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The Spherical Model of a Ferromagnet*†

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A mathematical model, the spherical model, of a ferromagnet is described. The model is a generalization of the Ising model; and one-, two-, and three-dimensional lattices of infinite extent can be extensively discussed. A three-dimensional lattice shows ferromagnetic behavior and provides a statistical model of the Weiss phenomenological theory. The limiting free energy appears in a form which contains two of the essential features of the exactly known Ising model results in one and two dimensions. This suggests the probable form of the limiting free energy for the three-dimensional Ising model. A simplified model, the Gaussian model, is briefly discussed because this model also contains some of the significant features of the Ising model. However, the Gaussian model, unlike the spherical model, is not defined for all temperatures.

INTRODUCTION

THE subtlety and difficulty of the theoretical problem of the phase transition of a ferromagnet has been well established by the work of Bloch, Kramers, Heisenberg, and Onsager. In fact, the only nontrivial systems exhibiting a phase transition which can be exactly discussed are the Bose-Einstein gas and the two-dimensional Ising model of a ferromagnet. One may also include the work on the condensation of a non-ideal gas by Mayer and by Kahn and Uhlenbeck.

The problems are purely statistical mechanical, and the idealizations of the underlying physical problems are readily formulated. All that remains is the explicit evaluation of the partition function (even if only in the limiting case of an infinite number of particles). This evaluation is, of course, the difficulty.

There does not appear to be any single technique of sufficient generality which can be applied to the evaluation of partition functions. This lack of a general technique is very apparent now because of the work of Onsager on the Ising model. Onsager evaluated the partition function of the two-dimensional Ising model by an algebraic technique.[1] This method, a magnificent achievement, is apparently restricted to the two-dimensional case. Nevertheless, the situation that presents itself is that no analytical method is available for the Ising model, whereas the Bose-Einstein condensation is demonstrated by a purely analytical method and the appropriate algebra is not available.

The partition function is the result of a generally complicated interplay between the Boltzmann factor and the weighting factor. One can expect that the characteristics of either factor may be responsible for a transition or the characteristics of both factors may be required. It is difficult to separate the relative importance of these factors with respect to their influence for a transition and also to discover the derivation of particular features of a transition. For the Bose-Einstein gas, condensation occurs in three dimensions but not in one or two dimensions. In this case, the transition can be ascribed to the weighting of the momentum states for the given Boltzmann factor.

We agree with Onsager that it is desirable to investigate models which yield to exact analysis and show transition phenomena. It is irrelevant that the models may be far removed from physical reality if they can illuminate some of the complexities of the transition phenomena.

We shall analyze two mathematical models: the Gaussian model, and the spherical model. These models

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[1] L. Onsager, Phys. Rev. 65, 117 (1944).

are continuum modifications of the Ising model of a ferromagnet. Montroll[2] has formulated more general continuum models in the hope that they will converge on the Ising model. The low temperature features of continuum models are obviously spurious. Nevertheless, we do not consider this aspect as detrimental to the discussion of possible transition phenomena. The Gaussian model becomes invalid for temperatures below a certain critical temperature (the partition function becomes complex). The reason for this behavior will become apparent, but it is surprising that the Gaussian model exhibits some of the general features of the exactly calculated one- and two-dimensional Ising models. The spherical model is a valid model for all temperatures. The one- and two-dimensional models do not exhibit transitions, whereas the three-dimensional model does. This model, in fact, can be regarded as a model for the Weiss phenomenological theory of ferromagnetism.

THE ISING MODEL

It is assumed that there is a spin at each site of a regular lattice of N sites. The interaction energy between neighboring spins may be written as $-J\epsilon_i\epsilon_j$, where J is the interaction energy and each spin can take on the discrete values ± 1. The partition function, normalized to unity, is

$$Q_N(I)=2^{-N}\sum_{\{\epsilon_j=\pm 1\}}\exp[(J/kT)\textstyle\sum'\epsilon_i\epsilon_j], \quad (1)$$

where $\{\epsilon_j\}$ denotes a given configuration of spins and $\sum'$ denotes the sum over nearest neighbors. If we write $K=J/2kT$,

$$Q_N(I)=2^{-N}\sum_{\{\epsilon_j=\pm 1\}}\exp[K\sum_{i,j}{}'\epsilon_i\epsilon_j], \quad (2)$$

with $\sum_{i,j}{}'$ counting a given i, j twice, that is the matrix of the quadratic form is symmetric.

We are essentially interested in the limiting free energy per particle which means that

$$-\psi/kT=\lim_{N\to\infty}N^{-1}\ln Q_N(I) \quad (3)$$

THE GAUSSIAN MODEL

This model assumes that the probability of finding a given spin ϵ_j between ϵ_j and $\epsilon_j+d\epsilon_j$ is given by

$$(2\pi)^{-\frac{1}{2}}\exp[-\epsilon_j^2/2]d\epsilon_j. \quad (4)$$

The model simulates the Ising model insofar as $\langle\epsilon_j\rangle=0$ and $\langle\epsilon_j^2\rangle=1$.

The normalized partition function is

$$Q_N(G)=(2\pi)^{-N/2}\int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N \times\exp[-\tfrac{1}{2}\sum_{j=1}^{N}\epsilon_j^2+K\sum_{i,j}{}'\epsilon_i\epsilon_j]. \quad (5)$$

[2] E. W. Montroll, Nuovo cimento **VI**, 264 (1949).

