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An Improved Spherical Approximation of an Ising Spin System

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§ 1. Introduction.

In 1952, Berlin and Kac[1] proposed the spherical model, which is a continuum modification of the Ising model of a ferromagnet. In this model, one-, two-, and three-dimensional lattices of infinite extent can be extensively discussed. The one- and two-dimensional spherical models do not exhibit phase transition, whereas the three-dimensional model does.

In 1977, N. Nagai, Y. Ohkawa, M. Shingu, S. Yagi and G. Iwata[2] improved the spherical approximation by Berlin and Kac. They rewrote the partition function of an Ising system as a multiple integral, and divided the integration space by a set of concentric spherical surfaces and sets of parallel planes into small domains. The two factors constituting the integrand of the multiple integral were separately averaged over a domain, and the product of the averaged two factors was summed up over all domains. If the integration space is divided only by a set of spherical surfaces, their approximation is equivalent to the spherical approximation by Berlin and Kac.

For an illustrative example of their method, they computed the partition function for the two-dimensional square lattice where only nearest neighbor spins interact with each other and no external field is present, by using a set spherical surfaces and only a set of planes. While the spherical approximation predicts no phase transition, their method gives a phase transition in the vicinity of the exact transition point.

To improve the approximation by N. Nagai et al., we add further a set of quadratic surfaces to a set of spherical surfaces and a set of planes, and divide the integration space by them. By this method we campute the partition function, the specific heat, magnetization and susceptibility for the two-dimensional square lattice with nearest neighbor interaction and no external field. The partition function and the specific heat are compared with those by the exact method, the spherical approximation and the improved spherical approximation by N. Nagai et al. Among those three approximations our results are the closest to the exact ones.

By the way, we compute Curie temperatures of three-dimensional anisotropic

Ising systems with the use of the improved spherical approximation by N. Nagai et al., and investigate the influence of anisotropy on Curie temperature.

§ 2. Division of the integration space.

The partition function Z of an Ising spin system consisting of N Ising spins x_r situated at N lattice points r of a lattice may be expressed as the sum

$$Z=2^{-N}\sum\exp\left[\frac{1}{2}\sum_{r,r'}K(r-r')x_rx_{r'}+h\sum_r x_r\right] \tag{1}$$

where the first $\sum$ means the summation over each variable x_r on 1 and -1, the lattice point r ranging over the whole lattice, $-K(r-r')x_rx_{r'}$ representing the interaction of the Ising spins x_r and $x_{r'}$, divided by the product of the Boltzmann constant and the absolute temperature, and $-hx_r$ representing the interaction of the Ising spin x_r and an external field divided by the same product as above. The factor 2^{-N} is inserted for later convenience.

The sum (1) may be transformed into a multiple integral

$$Z=\int\cdots\int A\cdot B\,dX \tag{2}$$

by virtue of the property of the delta function

$$\delta(x^2-1)=\frac{1}{2}\{\delta(x-1)+\delta(x+1)\}$$

where

$$A=\exp\left[\frac{1}{2}\sum K(r-r')x_rx_{r'}+h\sum x_r\right]$$

$$B=\Pi\delta(x_r^2-1)$$

$$dX=dx_1dx_2\cdots dx_N\,.$$

To improve the approximation by N. Nagai et al., we divide the integration space by a set of spherical surfaces

$$R=\sum x_r^2\,,\qquad 0<R<\infty\,, \tag{3}$$

a set of planes

$$L=\sum x_r\,,\qquad -\infty<L<\infty \tag{4}$$

and a set of quadratic surfaces

$$Q=M_{rr'}x_rx_{r'}\,,\qquad -\infty<Q<\infty\,. \tag{5}$$

The concrete form of $M_{rr'}$ will be given later.

We regard the multiple integral (2) as the sum of the product of $\langle A\cdot B\rangle$ and Ω over all sets of R, L, Q, that is,

$$Z=\int_0^\infty dR\int_{-\infty}^\infty dL\int_{-\infty}^\infty dQ\langle A\cdot B\rangle\Omega \tag{6}$$

where

$$\langle A\cdot B\rangle=\frac{1}{\Omega}\int\cdots\int A\cdot B\delta(R-\sum x_r^2)\delta(L-\sum x_r)\delta(Q-\sum M_{rr'}x_rx_{r'})dX$$

$$\Omega=\int\cdots\int\delta(R-\sum x_r^2)\delta(L-\sum x_r)\delta(Q-\sum M_{rr'}x_rx_{r'})dX\,.$$

$\langle A\cdot B\rangle$ represents the average of $A\cdot B$ over the domain which is defined by a set of R, L, Q, and Ω is the volume of the same domain.

