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An Improvement in the Spherical Approximation of an Ising Spin System

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Rewriting the partition function of an Ising system as a multiple integral, dividing the integration space by a set of concentric spherical surfaces and sets of parallel planes into small domains, averaging separately the two factors constituting the integrand of the multiple integral over each of these domains, and replacing the two factors by their respective averages, logarithm of the partition function per spin is given by the extremum of a function with respect to a complex variable and a number of real variables. The specific heat curve of an Ising square lattice obtained by the present method is compared with those by the exact method, the spherical approximation and the mean field approximation.

§ 1. 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

$$Z=2^{-N}\sum\exp\left[\frac{1}{2}\cdot\sum_{\mathrm{r},\mathrm{r}'}K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+\sum_{\mathrm{r}}h_{\mathrm{r}}x_{\mathrm{r}}\right] \tag{1}$$

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, $-K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}$ representing the interaction of the Ising spins x_{r} and $x_{\mathrm{r}'}$, divided by the product of the Boltzmann factor and the absolute temperature, and $-h_{\mathrm{r}}x_{\mathrm{r}}$ 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

$$Z=\iint\cdots\int\exp\left[\frac{1}{2}\sum K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+\sum h_{\mathrm{r}}x_{\mathrm{r}}\right]\cdot\prod\delta(x_{\mathrm{r}}^2-1)dX \tag{2}$$

$$dX=dx_1dx_2\cdots dx_N$$

by virtue of the property of the delta function

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

If we compare the representation (2) of the partition function with the expressions (11) and (12) in the paper by Berlin and Kac, the spherical approximation initiated by Berlin and Kac may be interpreted to consist in replacing the factor $\Pi\delta(x_r^2-1)$ by its average over a spherical surface $R=\sum x_r^2$. The average is given by

$$\langle\Pi\,\delta(x_r^2-1)\rangle=\int\Pi\,\delta(x_r^2-1)\cdot\delta(R-\sum x_r^2)dX\Big/\int\delta(R-\sum x_r^2)dX$$
$$=\delta(R-N)/((\pi R)^{N/2}/R\Gamma(N/2))\,.$$

To improve the approximation, we divide the integration space by a set of spherical surfaces

$$R=\sum x_r^2\,,\qquad 0<R<\infty$$

and n sets of linearly independent planes

$$L_j=\sum c_{jr}x_r\,,\qquad j=1,2,\cdots,n\,,\qquad -\infty<L_j<\infty\,.$$

How to choose the sets of planes L_j is very crucial to our method. We consider that the planes should include the plane $\sum h_r x_r=L$, or the plane $\sum h_r x_r=L$ should be expressed as the linear combination of planes L_j as few as possible

$$\sum h_r x_r=\sum\alpha_j\sum c_{jr}x_r\,.$$

Over a domain defined by $R, L_1, L_2, \cdots, L_n$, we compute the integral A of the factor $\Pi\,\delta(x_r^2-1)$ and the integral B of the factor

$$\exp\left[\frac{1}{2}\cdot\sum K(\mathrm{r}-\mathrm{r}')x_r x_{r'}+\sum h_r x_r\right]$$

in (2) separately, and replace the integral in (2) by

$$Z'=\int_0^\infty dR\int_{-\infty}^\infty dL_1\cdots\int_{-\infty}^\infty dL_n\,A\cdot B/\Omega \tag{3}$$

Ω being the volume of the domain defined by $R, L_1, L_2, \cdots, L_n$.

The spherical approximation by Berlin and Kac uses only the division by R. If $n=N-1$, the integral Z' of (3) is equal to the integral Z of (2) exactly. In the following, we fix the number n and make the number N tend to infinity. We note here that if $L=\sum x_r$ is included in the sets of planes, the integration space is divided by planes, in which the difference of the number of upward spins and that of downward spins is constant.

§ 2. Computation of the integrals over the domain

First we compute the volume Ω defined by $R, L_1, L_2, \cdots, L_n$, or

$$\Omega=\int\delta(R-\sum x_r^2)\cdot\prod_j\delta(L_j-\sum c_{jr}x_r)dX\,.$$

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

$$\begin{aligned}\Omega&=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{u}{2}(R-\sum x_{\mathrm{r}}^2)+\sum v_j(L_j-\sum c_{j\mathrm{r}}x_{\mathrm{r}})\Big]du\prod dv_j dX\\&=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{u}{2}R+\sum v_jL_j+\frac{N}{2u}\sum\rho_{jk}v_jv_k\Big]\Big(\frac{2\pi}{u}\Big)^{N/2}du\prod dv_j\end{aligned}$$

