta}e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle\langle\beta_{ij}|e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle \tag{2·11}$$

with $\beta_{00}\equiv\beta_{n,p}\equiv\alpha$. In the Monte Carlo simulation (MCS), the state $|\alpha,\{\beta_{ij}\}\rangle$ is approximately selected with the probability $\mathrm{Prob}_n(\alpha,\{\beta_{ij}\})$ for a large number of

steps of MCS. Thus, the energy is calculated from the following n-th approximant

$$\langle E\rangle_{\text{M.C.}}=\sum_{|\alpha,\{\beta_{ij}\}\rangle}\sum E_n(\alpha;\{\beta_{ij}\})/(\text{the number of MCS}), \tag{2·12}$$

in our Monte Carlo method. Similarly, an arbitrary physical quantity Q is calculated from the n-th approximant of the form

$$\langle Q\rangle_{\text{M.C.}}=\sum_{|\alpha,\{\beta_{ij}\}\rangle}\sum Q_n(\alpha;\{\beta_{ij}\})/(\text{the number of MCS}). \tag{2·13}$$

It is quite easy to find the expression for $Q_n(\alpha;\{\beta_{ij}\})$ for any Q, as for the energy. For example, the specific heat function $C_n(\alpha,\{\beta_{ij}\})$ is given by

$$\begin{aligned}k_BT^2C_n(\alpha;\{\beta_{ij}\})&=[E_n(\alpha,\{\beta_{ij}\})-\langle E\rangle_{\text{M.C.}}]^2\\&-\sum_k\left[\langle\beta_{ij}|\frac{\partial}{\partial\beta}e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle/\langle\beta_{ij}|e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle\right]^2\\&+\sum_k\langle\beta_{ij}|\frac{\partial^2}{\partial\beta^2}e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle/\langle\beta_{ij}|e^{-\hat{\mathcal{H}}_i}|\beta_{ij+1}\rangle\,.\end{aligned} \tag{2·14}$$

The susceptibility is calculated from the formula

$$\chi=\beta\mu_B^2\sum_{|\alpha,\{\beta_{ij}\}\rangle}\sum(M_n(\alpha)-\langle M_n(\alpha)\rangle_{\text{M.C.}})^2/(\text{the number of MCS}), \tag{2·15}$$

where

$$M_n(\alpha)=\langle\alpha|\sum_j\sigma_j|\alpha\rangle. \tag{2·16}$$

For a spin Hamiltonian of the form

$$\hat{\mathcal{H}}=\sum_{\langle ij\rangle}\mathcal{H}_{ij}\equiv\sum_{\langle ij\rangle}(K_x\sigma_i^x\sigma_j^x+K_y\sigma_i^y\sigma_j^y+K_z\sigma_i^z\sigma_j^z), \tag{2·17}$$

the matrix elements of the partial Boltzmann factor are given by[14]

$$(\langle\sigma_i,\sigma_j|\exp(-\mathcal{H}_{ij})|\sigma_i',\sigma_j'\rangle)=\tilde{a}\begin{pmatrix}1+X_3, & 0, & 0, & X_1-X_2\\ 0, & 1-X_3, & X_1+X_2, & 0\\ 0, & X_1+X_2, & 1-X_3, & 0\\ X_1-X_2, & 0, & 0, & 1+X_3\end{pmatrix}\begin{matrix}|\uparrow\uparrow\rangle\\|\uparrow\downarrow\rangle\\|\downarrow\uparrow\rangle\\|\downarrow\downarrow\rangle\end{matrix}, \tag{2·18}$$

where

$$\begin{aligned}\tilde{a}&=\cosh K_x\cosh K_y\cosh K_z-\sinh K_x\sinh K_y\sinh K_z\,,\\X_1&=(\tanh K_x-\tanh K_y\tanh K_z)/(1-\tanh K_x\tanh K_y\tanh K_z),\end{aligned} \tag{2·19}$$

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

These expressions will be used in the following sections.