The basic approximation in our method is to replace $\langle A\cdot B\rangle$ by $\langle A\rangle\langle B\rangle$. If the average $\langle A\cdot B\rangle$ is taken over the domain which is defined by a set of quadratic surfaces

$$S=\sum K(\mathrm{r}-\mathrm{r}')x_rx_{r'}\,,\qquad -\infty<S<\infty \tag{7}$$

and a set of planes defined by eq. (4), $\langle A\cdot B\rangle$ is exactly equal to $\langle A\rangle\langle B\rangle$, because the factor A contains the quadratic form $\sum K(\mathrm{r}-\mathrm{r}')x_rx_{r'}$ and the linear combination $\sum x_r$, so that A is constant over the domain defined by S, L. Therefore if we add a set of quadratic furfaces Q in (5) which resemble $S=\sum K(\mathrm{r}-\mathrm{r}')x_rx_{r'}$ to a set of spherical surfaces R in (3) and a set of planes L in (4), our approximation will be improved better than when only spherical surfaces and planes are used.

To define $M_{rr'}$, we divide the lattice into m sublattices or blocks each of which has $n=N/m$ lattice points. $M_{rr'}$ is defined to be equal to $K(\mathrm{r}-\mathrm{r}')$ except that $M_{rr'}=0$ if r and r′ belong to different blocks. Then eq. (5) is written as

$$Q=\sum_{\mathrm{l}}\sum_{\mathrm{j},\mathrm{j}'}\tilde{M}_{\mathrm{jj}'}x_{\mathrm{l},\mathrm{j}}x_{\mathrm{l},\mathrm{j}'} \tag{8}$$

where $\tilde{M}_{\mathrm{jj}'}$ is the interaction matrix in a block and $x_{\mathrm{l},\mathrm{j}}$ is the spin of the j-th lattice point in the l-th block. The summation with respect to j and j′ is taken over the lattice points in a block, l being summed up over all of the blocks.

§ 3. Computation of Z.

We compute the partition function Z by replacing $\langle A\rangle\langle B\rangle\Omega$ by $\langle A\rangle\Omega\cdot\langle B\rangle\Omega/\Omega$.

Using the representation of the delta function

$$\delta(x)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}e^{ux}du$$

we get

$$\Omega=\int\cdots\int\delta(R-\sum x_r^2)\delta(L-\sum x_r)\delta(Q-\sum\sum\tilde{M}_{\mathrm{jj}'}x_{\mathrm{l},\mathrm{j}}x_{\mathrm{l},\mathrm{j}'})dX$$

$$=\frac{(2\pi)^{N/2}}{4(2\pi i)^3}\iiint\exp\left[\frac{u}{2}R+\frac{v}{2}Q+wL+m\ln f(u,v,w)\right]dudvdw \tag{9}$$

$$\langle A\rangle\Omega=\int\cdots\int\exp\Big[\frac{1}{2}\sum K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+h\sum x_{\mathrm{r}}\Big]\delta(R-\sum x_{\mathrm{r}}{}^2)\delta(L-\sum x_{\mathrm{r}})$$
$$\cdot\delta(Q-\sum\sum\tilde{M}_{\mathrm{jj}'}x_{1,\mathrm{j}}x_{1,\mathrm{j}'})dX$$
$$=\frac{(2\pi)^{N/2}}{4(2\pi i)^3}\iiint\exp\Big[\frac{r}{2}R+\frac{s}{2}Q+tL-\frac{1}{2}\ln\det(r+sM-K)$$
$$+\frac{(t-h)^2}{2}\sum_{\mathrm{r},\mathrm{r}'}\Big(\frac{1}{r+sM-K}\Big)_{\mathrm{rr}'}\Big]drdsdt \tag{10}$$

$$\langle B\rangle\Omega=\int\cdots\int\Pi\delta(x_{\mathrm{r}}{}^2-1)\cdot\delta(R-\sum x_{\mathrm{r}}{}^2)\delta(L-\sum x_{\mathrm{r}})\delta(Q-\sum\sum\tilde{M}_{\mathrm{jj}'}x_{1,\mathrm{j}}x_{1,\mathrm{j}'})dX$$
$$=\frac{1}{4(2\pi i)^3}\iiint\exp\Big[\frac{u}{2}R+\frac{v}{2}Q+wL+m\ln g(u,v,w)\Big]dudvdw \tag{11}$$

where

$$f(u,v,w)=\exp\Big[-\frac{1}{2}\ln\det(u+v\tilde{M})+\frac{w^2}{2}\sum_{\mathrm{j},\mathrm{j}'}\Big(\frac{1}{u+v\tilde{M}}\Big)_{\mathrm{jj}'}\Big]$$

$$g(u,v,w)=\int\cdots\int\exp\Big[-\frac{u}{2}\sum_{\mathrm{j}}x_{1,\mathrm{j}}^2-\frac{v}{2}\sum_{\mathrm{j},\mathrm{j}'}\tilde{M}_{\mathrm{jj}'}x_{1,\mathrm{j}}x_{1,\mathrm{j}'}-w\sum_{\mathrm{j}}x_{1,\mathrm{j}}\Big]$$
$$\cdot\prod_{\mathrm{j}}dx_{1,\mathrm{j}}\delta(x_{1,\mathrm{j}}^2-1)\,. \tag{13}$$