ρ_{jk} being defined as

$$\rho_{jk}=\sum c_{j\mathrm{r}}c_{k\mathrm{r}}/N.$$

Integration with respect to v_j and u gives

$$\begin{aligned}\Omega&=\frac{i^n}{2(2\pi i)^{n+1}}\int\exp\Big[\frac{u}{2}(R-\sum(\rho^{-1})_{jk}L_jL_k/N)\Big]\cdot\Big(\frac{2\pi}{u}\Big)^{N/2}\Big(\frac{2\pi u}{N}\Big)^{n/2}\frac{1}{\sqrt{\det\rho}}du\\&=\frac{\pi^{(N-n)/2}}{N^{n/2}}\frac{1}{\sqrt{\det\rho}}\frac{1}{\Gamma((N-n)/2)}(R-\sum(\rho^{-1})_{jk}L_jL_k/N)^{(N-n)/2-1}\end{aligned}\tag{4}$$

$\det\rho$ denoting the determinant of the matrix $\rho\equiv(\rho_{jk})$ and $(\rho^{-1})_{jk}$ the (i,k) element of the inverse of the matrix ρ.

Next we compute the integral A to get

$$\begin{aligned}A&=\langle\prod\delta(x_{\mathrm{r}}^2-1)\rangle\Omega=\int\cdots\int\prod\delta(x_{\mathrm{r}}^2-1)\cdot\delta(R-\sum x_{\mathrm{r}}^2)\prod\delta(L_j-\sum c_{j\mathrm{r}}x_{\mathrm{r}})dX\\&=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{u}{2}(R-\sum x_{\mathrm{r}}^2)+\sum v_j(L_j-\sum c_{j\mathrm{r}}x_{\mathrm{r}})\Big]\\&\quad\cdot\prod\delta(x_{\mathrm{r}}^2-1)dX\,du\prod dv_j\\&=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{u}{2}(R-N)+\sum v_jL_j+\sum_{\mathrm{r}}\log\cosh\sum_j v_jc_{j\mathrm{r}}\Big]du\prod dv_j\\&=\delta(R-N)\cdot\frac{1}{(2\pi i)^n}\int\cdots\int\exp\,[\sum v_jL_j+\sum_{\mathrm{r}}\log\cosh\sum_j v_jc_{j\mathrm{r}}]\prod dv_j\end{aligned}\tag{5}$$

Thirdly we compute the integral B and get

$$\begin{aligned}B&=\Big\langle\exp\Big[\frac{1}{2}\sum K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+\sum h_{\mathrm{r}}x_{\mathrm{r}}\Big]\Big\rangle\Omega\\&=\int\cdots\int\exp\Big[\frac{1}{2}\sum K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+\sum\alpha_jL_j\Big]\cdot\delta(R-\sum x_{\mathrm{r}}^2)\prod\delta(L_j-\sum c_{j\mathrm{r}}x_{\mathrm{r}})dX\\&=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{1}{2}\sum K(\mathrm{r}-\mathrm{r}')x_{\mathrm{r}}x_{\mathrm{r}'}+\sum\alpha_jL_j\\&\quad+\frac{s}{2}(R-\sum x_{\mathrm{r}}^2)+\sum s_j(L_j-\sum c_{j\mathrm{r}}x_{\mathrm{r}})\Big]dX\,ds\prod ds_j\end{aligned}$$

the lines of integration with respect to s, s_j being parallel to the imaginary axes. Integrating with respect to x_{r}, we have

$$B=\frac{(2\pi)^{N/2}}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{1}{2}sR+\Sigma(s_j+\alpha_j)L_j$$

$$-\frac{1}{2}\log\det(s-K)+\frac{N}{2}\Sigma\,\sigma_{jk}s_js_k\Big]ds\,\Pi\,ds_j$$

where we use the following abbreviations

$$\sigma_{jk}=\sum_{\mathrm{r,r'}}c_{j\mathrm{r}}c_{k\mathrm{r'}}\Big(\frac{1}{s-K}\Big)_{\mathrm{rr'}}\Big/N$$

$(1/(s-K))_{\mathrm{rr'}}$ representing the $(\mathrm{r},\mathrm{r'})$ element of the inverse of the matrix $s-K$. It is necessary that the eigenvalues of the matrix $s-K$ have positive real parts. Integrating with respect to s_j, we have

$$B=\frac{i^n(2\pi/N)^{n/2}}{2(2\pi i)^{n+1}}\int\exp\Big[\frac{1}{2}sR-\frac{1}{2}\log\det(s-K)$$

$$+\Sigma\,\alpha_jL_j-\frac{1}{2N}\Sigma\,(\sigma^{-1})_{jk}L_jL_k\Big]\frac{ds}{\sqrt{\det\sigma}} \tag{6}$$