§ 3. One-dimensional quantum spin systems

As a simple demonstration of Monte Carlo simulations of quantum systems, we study here the one-dimensional Heisenberg model and XY-model at finite temperatures. The simplest case is $n=1$ as shown in Fig. 1. In Fig. 1, the state $|\alpha\rangle$ is denoted by the symbol ○, the state $|\beta_{11}\rangle$ is expressed by the spins encircled by a solid line, and $|\beta_{12}\rangle$ by a dotted line. The trace operation requires that $\beta'\equiv\alpha$, namely periodic boundary conditions in our effective lattice. This has been already solved analytically by one of the present authors as a "pair-product" approximation[23] of the anisotropic Heisenberg model. The partition function in this approximation is given by

$$Z_1=(2\tilde{a})^N(1+X_1^N+X_2^N+X_3^N)\simeq(2\tilde{a})^N \tag{3·1}$$

with $\tilde{a}$ defined in (2·19). Then, we perform the Monte Carlo simulation for the case $n=2$, whose effective lattice is shown in Fig. 2. It should be remarked here that the most effective procedure of the MCS is to flip all spins (five spins

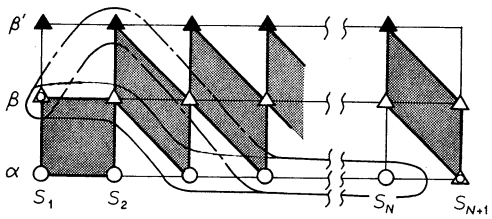


Fig. 1. Construction of the effective lattice for $n=1$ in one-dimension, where α denotes $|S_1\cdots S_N\rangle$, i.e., a state of N spins, and β and β' denote intermediate states.

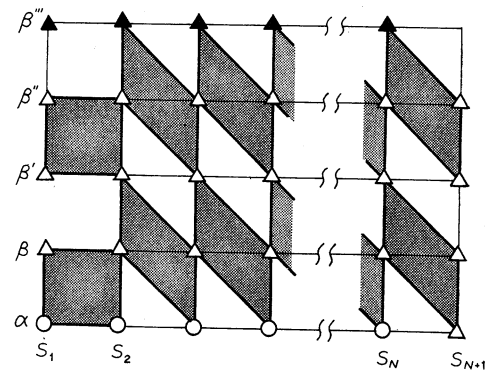


Fig. 2. Structure of the effective lattice for $n=2$ in one-dimension.

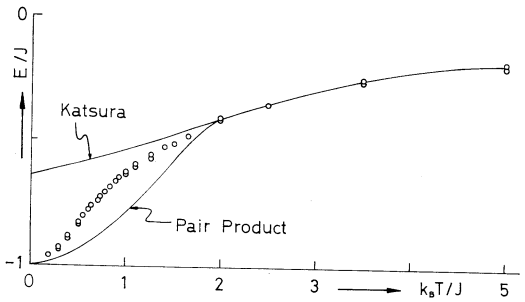


Fig. 3. Temperature-dependence of the total energy for the one-dimensional quantum XY-model ($N=33$, $n=2$); "Pair Product" means the analytic solution for $N=\infty$, $n=1$, and "Katsura" means the rigorous solution of this model.

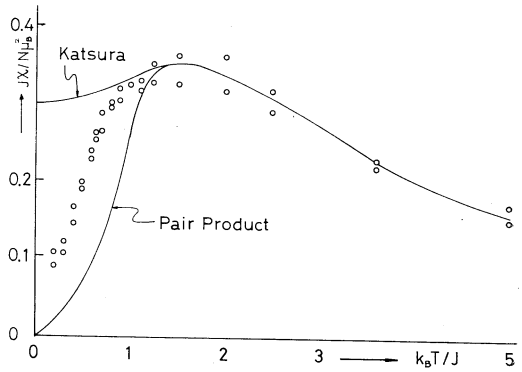


Fig. 4. Temperature-dependence of the perpendicular susceptibility for the one-dimensional quantum XY-model ($N=33$, $n=2$).