The function $g(u, v, w)$ is independent of l. The lines of integration with respect to u, v, w, r, s, t are parallel to the imaginary axis. $(1/(r+sM-K))_{\mathrm{rr}'}$ represents the (r, r') element of the inverse of the matrix $r+sM-K$. It is necessary that the eigenvalues of the matrix $r+sM-K$ and the matrix $u+v\tilde{M}$ have positive real parts.

The inverse of Ω will be computed by the following expression.

$$\frac{1}{\Omega}=(2\pi)^{-N/2}\int_0^\infty du'\int_0^\infty dv'\int_{-\infty}^\infty dw'\exp\Big[-\frac{u'}{2}R-\frac{v'}{2}Q-w'L-m\ln f(u',v',w')\Big]\cdot C \tag{14}$$

C being of a finite order in N.

Using the expressions (10), (11) and (14) we get

$$Z=\int_0^\infty dR\int_{-\infty}^\infty dL\int_{-\infty}^\infty dQ\langle A\rangle\Omega\cdot\langle B\rangle\Omega/\Omega$$
$$=\frac{C}{4^2(2\pi i)^6}\int\cdots\int\exp[NW]dudvdwdrdsdtdu'dv'dw'dRdLdQ$$
$$W=\frac{u+r-u'}{2}\frac{R}{N}+\frac{v+s-v'}{2}\frac{Q}{N}+(w+t-w')\frac{L}{N}+\frac{1}{n}\ln g(u,v,w)$$
$$-\frac{1}{2N}\ln\det(r+sM-K)+\frac{(t-h)^2}{2N}\sum\Big(\frac{1}{r+sM-K}\Big)_{\mathrm{rr}'},$$
$$-\frac{1}{n}\ln f(u',v',w')\,. \tag{15}$$

With n fixed, we make N tend to infinity and have, by the use of the method of the steepest descent,

$$F=\lim_{N\to\infty}\frac{1}{N}\ln Z=\min_{\substack{u,v,w\\r,s,t}}\max_{\substack{u',v',w'\\R,L,Q}}W \tag{16}$$

since u, v, w, r, s, t are complex variables, while u', v', w', R, L, Q are real variables.

Eliminating u', v', w' we get

$$\begin{aligned}W=&-\frac{1}{2N}\ln\det(r+sM-K)+\frac{(t-h)^2}{2}\frac{1}{N}\Sigma\left(\frac{1}{r+sM-K}\right)_{rr'}\\&+\frac{1}{n}\ln g(u,v,w)-\frac{1}{n}\ln f(u+r,v+s,w+t)\end{aligned} \tag{17}$$

$$F=\min_{\substack{u,v,w\\r,s,t}}W$$

since we get $u+r=u'$, $v+s=v'$ and $w+t=w'$ from the extremum conditions with respect to R, Q, L.

Hereafter we restrict ourselves to treat the two-dimensional square lattice with nearest neighbor interaction.

We divide the lattice into blocks each of which contains 2×2 lattice points as shown in Fig. 1. $\tilde{M}$ is written as

$$\tilde{M}=\bar{K}\begin{array}{c}\\1\\2\\3\\4\end{array}\begin{array}{c}\begin{array}{cccc}1&2&3&4\end{array}\\\begin{pmatrix}0&1&1&0\\1&0&0&1\\1&0&0&1\\0&1&1&0\end{pmatrix}\end{array} \tag{18}$$

where $\bar{K}$ is the exchange interaction divided by k_BT. $\bar{K}$ can be omitted in (18) if Q and corresponding integration variables s, v and v' are suitably redefined.

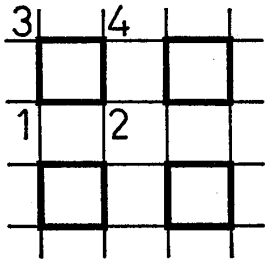

Fig. 1. The lattice divided into blocks each of which contains 2×2 lattice points.

We get

$$\begin{aligned}f(u+r,v+s,w+t)=\exp\Big[&-\frac{1}{2}\ln(u+r)^2\{(u+r)^2-4(v+s)^2\}\\&+\frac{(w+t)^2}{2}\cdot\frac{4}{u+r+2(v+s)}\Big]\end{aligned} \tag{19}$$

$$g(u,\ v,\ w)=\frac{e^{-2u}}{8}(e^{4v}+2+4\cosh 2w+e^{-4v}\cosh 4w) \tag{20}$$

$$\frac{1}{N}\Sigma\left(\frac{1}{r+sM-K}\right)_{rr'}=\frac{1}{r+2s-\lambda_0} \tag{21}$$

where $\lambda_0\equiv 4\bar{K}=4J/k_BT$. J is the exchange interaction.