§ 3. Computation of Z

Now we substitute the expressions (4), (5) and (6) into (3), replace R by N by virtue of $\delta(N-R)$ in (5), replace the variable L_j by Nu_j and get

$$Z'=\frac{C}{2(2\pi i)^{n+1}}\int\cdots\int\exp\Big[\frac{1}{2}sN-\frac{1}{2}\log\det(s-K)+N\,\Sigma\,\alpha_ju_j$$

$$-\frac{N}{2}\Sigma(\sigma^{-1})_{jk}u_ju_k+N\,\Sigma\,v_ju_j+\Sigma\log\cosh\Sigma\,v_jc_{j\mathrm{r}}\Big]$$

$$\cdot(1-\Sigma\,(\rho^{-1})_{jk}u_ju_k)^{1-(N-n)/2}(\det\sigma)^{-1/2}ds\,\Pi\,dv_j\,\Pi\,du_j\,.$$

C is a factor independent of integration variables.

With the fixed n, we make N tend to infinity under the assumption that ρ_{jk}, σ_{jk} and

$$\frac{1}{N}\cdot\log\det(s-K)=\frac{1}{N}\cdot\Sigma\log(s-\lambda)=\langle\log(s-\lambda)\rangle$$

λ's representing eigenvalues of the matrix K, tend to their respective limits. And further we assume $c_{j\mathrm{r}}$ to be periodic with respect to r with the period of n, then we have

$$\frac{1}{N}\cdot\sum_{\mathrm{r}}\log\cosh\Sigma\,v_jc_{j\mathrm{r}}=\frac{1}{n}\cdot\sum_{k}\log\cosh\Sigma\,v_jc_{jk}$$

k ranging over n lattice points.

As N tends to infinity, we see that

$$C=2^{(N-n)/2}\Gamma\Big(\frac{N-n}{2}\Big)N^{-N/2+3n/2+1}\sqrt{\det\rho}\longrightarrow e^{-N/2}c'$$

C' being of a finite order in N.

Then we can rewrite Z' as

$$Z'=\frac{1}{2(2\pi i)^{n+1}}\int\cdots\int\exp[NW]\cdot ds\,\Pi\,dv_j\,\Pi\,du_j C''$$

$$W=\frac{s}{2}-\frac{1}{2}\langle\log(s-\lambda)\rangle+\sum\alpha_j u_j-\frac{1}{2}\sum(\sigma^{-1})_{jk}u_j u_k$$

$$+\sum u_j v_j+\frac{1}{n}\sum\log\cosh\sum v_j c_{jk}-\frac{1}{2}\log(1-\sum(\rho^{-1})_{jk}u_j u_k)-\frac{1}{2} \tag{8}$$

C'' being of a finite order in N, the real variables u_j ranging over the domain defined by

$$\sum(\rho^{-1})_{jk}u_j u_k<1\,,$$

the complex variables s and v_j running upward, parallel to the respective imaginary axes.

Therefore, we have, by the use of the method of steepest descent,

$$F=\lim_{N\to\infty}\frac{1}{N}\cdot\log Z'=\operatorname*{Min}_{s}\operatorname*{Min}_{v_j}\operatorname*{Max}_{u_j}W \tag{9}$$

since the s and v_j are complex variables, while the u_j are real variables.

§ 4. Transformation of W

Since $\sum c_{jr}x_r=L_j$, $j=1,2,\cdots,n$ are assumed to be linearly independent, and c_{jr} are assumed to be periodic with the period of n, the matrix (c_{jk}), $j,k=1,2,\cdots,n$ has the determinant different from zero. If we denote the matrix inverse to the matrix (c_{jk}) by (c'_{jk}), we see that

$$\sum_k c_{jk}c'_{kl}=\delta_{jl}\,,\qquad \sum_k c'_{jk}c_{kl}=\delta_{jl}\,. \tag{10}$$

If we replace the variables v_j, u_j by the variables w_j, t_j defined by

$$\left.\begin{aligned} w_k&=\sum_j v_j c_{jk}\,, & v_j&=\sum_k w_k c'_{kj}\\ \frac{1}{n}t_k&=\sum_j c'_{kj}u_j\,, & u_j&=\frac{1}{n}\sum_k c_{jk}t_k\end{aligned}\right\} \tag{11}$$

we have

$$\sum_j u_j v_j+\frac{1}{n}\sum_k\log\cosh\sum_j v_j c_{jk}=\frac{1}{n}\sum_k(t_k w_k+\log\cosh w_k)\,.$$