Assuming that the quadratic form is negative definite,

$$Q_N(G)=\prod_{p=1}^{N}(1-2K\lambda_p)^{-\frac{1}{2}} =\exp[-\tfrac{1}{2}\sum_{p=1}^{N}\ln(1-2K\lambda_p)], \quad (6)$$

where λ_p is given in Appendix A for the several simple lattices. The free energy per particle is then, in the limit,

$$-\frac{\psi}{kT}=\lim_{N\to\infty}\left[-\frac{1}{2N}\sum_{p=1}^{N}\ln(1-2K\lambda_p)\right]. \quad (7)$$

The limit of the above sum over the characteristic values is discussed in Appendix B. The following results are obtained.

One-dimensional lattice:

$$-\frac{\psi}{kT}=-\frac{1}{2}\cdot\frac{1}{2\pi}\int_0^{2\pi}d\omega_1\ln[1-4K\cos\omega_1]; \quad (8a)$$

Two-dimensional square lattice:

$$-\frac{\psi}{kT}=-\frac{1}{2}\cdot\frac{1}{(2\pi)^2}\int_0^{2\pi}\int d\omega_1 d\omega_2 \times\ln[1-4K(\cos\omega_1+\cos\omega_2)]; \quad (8b)$$

Three-dimensional cubic lattice:

$$-\frac{\psi}{kT}=-\frac{1}{2}\cdot\frac{1}{(2\pi)^3}\int_0^{2\pi}\int\int d\omega_1 d\omega_2 d\omega_3 \times\ln[1-4K(\cos\omega_1+\cos\omega_2+\cos\omega_3)]. \quad (8c)$$

It is to be noticed that these results break down at a critical K which is $K_c=1/4n$, where n is the dimensionality of the lattice. For temperatures smaller than the critical temperature, the model is not defined since the free energy becomes complex. The source of this difficulty is obvious. Inspection of the characteristic values of the quadratic form shows that the form is not definite. Consequently, $Q_N(G)$ diverges for $T<T_c$.

This failure of the Gaussian model is trivial and is not the point. What is of interest is the comparison with the known results for the one- and two-dimensional Ising models.

One-dimensional Ising:

$$-\frac{\psi}{kT}=\frac{1}{2}\cdot\frac{1}{2\pi}\int_0^{2\pi}d\omega_1\ln[\cosh 4K-\sinh 4K\cos\omega_1]; \quad (9a)$$

Two-dimensional Ising:

$$-\frac{\psi}{kT}=\frac{1}{2}\cdot\frac{1}{(2\pi)^2}\int_0^{2\pi}\int d\omega_1 d\omega_2 \times\ln[\cosh^2 4K-\sinh 4K(\cos\omega_1+\cos\omega_2)]. \quad (9b)$$

The comparison is striking in the closeness in the formal structure of the expressions for ψ. The two features are the appearance of the logarithmic form and the structure of the cosines. The source of the formal appearance of the Ising model results is not clear. But the source is clear in the Gaussian model. The number and structure of the cosine terms arise from the "periodicity" in the interaction matrix. This periodicity is not simply due to the number of nearest neighbors because, for example, a doubly periodic interaction matrix is obtained for a plane regardless of the number of nearest neighbor interactions. Furthermore, we note that for a two-dimensional hexagonal lattice the structure of the cosine terms, easily obtained for the Gaussian and spherical models, is precisely that obtained by use of Onsager's method.

We shall now proceed to discuss the spherical model which retains the important formal features of the Gaussian model, but which also has the advantage of being valid for all temperatures.

THE SPHERICAL MODEL

A way of geometrically describing this model is the following. Let us suppose that we have N spins ϵ_j with $j=1, 2, \cdots, N$. Construct an N-dimensional cartesian space. A point P in this space is represented by the set of N coordinates $\{\epsilon_j\}$. The point P represents a spin configuration of the Ising model if $\epsilon_j=\pm 1$ for all j. The 2^N configurations in the Ising model are the vertices of an N-dimensional cube. Suppose that an N-dimensional sphere is circumscribed about the hypercube. The radius of this sphere is $N^{\frac{1}{2}}$, and the points on the sphere are given by the equation

$$\epsilon_1^2+\epsilon_2^2+\cdots+\epsilon_N^2=N. \tag{10}$$

The spherical model allows every point on this sphere to be an acceptable configuration. The model is a step closer to the Ising model than was the Gaussian model in that not only is $\langle\epsilon_j^2\rangle=1$, but also

$$\sum_{j=1}^{N}\epsilon_j^2=N$$

for every configuration. Furthermore, the interaction energy can now be replaced by a definite quadratic form so that a partition function valid for all temperatures is obtainable.

There are obvious defects in a continuum model. The entropy at absolute zero is infinite and the specific heat per particle is finite rather than zero. These defects, however, should not distract one's interest from the transition mechanism.

One can also raise the question that the spherical condition (10) allows configurations wherein a small number of spins can be very large, since $|\epsilon_j|\leq N^{\frac{1}{2}}$, so that these configurations could contribute a large magnetic moment to the system. It will be shown later that such states are not responsible for the behavior of the model. In fact, condition (10) implies that fluctuations are small.