Substituting eqs. (19), (20) and (21) into (17), and eliminating t, we get

$$W=-\frac{1}{2N}\ln\det(r+sM-K)-\frac{(w+h)^2}{2(u+2v+\lambda_0)}$$

$$-\frac{u}{2}+\ln\phi(v,\ w)+\frac{1}{2}\ln\varphi(u+r,\ v+s) \tag{22}$$

where

$$\phi(v,\ w)=\left[\frac{1}{8}(e^{4v}+2+4\cosh 2w+e^{-4v}\cosh 4w)\right]^{1/4}$$

$$\varphi(u+r,\ v+s)=[(u+r)^2\{(u+r)^2-4(v+s)^2\}]^{1/4}.$$

Using replacements

$$r=\lambda_0\bar{r},\quad s=\lambda_0\bar{s},\quad u=\lambda_0\bar{u},\quad v=\lambda_0\bar{v},\quad h=\lambda_0\bar{h}$$

we rewrite (22) and get

$$W=-\frac{1}{4}\Delta(\bar{r},\ \bar{s})-\frac{1}{2\lambda_0}\cdot\frac{(w+\lambda_0\bar{h})^2}{\bar{u}+2\bar{v}+1}-\frac{\lambda_0\bar{u}}{2}+\ln\phi(\lambda_0\bar{v},\ w)$$

$$+\frac{1}{2}\ln\varphi(\bar{u}+\bar{r},\ \bar{v}+\bar{s}) \tag{23}$$

$$F=\min_{\substack{\bar{u},\bar{v},\bar{w}\\ \bar{r},\bar{s}}} W$$

where

$$\Delta(\bar{r},\ \bar{s})\equiv\frac{1}{N}\ln\det\left(\bar{r}+\bar{s}M-\frac{K}{\lambda_0}\right).$$

We regard F as a function of λ_0 and $\bar{h}$. Computation of $\Delta(\bar{r},\ \bar{s})$ is given in Appendix A.

The specific heat, magnetization and susceptibility are given respectively by

$$\frac{C_H}{k_B}=\lambda_0^2\frac{\partial^2F}{\partial\lambda_0^2},\quad \frac{M}{m}=\frac{1}{\lambda_0}\frac{\partial F}{\partial\bar{h}},\quad \frac{4J\chi}{m^2}=\frac{1}{\lambda_0}\frac{\partial^2F}{\partial\bar{h}^2} \tag{25}$$

where m is the magnetic moment of a spin. Computation of $\partial^2F/\partial\lambda_0^2$, $\partial F/\partial\bar{h}$ and $\partial^2F/\partial\bar{h}^2$ is given in Appendix B.

§ 4. Results.

We have computed the partition function, the specific heat, magnetization and susceptibility for the two-dimensional square lattice with nearest neighbor

interaction and no external field.

In Fig. 2, logarithm of the partition function per spin is shown. Curves by some other methods are also illustrated. It is clear that our result is closer to the exact solution than that by N. Nagai et al. Computing F in (24), we get two branches corresponding to two solutions of w: $w=0$ and $w\neq 0$, which are given from the condition $\partial W/\partial w=0$. The method of the steepest descent forces us to employ the maximum values of F as the true F. We regard the cross point of the branches as Curie point. In case of method by N. Nagai et al. the branch without a fold is consistent with the spherical approximation. While the curve by spherical approximation deviates from the exact one with increasing λ_0, our curve converges to the exact one with increasing λ_0.