in our example) corresponding to each real spin S_j as a set, because many matrix elements of $\exp(-\hat{\mathcal{H}}_i)$ vanish as shown in (2·18). It is more effective to treat more spins as a set in each step, although programming becomes more complicated. Results thus obtained are shown in Figs. 3∼6, for the XY-model and Heisenberg model. Clearly the results of the XY-model agree very well with the well-known exact solution by Katsura[24] and by Lieb et al.,[25] except for low temperatures below J/k_B, in which region simulations for a larger value of n are necessary. In fact, as the value of n increases, the temperature region of validity of our simulation extends towards zero temperature, as seen from our results for $n=1$ and $n=2$ in Figs. 3∼6.

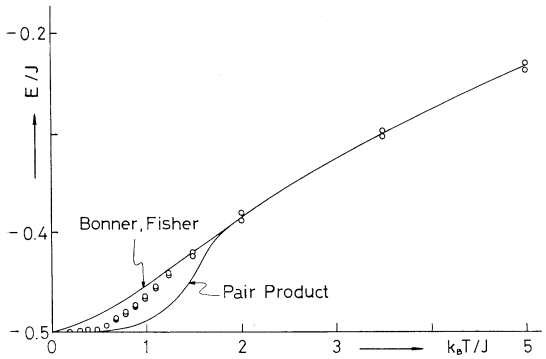


Fig. 5. Temperature-dependence of the total energy for the one-dimensional quantum Heisenberg model ($N=33$, $n=2$); "Bonner, Fisher" means an exterpolation from exact numerical solutions in finite systems.

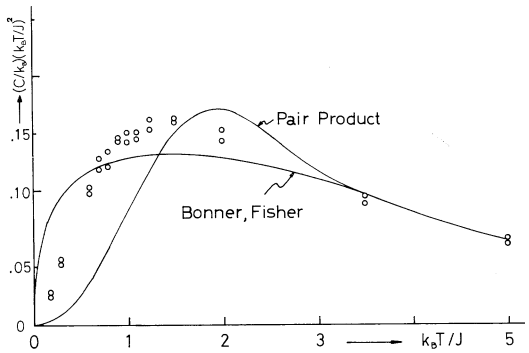


Fig. 6. Temperature-dependence of the energy-correlation (or specific heat) for the one-dimensional quantum Heisenberg model ($N=33$, $n=2$).

§ 4. Two-dimensional XY-model

It is very interesting to investigate the two-dimensional XY-model with the help of Monte Carlo simulations. We study here the following Hamiltonian:

$$\hat{\mathcal{H}} = \sum_{i,j} (K_x\sigma_{ij}^x\sigma_{i+1,j}^x + K_y\sigma_{ij}^y\sigma_{i+1,j}^y + K_z\sigma_{ij}^z\sigma_{i+1,j}^z) + \sum_{i,j} (K_x\sigma_{ij}^x\sigma_{i,j+1}^x + K_y\sigma_{ij}^y\sigma_{i,j+1}^y + K_z\sigma_{ij}^z\sigma_{i,j+1}^z). \quad (4\cdot1)$$

The effective classical representation of this system is obtained in a similar way[14] to the one-dimensional case discussed in § 3.

A unit cell of the effective lattice is shown in Fig. 7. These twenty spins of this unit cell are treated as a unit for each step of spin flips.

The temperature-dependence of energy for two-dimensional systems obtained by the present Monte Carlo simulation is shown in Fig. 8, together with the results of the Ising model for comparison. The specific heats multiplied with

$(k_BT)^2$ are shown in Fig. 9. The specific heat for the Heisenberg model is quite smooth, and that for the Ising model diverges at T_c, as is well known. The specific heat of the XY-model for $d=2$ is delicate and it might have a cusp, although our simulation shows that it does not diverge. In fact, the size dependence of the maximum value of it is very small, as shown in Fig. 10. This indicates that the specific heat is nondivergent. In order to see more clearly the temperature dependence of the specific heat, we have plotted the derivative of it, as shown in Fig. 11. This may have cusp. However, to draw a definite conclusion it will be necessary to perform a more detailed simulation, which will be published in future.