The partition function for the spherical model is

$$Q_N(S)=A_N^{-1}\underset{\sum_{j=1}^{N}\epsilon_j^2=N}{\int\cdots\int} d\epsilon_1\cdots d\epsilon_N \exp[K\sum_{i,j}{}'\,\epsilon_i\epsilon_j], \tag{11}$$

where

$$A_N=\underset{\sum_{j=1}^{N}\epsilon_j^2=N}{\int\cdots\int} d\epsilon_1\cdots d\epsilon_N=2\pi^{N/2}N^{\frac{1}{2}(N-1)}/\Gamma(N/2). \tag{12}$$

There are various ways of evaluating the multiple integral. One can use the method of von Neumann,[3] one can use the Dirichlet factor[2] to remove the condition on the variables, or one can most conveniently use the delta function to evaluate the integral. The integral is evaluated using the delta function technique in Appendix C, where the details are also discussed.

If we let n denote the dimensionality of the simple lattices, then the result of the evaluation in the limit of $N\rightarrow\infty$ is that

$$-\psi_n/kT=-\tfrac{1}{2}-\tfrac{1}{2}\ln 4K+2Kz_s-\tfrac{1}{2}f_n(z_s), \tag{13}$$

where ψ_n is the limiting free energy per particle. The parameter z_s is the saddle point of the steepest descent evaluation of the partition function. It is the solution of

$$4K=[df_n(z)/dz]_{z=z_s}. \tag{14}$$

A solution $z_s(K)$ is possible for all temperatures for $n=1$ and 2. The reason for this is that the right side of Eq. (14) approaches infinity as z_s approaches the branch point of $f_1(z)$ and $f_2(z)$. Therefore ψ_1 and ψ_2 are regular functions of T and no transitions are obtained. In the three-dimensional lattice, the right side of Eq. (14) has a finite value, called $4K_c$, when $z_s=3$, the branch point of $f_3(z)$. For $T<T_c$, or $K>K_c$, the new path of steepest descent has a cusp at $z=3$. Then for $T<T_c$, ψ_3 is given by Eq. (13) when we put $z_s\equiv 3$. This "sticking" of the saddle point corresponds to a phase transition. The phase transition corresponds thermodynamically to a discontinuity in the temperature coefficient of the specific heat.

If we let U_n, C_n denote the internal energy per particle and specific heat per particle, respectively, for an n-dimensional simple lattice, $n=1, 2, 3$, then

$$U_n=\tfrac{1}{2}J\frac{d}{dK}(\psi_n/kT);\quad C_n=-kK^2\frac{d^2}{dK^2}(\psi_n/kT). \tag{15}$$

[3] J. von Neumann, Ann. Math. Stat. 12, 367 (1941), in particular pp. 372–374.

Now

$$\frac{d}{dK}(\psi_n/kT)=\frac{\partial}{\partial K}(\psi_n/kT)$$
$$+\frac{dz_s}{dK}\frac{\partial}{\partial z_s}(\psi_n/kT)=\frac{\partial}{\partial K}(\psi_n/kT). \quad (16)$$

The last equality is true since $(\partial/\partial z_s)(\psi_n/kT)$ vanishes when the saddle point exists. In the case $n=3$, $T<T_c$, then $z_s=3$ and is independent of K so that dz_s/dK vanishes. We then have

$$\frac{d}{dK}(\psi_n/kT)=\frac{1}{2K}-2z_s,\ \frac{d^2}{dK^2}(\psi_n/kT)=-\frac{1}{2K^2}-2\frac{dz_s}{dK}. \quad (17)$$

Consequently,

$$U_n=J[(1/4K)-z_s], \quad (18)$$

and

$$C_n=\tfrac{1}{2}k[1+4K^2dz_s/dK]. \quad (19)$$

It is clear from the analysis that z_s is a continuous function of T so that U_n is continuous. It is shown in Appendix C that dz_s/dK is a continuous function of T and vanishes at T_c when $n=3$. Hence, C_n is a continuous function of T approaching $\frac{1}{2}k$ as T approaches absolute 0. However, for $n=3$, $C_3=\frac{1}{2}k$, for $T<T_c$, and it is shown in Appendix C that d^2z_s/dK^2 is discontinuous at $T=T_c$. Thus, C_3 has a break in slope at the critical temperature. A sketch of the behavior is shown in Fig. 1.

The mechanical nature of the transition may be elucidated without difficulty. We shall show that the transition corresponds to spontaneous magnetization.

If μ_0 denotes the magnetic moment associated with a single spin, then the magnetic moment per particle of a given spin configuration, μ, is given by

$$\mu=(\mu_0/N)\sum_{j=1}^{N}\epsilon_j. \quad (20)$$

The magnetic susceptibility is given by

$$\chi=(N/kT)\langle\mu^2\rangle. \quad (21)$$

We now compute $\langle\mu^2\rangle$. Using the orthogonal transformation of the variables $\{\epsilon_j\}$ to the variables $\{y_j\}$ discussed in Appendix A, we note that

$$y_1=N^{-\frac{1}{2}}\sum_{j=1}^{N}\epsilon_j.$$

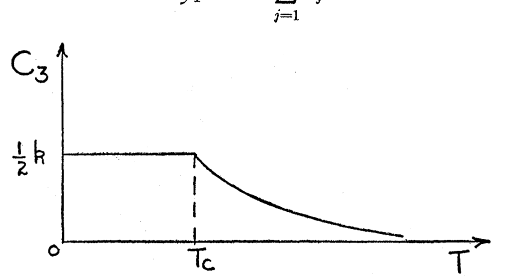

FIG. 1. The specific heat per particle *versus* temperature.