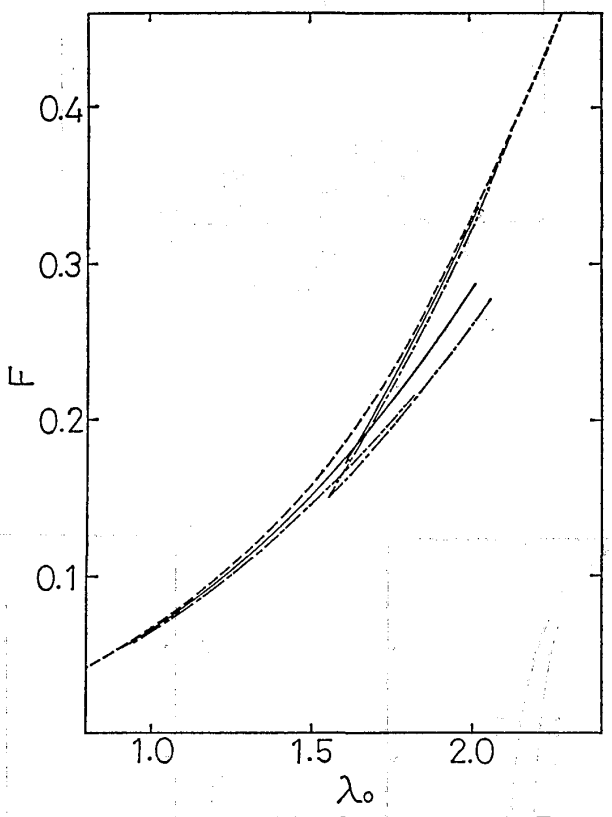

Fig. 2. $F=\lim N^{-1}\ln Z$ vs. $\lambda_0=4J/k_BT$.
- - - - - - - Onsager's exac method
— — — — — The method by N. Nagai et al.
——————— Present method

While the exact Curie point is 0.567 in unit of $4J/k_B$, that by N. Nagai et al. is 0.618 and ours is 0.604. The ratioes of respective Curie points to the exact one are 1.09 and 1.07.

Respective specific heat curves are shown in Fig. 3. It is clear that our result is closer to the exact one than that by N. Nagai et al. is.

Magnetization and susceptibility are shown in Fig. 4 and 5.

We have investigated the influence of anisotropy on Curie point with the use of the method by N. Nagai et al.

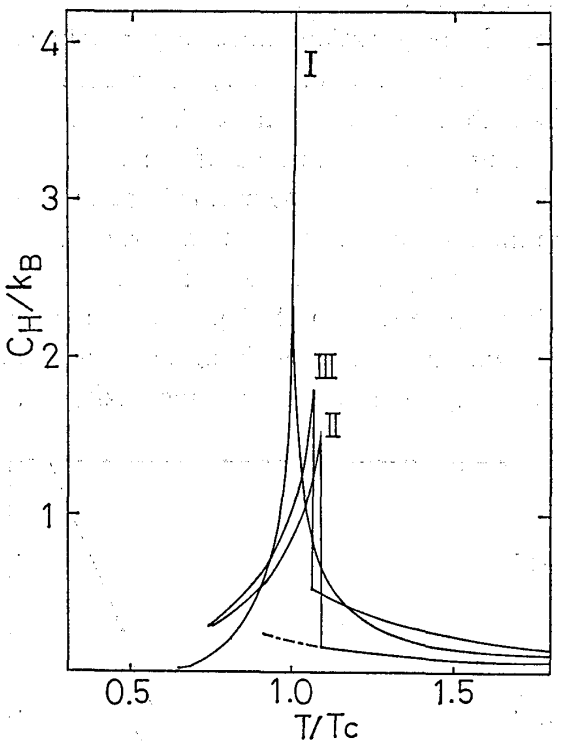

Fig. 3. Specific heat vs. temperature.
I Onsager's exact method
– – – – – Spherical approximation
II The method by N. Nagai et al.
III Present method

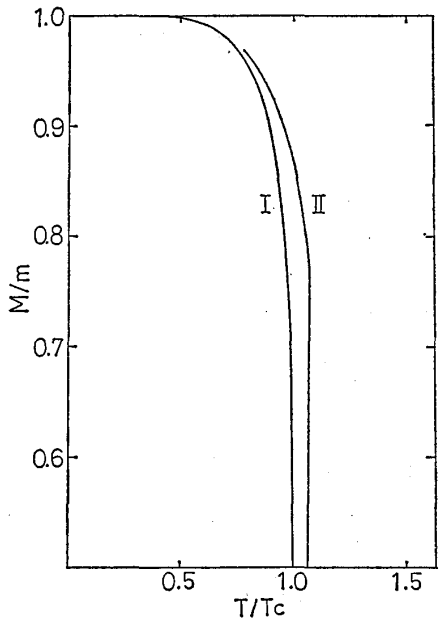

Fig. 4. Mognetization vs. temperature.
I Exact method
II Rresent method

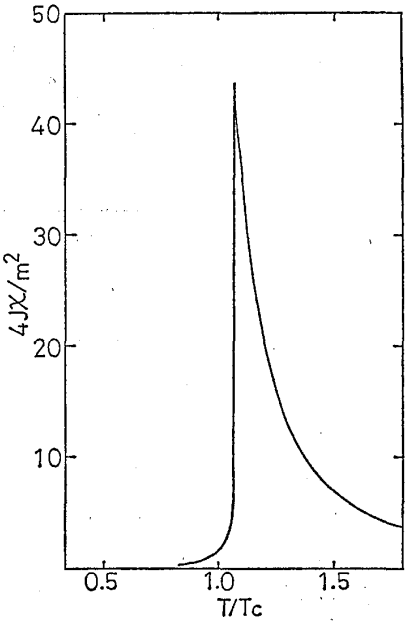

Fig. 5. Susceptibility vs. temperature given by present method.