A typical term $tw+\log\cosh w$ in the right hand side is minimum when $t+\tanh w=0$ or $w=1/2\cdot\log[(1-t)/(1+t)]$, and has the minimum

$$-\frac{1}{2}\{(1+t)\log(1+t)+(1-t)\log(1-t)\}\,.$$

This expression appears in the mean field approximation,[2] t standing for the long range order. Consequently we can eliminate v_j and replace

$$\operatorname*{Min}_{v_j}\Big[\sum u_j v_j+\frac{1}{n}\cdot\sum\log\cosh\sum v_j c_{jk}\Big]$$

by

$$-\frac{1}{2n}\cdot\sum_{k}\{(1+t_k)\log(1+t_k)+(1-t_k)\log(1-t_k)\}\,. \tag{12}$$

Now we must eliminate the variables u_j from (8). From (11), it follows that

$$\sum(\sigma^{-1})_{jk}u_ju_k=\frac{1}{n}\cdot\sum a_{lm}t_lt_m\,,\qquad a_{lm}=\sum(\sigma^{-1})_{jk}c_{jl}c_{km}/n \tag{13}$$

$$\sum(\rho^{-1})_{jk}u_ju_k=\frac{1}{n}\cdot\sum b_{lm}t_lt_m\,,\qquad b_{lm}=\sum(\rho^{-1})_{jk}c_{jl}c_{km}/n\,. \tag{14}$$

We remark here that if the set of L_j is replaced by the set of $L_j^*=\sum\alpha_{jk}L_k$, $(\alpha_{jk})=\alpha$ being a non-singular matrix, the matrices $a=(a_{lm})$ and $b=(b_{lm})$ remain invariant, as we will see in the following.

From $L_j^*=\sum\alpha_{jk}L_k$ we have

$$c_{jl}^*=\sum\alpha_{jk}c_{kl}\quad\text{or}\quad c^*=\alpha c\qquad\text{in matrix form.}$$

If a quantity obtained by replacing L_k by L_k^* may be denoted by the same symbol with an asterisk, we have

$$\rho_{jk}^*=\frac{1}{N}\cdot\sum c_{jr}^*c_{kr}^*=\sum\alpha_{jl}\alpha_{km}\rho_{lm}\qquad\text{or}\qquad\rho^*=\alpha\rho\alpha^t$$

α^t being the transposed matrix of α. Similarly we have

$$\sigma^*=\alpha\sigma\alpha^t\,.$$

On the other hand, (13) and (14) give

$$a=c^t\sigma^{-1}c/n\,,\quad\text{and}\quad b=c^t\rho^{-1}c/n\,.$$

Therfore we have

$$a^*=c^{*t}\sigma^{*-1}c^*/n=c^t\alpha^t(\alpha^t)^{-1}\sigma^{-1}\alpha^{-1}\alpha c/n=a$$

$$b^*=c^{*t}\rho^{*-1}c^*/n=b\,.$$

In other words, the matrices a and b are independent of the choice of c_{jk} so long as the condition $\det c=|c_{jk}|\neq 0$ is ensured. If we choose $c_{jk}=\delta_{jk}$, we have

$$\rho_{jk}=1/n\cdot\delta_{jk}$$

$$b_{jk}=\delta_{jk}\,.$$

The computation of a_{jk} is rather troublesome, so it will be presented in a succeeding paper. For the present we have

$$W=\frac{1}{2}s-\frac{1}{2}\langle\log(s-\lambda)\rangle+\frac{1}{n}\sum\alpha_jc_{jk}t_k-\frac{1}{2n}\sum a_{jk}t_jt_k$$