Therefore, using $Q_N(S)$ as given in Appendix C, Eqs. (C3) and (C4), we have

$$\mu=N^{-\frac{1}{2}}\mu_0y_1,\quad \chi=(\mu_0^2/kT)\langle y_1^2\rangle,$$

$$\langle y_1^2\rangle=Q_N^{-1}(S)A_N^{-1}\frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty}ds$$
$$\times\exp[Ns]\int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_Ny_1^2$$
$$\times\exp[-\sum_{j=1}^{N}(s-K\lambda_j)y_j^2]. \quad (22)$$

Hence,

$$\langle y_1^2\rangle\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}$$
$$=\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz(4K)^{-1}(z-\tfrac{1}{2}\lambda_1)^{-\frac{3}{2}}e^{Ng(z)}. \quad (23)$$

Whenever a normal saddle point z_s exists, then

$$\langle y_1^2\rangle=1/[4K(z_s-\tfrac{1}{2}\lambda_1)];\quad \chi=\mu_0^2/[2J(z_s-\tfrac{1}{2}\lambda_1)]. \quad (24)$$

We see that $\chi\rightarrow\infty$ when $z_s\rightarrow\frac{1}{2}\lambda_1$. In the one- and two-dimensional lattices, $T=0$ corresponds to $z_s=\frac{1}{2}\lambda_1$. In the three-dimensional lattice,

$$\chi=\mu_0^2/[2J(z_s-3)], \quad (25)$$

for $T>T_c$, and χ is infinite at the transition temperature. This result implies the finiteness of μ for $T<T_c$. We shall compute this magnetic moment. Because of the directional symmetry of the model $\langle\mu\rangle=0$, we therefore calculate

$$\langle|\mu|\rangle=N^{-\frac{1}{2}}\mu_0\langle|y_1|\rangle. \quad (26)$$

With the procedure used above,

$$\langle|y_1|\rangle\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}$$
$$=\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz(2\pi K)^{-\frac{1}{2}}(z-\tfrac{1}{2}\lambda_1)^{-1}e^{Ng(z)}. \quad (27)$$

When the normal saddle point exists, then

$$\langle|y_1|\rangle=[2\pi K(z_s-\tfrac{1}{2}\lambda_1)]^{-\frac{1}{2}},$$
$$\langle|\mu|\rangle=\mu_0[N2\pi K(z_s-\tfrac{1}{2}\lambda_1)]^{-\frac{1}{2}}\rightarrow 0, \quad (28)$$

in the limit $N\rightarrow\infty$. Hence, in the limit $N\rightarrow\infty$, $\langle|\mu|\rangle=0$ for the one- and two-dimensional models and also in the three-dimensional model for $T>T_c$.

For $T<T_c$, the numerator of Eq. (27) must be reconsidered. In the numerator, we note that the branch point, $z=3$, of the integrand is also a pole. Consequently, the contribution to the integral is obtained

from the infinitesimally small circle about the pole. The path of integration is shown in Fig. 2. We then find that for $T<T_c$,

$$\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-3)^{-1}e^{Ng(z)}\simeq e^{Ng(3)}, \tag{29}$$

and

$$\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-3)^{-\frac{1}{2}}e^{Ng(z)}\simeq[N2\pi(K-K_c)]^{-\frac{1}{2}}e^{Ng(3)}.$$

Therefore,

$$\begin{aligned}\langle|y_1|\rangle&=N^{\frac{1}{2}}[1-K_c/K]^{\frac{1}{2}};\\ \langle|\mu|\rangle&=\mu_0[1-K_c/K]^{\frac{1}{2}}=\mu_0[1-T/T_c]^{\frac{1}{2}}.\end{aligned} \tag{30}$$

This result proves the onset of spontaneous magnetization at the transition temperature T_c.

The possibility remains that the magnetization is due to a few spins taking on abnormally large values of the order $N^{\frac{1}{2}}$. We now show this possibility is not real by means of a calculation of the correlation between two spins.

The correlation C_{jk} between two spins ϵ_j, ϵ_k situated at the jth and kth lattice sites, respectively, is defined as

$$C_{jk}=\langle\epsilon_j\epsilon_k\rangle/\langle\epsilon_j^2\rangle^{\frac{1}{2}}\langle\epsilon_k^2\rangle^{\frac{1}{2}}. \tag{31}$$

Since the spherical condition, Eq. (10), requires $\langle\epsilon_j^2\rangle=1$ for all j, $C_{jk}=\langle\epsilon_j\epsilon_k\rangle$. In terms of the variables $\{y_j\}$,

$$\epsilon_j\epsilon_k=\left(\sum_{s=1}^{N} V_{js}y_s\right)\left(\sum_{t=1}^{N} V_{kt}y_t\right),$$

so that

$$C_{jk}=\sum_{s,t} V_{js}V_{kt}\langle y_sy_t\rangle.$$

However, $\langle y_sy_t\rangle=0$ unless $s=t$ because of the symmetry of the model. Thus,

$$C_{jk}=\sum_{s=1}^{N} V_{js}V_{ks}\langle y_s^2\rangle. \tag{32}$$

It is clear from Eq. (22) that

$$\begin{aligned}\langle y_s^2\rangle&\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}\\ &=\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz[4K(z-\tfrac{1}{2}\lambda_s)]^{-1}(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}.\end{aligned} \tag{33}$$