For the three-dimensional lattice with nearest neighbor interaction and no external field, we assume the lattice to have the interaction J_0 in the $x-y$ plane and the interaction J_1 between the two nearby planes. The behavior of Curie point against J_1/J_0 is shown in Fig. 6. Here λ_0 is $(4J_0+2J_1)/k_BT_c$, where T_c is Curie point. The three-dimensional lattice can be regarded as the two-dimensional one in case of $J_1/J_0\approx 0$. Curie point in the isotropic limit ($J_1/J_0=1$) is 0.734 in unit of $6J/k_B$, which is a little lower than the value 0.752[3] obtained from the high temperature susceptibility series.

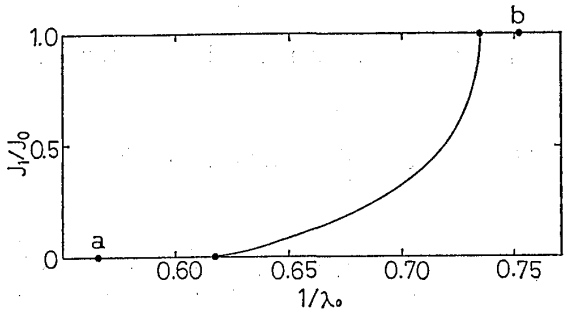

Fig. 6. The influence of anisotropy on Curie point.
a: 0.567 (Onsager's Exact Method)
b: 0.752 (High temperature susceptibility series)

§ 5. Discussion.

Our method, which inherits the merits of the spherical approximation, may open a wider scope of applicability to a system with or without an external field when the size of a sublattice is increased, although analysis may become more exacting.

Appendix A. Computation of $\Delta(\bar{r}, \bar{s})$

Since the interaction matrix $K(\mathrm{r}-\mathrm{r}')$ is real and symmetric, it is diagonalized by a unitary matrix

$$U_{\mathrm{ru}}=\frac{1}{\sqrt{N}}\exp\left[\frac{i2\pi}{N^*}\mathrm{r}\cdot\mathrm{u}\right], \qquad N^*\equiv N^{1/d}. \tag{A1}$$

Here d is the dimension of the lattice, and r and u are d-dimensional vectors which indicate actual and reciprocal lattice points respectively. The eigenvalues of $K(\mathrm{r}-\mathrm{r}')$ are given by

$$\lambda_{\mathrm{u}}=\sum_{\mathrm{x}}K(\mathrm{x})\exp\left[\frac{i2\pi}{N^*}\mathrm{x}\cdot\mathrm{u}\right] \tag{A2}$$

where the summation is taken all over the lattice points.

Let us divide the lattice into m sublattices or blocks each of which contains $n=N/m$ lattice points, and put $\mathrm{r}=\mathrm{j}+n^*\mathrm{l}$ ($n^*\equiv n^{1/d}$). Then the reciprocal lattice is divided into n blocks each of which contains $m=N/n$ lattice points, so $\mathrm{u}=\mathrm{p}+m^*\mathrm{q}$ ($m^*\equiv m^{1/d}$). Here the components of the vectors j and q take integers

from 0 to n^*-1, and those of the vectors l and p take integers from 0 to m^*-1.

Now $\det(\bar{r}+\bar{s}M-K/\lambda_0)$ is equal to $\det(U^{-1}(\bar{r}+\bar{s}M-K/\lambda_0)U)$. Since $\tilde{M}$ is the interaction matrix in a block, it is diagonalized by a small $(n\times n)$ unitary matrix

$$L_{jq}=\frac{1}{\sqrt{n}}\exp\left[\frac{i2\pi}{n^*}j\cdot q\right]. \tag{A3}$$

The eigenvalues are

$$\rho_q=\frac{1}{\bar{K}}\sum_y K(y)\exp\left[\frac{i2\pi}{n^*}y\cdot q\right] \tag{A4}$$

where the summation is taken all over the lattice points in a block. Then M is transformed as

$$(U^{-1}MU)_{uu'}=\delta_{pp'}\sum_{q''}\langle q|c(p)|q''\rangle\rho_{q''}\langle q''|\overline{c(p)}|q'\rangle \tag{A5}$$

where

$$\langle q|c(p)|q'\rangle\equiv\frac{1}{n}\sum_j\exp\left[i2\pi\left(\frac{q'-q}{n^*}-\frac{p}{N^*}\right)\cdot j\right]. \tag{A6}$$