The susceptibility calculated by our simulation is shown in Fig. 12. It seems that the susceptibility diverges near $k_BT\sim 2J$, although the existence of finite-size

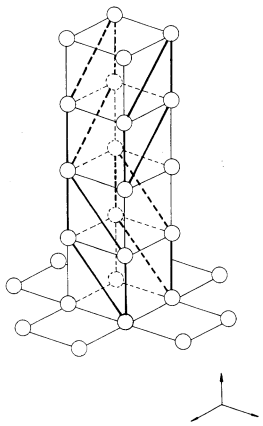


Fig. 7. Unit cell of the effective lattice: effective four-spin interactions are denoted by bold-faced solid or dotted lines.

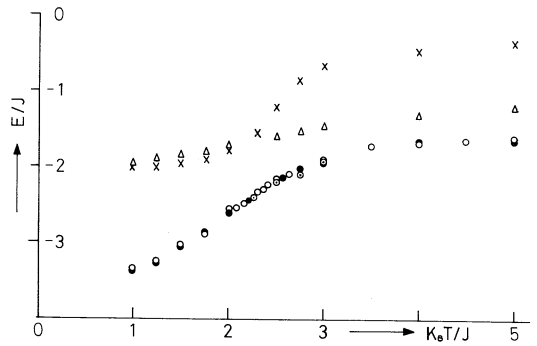


Fig. 8. Temperature-dependence of the energy for the two-dimensional models; "×", Ising model (9×9); "△", Heisenberg model (9×9); "●", XY-model (9×9); "○", XY-model (15×15) and "⊙", XY-model (30×30).

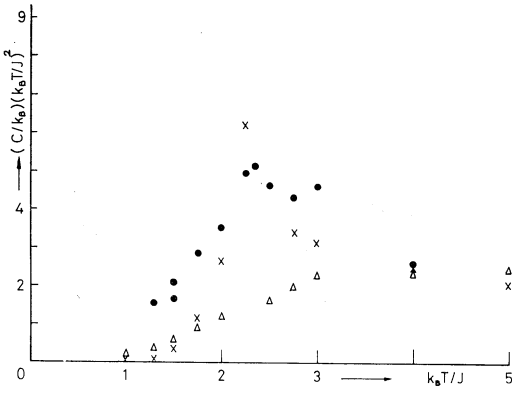


Fig. 9. Temperature-dependence of energy-correlation (or specific heat) for the two-dimensional models, with similar symbols to Fig. 8.

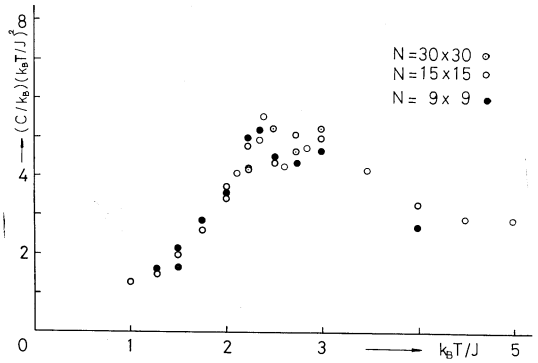


Fig. 10. Size-dependence of energy-correlation (or specific heat) for the two-dimensional XY-model.

effect cannot be excluded. In Fig. 13, the above result for the XY-model is compared with that for the Heisenberg model. It is seen that the former increases more rapidly than the latter.

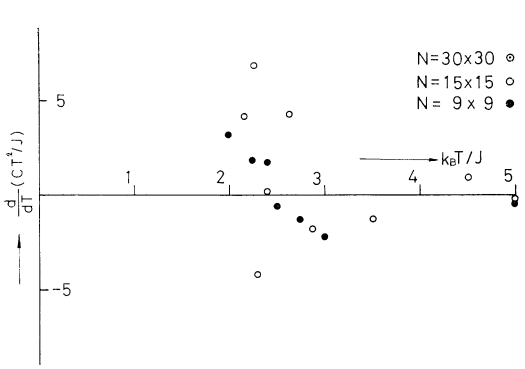


Fig. 11. Temperature derivative of energy correlation for the two-dimensional XY-model.