Consequently,

$$\begin{aligned}C_{jk}&\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}\\ &=\frac{(4K)^{-1}}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dzF_{jk}(z)(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)},\end{aligned} \tag{34}$$

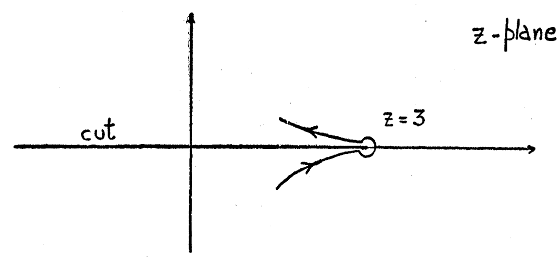

FIG. 2. The path of integration for $T<T_c$.

where

$$F_{jk}(z)=\sum_{s=1}^{N} V_{js}V_{ks}/(z-\tfrac{1}{2}\lambda_s).$$

The evaluation of a function such as F_{jk} as N becomes very large is described in Appendix B. We may write that

$$F_{jk}(z)=\frac{1}{N(z-3)}+\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi} d\omega_1d\omega_2d\omega_3 \times\frac{\cos(x'\omega_1/a+y'\omega_2/a+z'\omega_3/a)}{z-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}. \tag{35}$$

We now see that for $T>T_c$,

$$C_{jk}=\frac{(4K)^{-1}}{(2\pi)^3}\int\int\int_0^{2\pi} d\omega_1d\omega_2d\omega_3 \times\frac{\cos(x'\omega_1/a+y'\omega_2/a+z'\omega_3/a)}{z_s-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}. \tag{36}$$

Note that $C_{jj}=\langle\epsilon_j^2\rangle=1$ and from the above equation, putting $x'=y'=z'=0$,

$$C_{jj}=\frac{(4K)^{-1}}{(2\pi)^3}\int\int\int_0^{2\pi} \frac{d\omega_1d\omega_2d\omega_3}{z_s-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}=1,$$

because this is the equation determining z_s.

It is also apparent that as (x', y', z') increase, C_{jk} decreases so that the correlation monotonically approaches zero as the distance between spins increases.

For $T<T_c$ a closer examination is required because the first term in $F_{jk}(z)$ is a pole at $z=3$. However, since the integral part converges at $z=3$, this part is the same as Eq. (36) with $z_s=3$. A straightforward evaluation yields

$$\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz[N(z-3)]^{-1}(z-3)^{-\frac{1}{2}}e^{Ng(z)} \simeq4\left[\frac{(K-K_c)}{2\pi N}\right]^{\frac{1}{2}}e^{Ng(z)}. \tag{37}$$

We consequently find that

$$C_{jk}=1-\frac{T}{T_c}+\frac{(4K)^{-1}}{(2\pi)^3}\int\int_0^{2\pi}\int d\omega_1 d\omega_2 d\omega_3 \times\frac{\cos(x'\omega_1/a+y'\omega_2/a+z'\omega_3/a)}{3-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}. \quad (38)$$

This result demonstrates that below the transition temperature an extended correlation exists of magnitude $1-T/T_c$. Superimposed on the correlation extending over the whole lattice is a correlation monotonically decreasing with increasing distance.

As a check on this result we note that

$$C_{jj}=1-\frac{T}{T_c}+\frac{(4K)^{-1}}{(2\pi)^3}\int\int_0^{2\pi}\int\frac{d\omega_1 d\omega_2 d\omega_3}{3-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}.$$

However, we have defined K_c so that

$$4K_c\equiv\frac{1}{(2\pi)^3}\int\int_0^{2\pi}\int\frac{d\omega_1 d\omega_2 d\omega_3}{3-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}.$$

Hence,

$$C_{jj}=1-T/T_c+4K_c/4K=1.$$

The integrals are readily evaluated in the case of the one-dimensional lattice. We have then for all T,

$$C_{jk}=\frac{(4K)^{-1}}{2\pi}\int_0^{2\pi}d\omega_1\frac{\cos(x'\omega_1/a)}{z_s-\cos\omega_1}.$$

This gives

$$C_{jk}=[z_s-(z_s^2-1)^{\frac{1}{2}}]^{x'/a}/4K(z_s^2-1)^{\frac{1}{2}} =[z_s-(z_s^2-1)^{\frac{1}{2}}]^{x'/a}, \quad (39)$$

since $4K(z_s^2-1)^{\frac{1}{2}}=1$. Thus the correlation falls off with distance exponentially.

The connection between the spherical and Gaussian models is rather transparent. In the spherical model, if we ask for the distribution of a finite number of spins, that is, a number independent of N for large N, then this distribution is Gaussian, at least above the transition temperature. The spherical condition forces a cooperation among the spins which does not exist in the Gaussian model. Therefore, deviations from a Gaussian distribution are obtained when the cooperation sets in, that is, below the transition temperature. We can see this by means of a calculation of $\langle\epsilon_j^4\rangle$.