Hereafter we consider a two-dimensional square lattice with nearest neighbor interaction. We divide the actual lattice into $m=N/4$ blocks. Each block has 2×2 lattice points. Then there are four blocks in the reciprocal lattice space, each of which is assigned by a vector such as

$$q=(0,0),\quad (0,1),\quad (1,0),\quad (1,1). \tag{A7}$$

From (A5), $(U^{-1}MU)_{uu'}$ is zero if $p\neq p'$. Namely it is diagonal in a reciprocal lattice block as shown in Fig. 7. The matrix $U^{-1}(\bar{r}+\bar{s}M-K/\lambda_0)U$ is also of the type of Fig. 7. By reconstructing the rows and columns suitably, the determinant of such a matrix is calculated to be

$$\begin{vmatrix} a_1 & & b_1 & & \cdots \\ & a_2 & & b_2 & \\ c_1 & & d_1 & & \cdots \\ & c_2 & & d_2 & \\ \vdots & & \vdots & & \end{vmatrix} = \begin{vmatrix} a_1b_1\cdots & & \cdots \\ c_1d_1\cdots & 0 & \\ \cdots & & \cdots \\ 0 & a_2b_2\cdots & \\ & c_2d_2\cdots & \cdots \\ \cdots & \cdots & \end{vmatrix} = \prod_i \begin{vmatrix} a_i & b_i & \cdots \\ c_i & d_i & \cdots \\ \cdots & \cdots & \end{vmatrix}. \tag{A8}$$

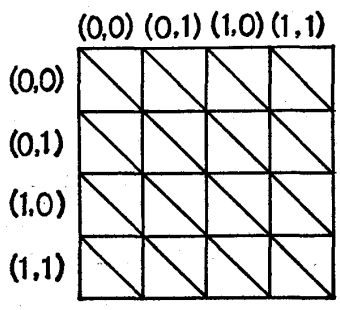

Fig. 7. The matrix diagonalized in each block.

After some calculation we get

$$\left|\bar{r}+\bar{s}M-\frac{K}{\lambda_0}\right|=\prod_{\mathrm{p}}G_{\mathrm{p}} \tag{A9}$$

where

$$G_{\mathrm{p}}=\begin{vmatrix} \bar{r}-\left(\frac{1}{2}-\bar{s}\right)(\cos\theta_1+\cos\theta_2) & -i\bar{s}\sin\theta_2 & -i\bar{s}\sin\theta_1 & 0 \\ i\bar{s}\sin\theta_2 & \bar{r}-\left(\frac{1}{2}-\bar{s}\right)(\cos\theta_1-\cos\theta_2) & 0 & -i\bar{s}\sin\theta_1 \\ i\bar{s}\sin\theta_1 & 0 & \bar{r}+\left(\frac{1}{2}-\bar{s}\right)(\cos\theta_1-\cos\theta_2) & -i\bar{s}\sin\theta_2 \\ 0 & i\bar{s}\sin\theta_1 & i\bar{s}\sin\theta_2 & \bar{r}+\left(\frac{1}{2}-\bar{s}\right)(\cos\theta_1+\cos\theta_2) \end{vmatrix} \tag{A10}$$

$$\theta_1=\frac{\pi}{\sqrt{m}}p_1, \qquad \theta_2=\frac{\pi}{\sqrt{m}}p_2,$$

p_1 and p_2 being the components of the vector p.

From (A9) and (A10), we get

$$\begin{aligned} \Delta(\bar{r},\bar{s})&=\frac{1}{N}\ln\det\left(\bar{r}+\bar{s}M-\frac{K}{\lambda_0}\right) \\ &=\frac{1}{N}\ln\prod_{\mathrm{p}}G_{\mathrm{p}} \\ &=\frac{1}{N}\sum_{p_1=0}^{\sqrt{m}-1}\sum_{p_2=0}^{\sqrt{m}-1}\ln G_{p_1p_2}(\theta_1,\theta_2,\bar{r},\bar{s}). \end{aligned} \tag{A11}$$

Taking N to infinity, we have

$$\Delta(\bar{r},\bar{s})=\frac{1}{(2\pi)^2}\int_0^\pi\int_0^\pi\ln G(\theta_1,\theta_2,\bar{r},\bar{s})d\theta_1 d\theta_2. \tag{A12}$$

If $\bar{r}$ and $\bar{s}$ are given, integration is carried out numerically.

Appendix B. Computation of $\partial^2F/\partial\lambda_0^2$, $\partial F/\partial\bar{h}$ and $\partial^2F/\partial\bar{h}^2$

To compute $\partial^2F(\lambda_0,\bar{h})/\partial\lambda_0^2$, $\partial F(\lambda_0,\bar{h})/\partial\bar{h}$ and $\partial^2F(\lambda_0,\bar{h})/\partial\bar{h}^2$ systematically we replace $\bar{r}$, $\bar{s}$, $\bar{u}$, $\bar{v}$, w, λ_0, $\bar{h}$ by $x_1, x_2, \cdots, x_5, \alpha_1, \alpha_2$ respectively. Since $F(\alpha_1,\alpha_2)$ is the extremum of $W(x_1, x_2, \cdots, x_5, \alpha_1, \alpha_2)$, it is given by solving the equations

$$\frac{\partial W}{\partial x_1}=0, \quad \frac{\partial W}{\partial x_2}=0, \quad \cdots\cdots, \quad \frac{\partial W}{\partial x_5}=0.$$