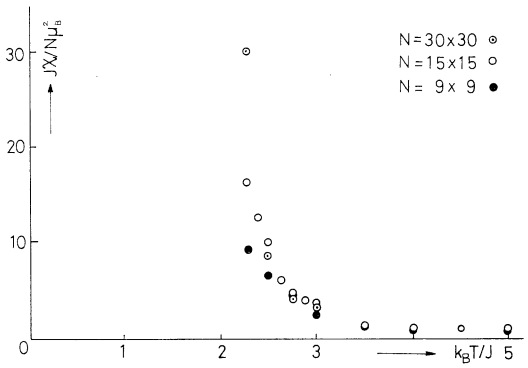


Fig. 12. Temperature- and size-dependence of susceptibility in the XY-plane for the two-dimensional XY-model.

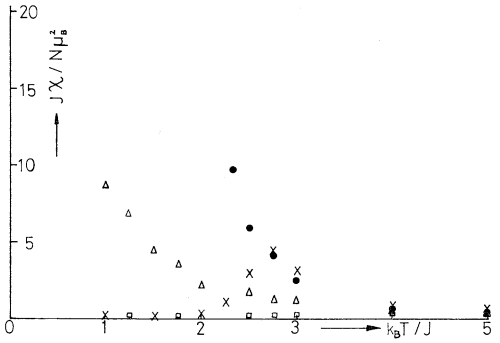


Fig. 13. Temperature-dependence of susceptibility for two-dimensional models; "●", XY-model (15×15); "△", Heisenberg model; "×", Ising model and "□", $\chi_{\parallel}$ in the XY-model.

§ 5. Some theoretical considerations and remarks

In this paper, we have demonstrated that it is practically possible to perform Monte Carlo simulations of quantum systems such as the Heisenberg model and XY-model. The present calculations are still preliminary and more thorough simulations will be performed in the near future.

From our preliminary results, it may be expected already that there occurs a phase transition with a divergent susceptibility and without long-range order.

It should be remarked that there exist some similarities between the above phase transition of the XY-model and spin-glass phase transitions.[27),28)] In both systems, there exists no ordinary long-range order, and the singularities of specific heat are very weak. Thus, there is a possibility to construct a phenomenological

theory of the phase transition of the XY-model, as for the spin-glass transition.[28]

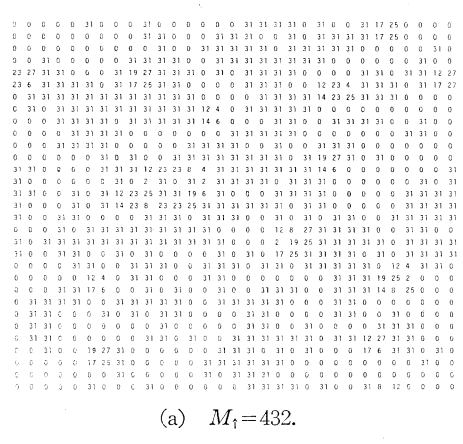
In fact, we have already proposed a very simple phenomenological theory.[22] It was discussed before[22] for the classical XY-model with vortices.[15),21),22] However, this theory is also valid for the two-dimensional quantum XY-model. That is, we introduce a disorder parameter n, which vanishes for $T<T_c$ and which does not vanish for $T>T_c$. In the classical XY-model, this parameter has been interpreted as the number density of vortices or more general disclinations. In the present quantum system, it is difficult to define clearly this disorder parameter. However, the physical mechanism of phase transitions is expected to be essentially the same. In fact, spin configurations of our simulations show a *cluster property* near the "critical point", as shown in Fig. 14, which may correspond*) to vortices in the classical systems. Thus, the number density of clusters may be taken as the disorder parameter. As in the phenomenological theory of spin-glasses,[28] the free energy of this system may be expanded in a power series of m (magnetization density) as