A Gaussian distribution of ϵ_j with $\langle\epsilon_j\rangle=0$, $\langle\epsilon_j^2\rangle=1$, yields $\langle\epsilon_j^4\rangle=3$. In the spherical model,

$$\langle\epsilon_j^4\rangle=\left\langle\left[\sum_{s=1}^N V_{js}y_s\right]^4\right\rangle =\sum_{s=1}^N V_{js}^4\langle y_s^4\rangle+3\sum_{r\neq s}V_{js}^2V_{jr}^2\langle y_s^2y_r^2\rangle, \quad (40)$$

because the average of odd powers of the y's vanishes. Then

$$\langle\epsilon_j^4\rangle\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz(z-3)^{-\frac{1}{2}}e^{Ng(z)}=\frac{3}{16K^2}\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz \times\left[\sum_{s=1}^N V_{js}^2(z-\tfrac{1}{2}\lambda_s)^{-1}\right]^2(z-3)^{-\frac{1}{2}}e^{Ng(z)}. \quad (41)$$

However,

$$\sum_{s=1}^N V_{js}^2(z-\tfrac{1}{2}\lambda_s)^{-1}=\frac{1}{N(z-3)} +\frac{1}{(2\pi)^3}\int\int_0^{2\pi}\int\frac{d\omega_1 d\omega_2 d\omega_3}{z-(\cos\omega_1+\cos\omega_2+\cos\omega_3)} \quad (42)$$

for the simple three-dimensional lattice.

When $T>T_c$, $(K<K_c)$, a normal saddle point exists and we may use

$$\sum_{s=1}^N V_{js}^2(z_s-\tfrac{1}{2}\lambda_s)^{-1}=4K. \quad (43)$$

Consequently $\langle\epsilon_j^4\rangle=3$ for $T>T_c$. (44)

Below the transition temperature the integral in Eq. (42) is finite and we may use

$$\sum_{s=1}^N V_{js}^2(z-\tfrac{1}{2}\lambda_s)^{-1}=\frac{1}{N(z-3)}+4K_c. \quad (45)$$

It is then found that

$$\langle\epsilon_j^4\rangle=3-2(1-T/T_c)^2 \quad \text{for} \quad T<T_c. \quad (46)$$

Note that at $T=0$, $\langle\epsilon_j^4\rangle=1$, which is as it should be because all the spins are lined up. Equation (46), by showing that $\langle\epsilon_j^4\rangle$ is finite, proves (along with the correlation) that configurations in which a small number of spins have moments of the order $N^{\frac{1}{2}}$ are not responsible for the behavior of the spherical model.

In concluding this section we wish to point out that we may write the limiting free energy per particle for the spherical model in the form

$$-\frac{\psi_n}{kT}=-\frac{1}{2}\cdot\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int d\omega_1\cdots d\omega_n \times[F(T)-G(T)\sum_{j=1}^n\cos\omega_j], \quad (47)$$

where $F=z_sG$, $G=4Ke^{1-4kz_s}$, and n is the dimensionality of the simple lattice.

The analogy with the Ising model solutions is close. Furthermore, we have noted that the structure of the cosine terms in the integrand is simply determined from the cyclized interaction energy matrix of the Boltzmann factor. If we consider a two-dimensional hexagonal lattice with six nearest neighbors, then we easily find that, with $n=2$, the cosine terms $[\cos\omega_1+\cos\omega_2]$ for the square lattice are replaced by $[\cos\omega_1+\cos\omega_2+\cos(\omega_2-\omega_1)]$.

These same cosine terms were found by Onsager in his solution of the corresponding Ising model. It may then be conjectured that the solution of the three-dimensional simple cubic Ising model is of the form

$$-\frac{\psi_3}{kT}=\frac{1}{2}\cdot\frac{1}{(2\pi)^3}\iiint_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times\ln[F(T)-G(T)(\cos\omega_1+\cos\omega_2+\cos\omega_3)], \quad (48)$$

where $F(T)$, $G(T)$ are the appropriate functions of temperature.

THE SPHERICAL MODEL IN AN HOMOGENEOUS MAGNETIC FIELD

Let us assume that the lattice is in an homogeneous magnetic field of strength H and that the direction of the spins is in the direction of the magnetic field. Then the additional energy of the system is

$$-H\mu_0\sum_{j=1}^{N}\epsilon_j=-N^{\frac{1}{2}}H\mu_0 y_1. \quad (49)$$

This then yields for the partition function

$$Q_{NH}(S)=\frac{A_N^{-1}}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} ds\exp[Ns]\int\cdots\int_{-\infty}^{\infty} dy_1\cdots dy_N \times\exp\left[-\sum_{j=1}^{N}(s-K\lambda_j)y_j^2+2N^{\frac{1}{2}}My_1\right], \quad (50)$$

with $M=\mu_0 H/2kT$.