$$-\frac{1}{2n}\sum\{(1+t_k)\log(1+t_k)+(1-t_k)\log(1-t_k)\}$$

$$-\frac{1}{2}\log\Bigl(1-\frac{1}{n}\sum t_k^2\Bigr)-\frac{1}{2}$$

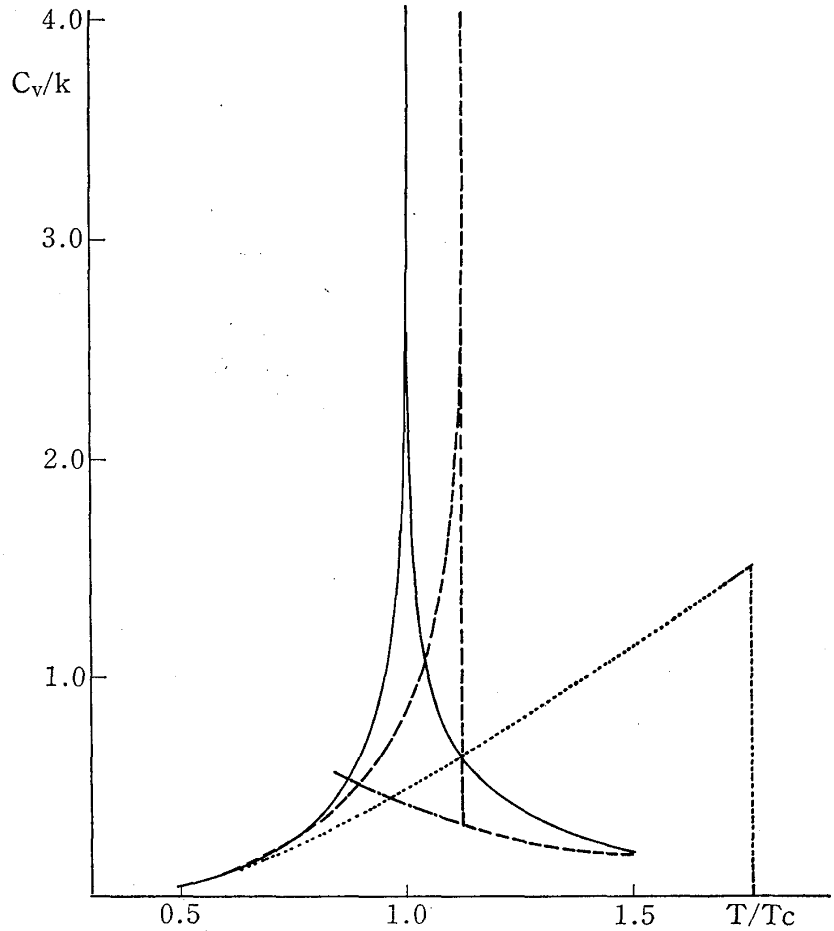
$$F = \operatorname*{Min}_{s} \operatorname*{Max}_{t_k} W .$$

§ 5. An illustrative example, square lattice

For the square lattice where only nearest neighbor spins interact with each other and no external field is present, we take only one plane $L_1 = \sum x_r$ and use only one variable t for the sake of simplicity, so we have

$$W = \frac{1}{2} s - \frac{1}{2} \langle \log (s-\lambda) \rangle - \frac{1}{2} a_{11} t^2 - \frac{1}{2} (1+t) \log (1+t) - \frac{1}{2} (1-t) \log (1-t)$$
$$- \frac{1}{2} \log (1-t^2) - \frac{1}{2} .$$

If we put $t=0$, W reduces to that of the spherical approximation. The terms dependent on the variable t originate from the divison of the space by planes $\sum x_r = L_1 = Nt$. The constant a_{11} is to be computed from the relation



Comparison of specific heat curves given by
Onsager's exact method ————
Mean field approximation ....
Spherical approximation —·—·—
Present method – – – –

$$\frac{1}{a_{11}}=\sigma_{11}=\frac{1}{N}\sum_{\mathrm{r},\mathrm{r}'}\left(\frac{1}{s-K}\right)_{\mathrm{rr}'}.$$

For the nearest neighbor interaction, non-zero element of the interaction matrix $K(\mathrm{r}-\mathrm{r}')$ are

$$K(1,0)=K(-1,0)=K(0,1)=K(0,-1)=K.$$

We have then

$$\lambda=2K(\cos\theta_1+\cos\theta_2), \qquad \lambda_0=4K$$

$$\sigma_{11}=\frac{1}{a_{11}}=\frac{1}{s-\lambda_0}.$$

Putting $s=\lambda_0 y$, we have

$$\langle\log(s-\lambda)\rangle=\log\lambda_0+C(y),$$

$$C(y)=\left\langle\log\left(y-\frac{\cos\theta_1+\cos\theta_2}{2}\right)\right\rangle$$

$$=\frac{1}{\pi^2}\int_0^\pi\int_0^\pi\log\left(y-\frac{\cos\theta_1+\cos\theta_2}{2}\right)d\theta_1 d\theta_2$$

$$C'(y)=\frac{2}{\pi}\frac{1}{y}K\left(\frac{1}{y}\right),$$

$K(x)$ denoting the complete elliptic integral of modulus x.

In the figure we show the specific heat curves obtained by the exact method of Onsager,[3] the spherical approximation, the mean field approximation and our method. While the spherical approximation predicts no phase transition, our method gives a phase transition in the vicinity of the point where the exact method predicts a phase transition.

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