$$f(m,n)=F_0(n)+A(n)m^2+B(n)m^4+\cdots. \tag{5·1}$$

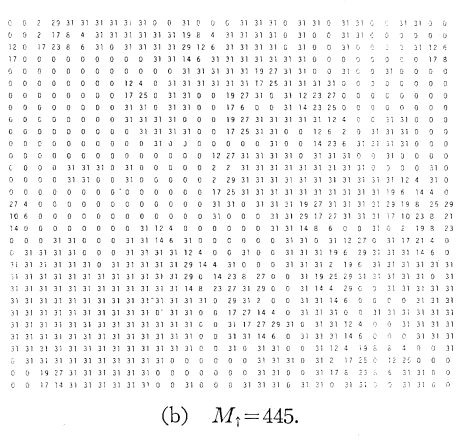
The expansion coefficients may be expanded again in a power series of n as

$$\begin{aligned} &F_0(n)=f_0(T)+c(T)n+dn^2+\cdots, \\ &A(n)=A_0+an+\cdots \quad\text{and}\quad B(n)=b+b_1n+\cdots. \end{aligned} \tag{5·2}$$

Here, we assume that $A_0\equiv 0$, only because results thus obtained are quite reason-



(a) $M_\uparrow=432$.



(b) $M_\uparrow=445$.

Fig. 14. Typical spin configurations of the effective lattice: (a) $k_BT=3.0J$, (b) $k_BT=2.25J$, where each number in the figures represents states of five Ising spins corresponding to each real spin in the binary system: $0=(\downarrow,\downarrow,\downarrow,\downarrow,\downarrow)$, $31=(\uparrow,\uparrow,\uparrow,\uparrow,\uparrow)$ or $12=(\downarrow,\uparrow,\uparrow,\downarrow,\downarrow)$. $M_\uparrow$ denotes the number of up spins in the real space.

*) K. Hirakawa has kindly informed the present authors his preliminary experimental data on K_2CuF_4 ($S=\frac{1}{2}$) by neutron scattering, which seem to show the appearance of a new type of peak near T_c, which might be relevant to vortices.

able. That is, this assumption represents the characteristic feature of the phase transition of the two-dimensional XY-model. Thus, we obtain

$$f(m,n)=f_0(T)+anm^2+bm^4+\cdots+c(T)n+dn^2+\cdots . \tag{5·3}$$

From the stability condition of the system and from the condition that $m_s\equiv 0$ for $T>0$, if follows further that

$$a>0,\ b>0 \quad \text{and} \quad d>0 . \tag{5·4}$$

By minimizing $f(m,n)-hm$ with respect to m and n for a fixed magnetic field h, we obtain the following results:

(i) $m_s\equiv 0$ for $h=0$,

(ii) $n=-c(T)/(2d)$ for $T>T_c$ and $n=0$ for $T<T_c$,

(iii) the critical point T_c is defined by $c(T_c)=0$; $c(T)<0$ for

$$T>T_c \quad \text{and} \quad c(T)>0 \quad \text{for} \quad T<T_c ,$$

(iv) the susceptibility χ_0 is given by $\chi_0=1/[2an(T)]$, which diverges at T_c and is always infinite for $T<T_c$,

(v) the specific heat shows the singularity of the form

$$C_0\sim\frac{\partial^2}{\partial T^2}[c(T)n+dn^2+\cdots]\sim\frac{\partial^2}{\partial T^2}[c^2(T)/d(T)]$$
$$\sim(T-T_c)^{2\gamma-2-\varphi}, \tag{5·5}$$

where γ and φ are defined by

$$c(T)\sim(T-T_c)^{\gamma} \quad \text{and} \quad d(T)\sim(T-T_c)^{\varphi} . \tag{5·6}$$

Consequently C_0 is smooth near T_c up to its first derivative for $2\gamma>\varphi+3$. This condition may be easily satisfied in the two-dimensional XY-model, because the value of γ is believed to be very large[8] in this system. This explains well our results from the Monte Carlo simulation.

More microscopic explanations of this phenomenological theory will be given in future.

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