The integration of y_1 introduces a new factor $\exp[NM^2/(s-K\lambda_1)]$. This then gives

$$-\psi_n(H)/kT=-\tfrac{1}{2}-\tfrac{1}{2}\ln 4K+2Kz_s -\tfrac{1}{2}f_n(z_s)+M^2/2K(z_s-\tfrac{1}{2}\lambda_1), \quad (51)$$

where the saddle point $z_s(K, H)$ is given by

$$4K=[df_n(z)/dz]_{z=z_s}+M^2/[K(z_s-\tfrac{1}{2}\lambda_1)^2]. \quad (52)$$

We see immediately that for $M\neq 0$, a normal saddle point always exists because the M dependent term approaches ∞ as z_s approaches $\frac{1}{2}\lambda_1=n$. This means that a magnetic field destroys the transition to a spontaneously magnetized state for the three-dimensional lattice.

The mean magnetic moment per particle is $\langle\mu\rangle=\mu_0 N^{-\frac{1}{2}}\langle y_1\rangle$. Since a normal saddle point always exists, we easily find that

$$\langle y_1\rangle=\frac{N^{\frac{1}{2}}M}{2K(z_s-\frac{1}{2}\lambda_1)}=\tfrac{1}{2}N^{\frac{1}{2}}\frac{\partial}{\partial M}(-\psi_n/kT), \quad (53)$$

so that

$$\langle\mu\rangle=\mu_0 M/[2K(z_s-n)]=H\mu_0^2/[2J(z_s-n)], \quad (54)$$

and we have the magnetic equation of state for the model through Eqs. (51), (52), and (54). The magnetic susceptibility per particle is

$$\chi=\langle\mu\rangle/H=\mu_0^2/[2J(z_s-n)]. \quad (55)$$

The high temperature and saturation behavior of $\langle\mu\rangle$, χ, is precisely as expected. In fact, this model provides a mechanism for and essentially the formulas of the Curie-Weiss phenomenological theory of ferromagnetism.

In the Curie-Weiss theory,

$$\chi=T_c^*/[\alpha^*(T-T_c^*)], \quad (56)$$

where T_c^* is the transition temperature and α^* is a parameter controlling the strength of the local field. (α^* is chosen to enable the theory to fit the experimental data.)

Putting Eq. (55) in a form similar to that of Eq. (56), we find that, with $n=3$,

$$\chi=T_c/\alpha[h(T)T-T_c], \quad (57)$$

where

$$\alpha=6J/\mu_0^2,\quad h(T)=T_c z_s/3T.$$

The quantity α is to be identified with α^*. According to the Curie-Weiss theory, $T_c^*=6J/k$. The present model yields $T_c\simeq 6J/1.5k$. If we set $T_c^*=\gamma T_c$, then

$$\chi=T_c^*/\alpha[\gamma h(T)T-T_c^*]. \quad (58)$$

We find that for $T_c\leqslant T<\infty$, $3/2\geqslant\gamma h(T)\geqslant 1$, so that the spherical model yields a slightly modified Curie-Weiss formula for the case of zero magnetic field strength. Equation (57) holds for all field strengths when z_s is determined by Eq. (52).

DISCUSSION

The virtue of the spherical model of a ferromagnet is that its properties can be rather extensively discussed and that a three-dimensional lattice has ferromagnetic properties. It is of further interest that the model provides a classical mechanism for the Weiss phenomenological theory.

With respect to the physical ferromagnet, the model has nothing to say positively. We may briefly consider, however, the bearing of our results on the nature of the transition.

The Bloch spin wave theory, which is valid near saturation or low temperature, has the result that a two-dimensional net is nonferromagnetic and a three-dimensional lattice is ferromagnetic. The spherical model yields the same result. On the other hand, the two-dimensional Ising model is ferromagnetic.

A recent paper by Herring and Kittel[4] illuminates the Ising model transition. These authors discussed a phenomenological theory based on the spin-wave treatment

[4] C. Herring and C. Kittel, Phys. Rev. 81, 869 (1951).

and they demonstrate that ferromagnetism may be induced in a two-dimensional lattice by the presence of anisotropic interactions. This they suggest, lies behind the Ising transition. The spherical model weakens the anisotropy of the Ising model, and, in fact, has destroyed the transition in the two-dimensional lattice.

One might now infer that although the three-dimensional Ising model certainly will provide a transition, this transition may still be more descriptive of the anisotropy of the Ising model rather than descriptive of the transition in an ideal isotropic ferromagnet. It is more likely that the spherical model transition is closer to the actual transition behavior.

There is a further feature of the spherical model which is probably of significance. The point in question is also shown by the Gaussian model. Comparing, say, Eq. (8) with (11), note that the Gaussian model (and the spherical model) have a minus sign before the integral representation, whereas the Ising model has a plus sign. Although the minus sign can be converted into a plus sign by an appropriate transformation, it is true that the conversion is not unique. We cannot throw any light on this point, but it may be indicative of an essential difference between the transition mechanisms of the two models (spherical and Ising).

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APPENDIX A. ON THE QUADRATIC FORM $\sum_{i,j}'\varepsilon_i\varepsilon_j$

It will be convenient to set down here properties associated with the quadratic form describing the interaction energy which will be useful in the body of the paper. The properties are all connected with the diagonalization of the quadratic form. Since the form is symmetric, its diagonalization is always possible by means of an orthogonal transformation.

It is also particularly convenient to make the matrix of the coefficients of the form cyclic. Cyclization is achieved by postulating an appropriate periodicity. In a one-dimensional lattice, the chain is bent into a ring so that the Nth site is a nearest neighbor of the 1st site. In two dimensions, the simple lattice is constructed on a torus. These are the obvious geometrical representations.