Therefore,

$$\frac{\partial F}{\partial\alpha_\mu}=\sum_i\frac{\partial W}{\partial x_i}\cdot\frac{\partial x_i}{\partial\alpha_\mu}+\frac{\partial W}{\partial\alpha_\mu}=\frac{\partial W}{\partial\alpha_\mu} \tag{B1}$$

$$\frac{\partial^2F}{\partial\alpha_\nu\partial\alpha_\mu}=\sum_i\frac{\partial^2W}{\partial x_i\partial\alpha_\mu}\cdot\frac{\partial x_i}{\partial\alpha_\nu}+\frac{\partial^2W}{\partial\alpha_\nu\partial\alpha_\mu}\equiv Y+\frac{\partial^2W}{\partial\alpha_\nu\partial\alpha_\mu} \tag{B2}$$

$$(\mu=1,2;\ \nu=1,2).$$

To compute Y in (B2) we consider the following six equations

$$\left\{\begin{array}{l}\dfrac{\partial}{\partial\alpha_\nu}\left(\dfrac{\partial W}{\partial x_1}\right)=\sum_i \dfrac{\partial^2 W}{\partial x_i\partial x_1}\cdot\dfrac{\partial x_i}{\partial\alpha_\nu}+\dfrac{\partial^2 W}{\partial\alpha_\nu\partial x_1}=0\\ \dfrac{\partial}{\partial\alpha_\nu}\left(\dfrac{\partial W}{\partial x_2}\right)=\sum_i \dfrac{\partial^2 W}{\partial x_i\partial x_2}\dfrac{\partial x_i}{\partial\alpha_\nu}+\dfrac{\partial^2 W}{\partial\alpha_\nu\partial x_2}=0\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ \dfrac{\partial}{\partial\alpha_\nu}\left(\dfrac{\partial W}{\partial x_5}\right)=\sum_i \dfrac{\partial^2 W}{\partial x_i\partial x_5}\dfrac{\partial x_i}{\partial\alpha_\nu}+\dfrac{\partial^2 W}{\partial\alpha_\nu\partial x_5}=0\\ \qquad\qquad \sum_i \dfrac{\partial^2 W}{\partial x_i\partial\alpha_\mu}\dfrac{\partial x_i}{\partial\alpha_\nu}-Y=0\,.\end{array}\right. \tag{B3}$$

If we put

$$W_{ij}=W_{ji}=\frac{\partial^2 W}{\partial x_i\partial x_j},\quad W_{\alpha_\nu i}=W_{i\alpha_\nu}=\frac{\partial^2 W}{\partial\alpha_\nu\partial x_i},\quad X_i=\frac{\partial x_i}{\partial\alpha_\nu} \tag{B4}$$

we can write (B3) in a matrix form:

$$\begin{pmatrix} W_{11} & W_{12} & \cdots & W_{15} & 0\\ W_{21} & W_{22} & \cdots & W_{25} & 0\\ & \cdots\cdots & & & \\ & \cdots\cdots & & & \\ W_{51} & W_{52} & \cdots & W_{55} & 0\\ W_{\alpha_\mu 1} & W_{\alpha_\mu 2} & \cdots & W_{\alpha_\mu 5} & -1\end{pmatrix}\begin{pmatrix} X_1\\ X_2\\ \vdots\\ X_5\\ Y\end{pmatrix}=\begin{pmatrix} -W_{1\alpha_\nu}\\ -W_{2\alpha_\nu}\\ \vdots\\ -W_{5\alpha_\nu}\\ 0\end{pmatrix}. \tag{B5}$$

From (B5), we get

$$Y=\begin{vmatrix} W_{11} & W_{12} & \cdots & W_{15} & W_{1\alpha_\nu}\\ W_{21} & W_{22} & \cdots & & W_{2\alpha_\nu}\\ & \cdots\cdots & & & \\ W_{51} & W_{52} & \cdots & W_{55} & W_{5\alpha_\nu}\\ W_{\alpha_\mu 1} & W_{\alpha_\mu 2} & \cdots & W_{\alpha_\mu 5} & 0\end{vmatrix}\Bigg/\begin{vmatrix} W_{11} & W_{12} & \cdots & W_{15}\\ W_{21} & W_{22} & \cdots & \\ & \cdots\cdots & & \\ W_{51} & W_{51} & \cdots & W_{55}\end{vmatrix}. \tag{B6}$$

Putting $\mu=\nu=1$ in (B2), we get a formula for C_H; putting $\mu=\nu=2$ in (B2) we get χ; and putting $\mu=2$ in (B1) we get M.

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