Consider first the cyclic matrix $M(c_1, c_2, \cdots, c_N)$.

$$M\equiv\begin{Bmatrix} c_1 & c_2 & c_3 & \cdots & c_{N-1} & c_N \\ c_N & c_1 & c_2 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_N & c_1 & \cdots & c_{N-3} & c_{N-2} \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot \\ c_2 & c_3 & c_4 & \cdots & c_N & c_1 \end{Bmatrix}. \tag{A1}$$

We wish to find the characteristic values and vectors associated with M, that is

$$MV=\lambda V. \tag{A2}$$

For the characteristic values we must solve the equation

$$|M(c_1-\lambda, c_2, \cdots, c_N)|=0. \tag{A3}$$

Following Kowaleski,[5] let $r_1, r_2, \cdots, r_N$ denote the N roots of unity and we shall choose

$$r_k=\exp[2\pi i(k-1)/N].$$

Construct the determinant

$$\Delta\equiv\begin{vmatrix} 1 & 1 & \cdots & 1 \\ r_1 & r_2 & \cdots & r_N \\ r_1^2 & r_2^2 & \cdots & r_N^2 \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ r_1^{N-1} & r_2^{N-1} & \cdots & r_N^{N-1} \end{vmatrix}\neq 0. \tag{A4}$$

We next form the product $|M|\Delta\equiv|P_{jk}|$. Now

$$P_{jk}=\sum_{s=1}^{N} M_{js}r_k^{s-1}.$$

But $M_{js}=c_{N-j+1+s}$, where we define $c_{N+s}\equiv c_s$. Hence, if we define

$$f(r_k)=\sum_{s=1}^{N} c_s r_k^{s-1}, \tag{A5}$$

then

$$P_{jk}=\sum_{s=1}^{N} c_{N-j+1+s}r_k^{s-1}=r_k^{j-1}f(r_k). \tag{A6}$$

It is apparent that

$$|P_{jk}|=\Delta\prod_{k=1}^{N} f(r_k),$$

so that

$$|M|=\prod_{k=1}^{N} f(r_k). \tag{A7}$$

This immediately yields the result that

$$\lambda_k=f(r_k). \tag{A8}$$

Let V_{ks} denote the sth component of the characteristic vector belonging to λ_k. Then, from (A2),

$$\sum_{s=1}^{N} c_{N-j+1+s}V_{ks}=\lambda_k V_{kj}. \tag{A9}$$

If we set $V_{ks}=\alpha r_k^{s-1}$, then

$$\alpha\sum_{s=1}^{N} c_{N-j+1+s}r_k^{s-1}=\alpha\lambda_k r_k^{j-1}.$$

Since the left sum is $r_k^{j-1}f(r_k)=r_k^{j-1}\lambda_k$, we have deter-

[5] G. Kowaleski, *Determinantentheorie* (Chelsea Publishing Company, New York, 1948), 3rd edition, p. 105.

mined the characteristic vector up to a multiplicative constant.

Now suppose that the matrix M is also symmetric. This requires that $M_{jk}=M_{kj}$ or $c_{N-j+1+k}=c_{N-k+1+j}$. Setting $j=1$,

$$c_{N+k}\equiv c_k=c_{N-k+2}. \tag{A10}$$

This implies that $\lambda_k=\lambda_{N-k+2}$, because

$$\lambda_k=\sum_{s=1}^{N} c_s r_k^{s-1}=\sum_{s=1}^{N} c_{N-s+2} r_k^{s-1}=\sum_{p=1}^{N} c_p r_k^{N-p+1},$$

and since

$$r_k^{N-p+1}=r_{N-k+2}^{p-1},$$

$$\lambda_k=\sum_{p=1}^{N} c_p r_{N-k+2}^{p-1}=\lambda_{N-k+2}. \tag{A11}$$

Consequently, the characteristic values of a symmetric, cyclic matrix are twofold except for λ_1, and $\lambda_{\frac{1}{2}N+1}$ if N is even.

The corresponding real, orthogonal characteristic vectors, normalized to unity, are given by

$$V_{ks}=N^{-\frac{1}{2}}\left[\cos\frac{2\pi}{N}(k-1)(s-1)+\sin\frac{2\pi}{N}(k-1)(s-1)\right]. \tag{A12}$$

Now consider the quadratic forms of immediate interest.

Let ϵ denote the column matrix with components $\epsilon_1, \epsilon_2, \cdots, \epsilon_N$. Then

$$\sum_{i,j}{}' \epsilon_i\epsilon_j=\epsilon' M\epsilon,$$

with M symmetric and cyclic. We make an orthogonal transformation $\epsilon=Vy$ with Jacobian unity. Thus

$$\epsilon' M\epsilon=\sum_{p=1}^{N}\lambda_p y_p^2 \quad\text{and}\quad \sum_{p=1}^{N}\epsilon_p^2=\sum_{p=1}^{N} y_p^2. \tag{A13}$$

The elements of V, V_{ks}, are given by (A12).

One-dimensional lattice:

$$c_2=c_N=1. \text{ All other } c\text{'s}=0. \qquad \lambda_p=2\cos(2\pi/N)(p-1). \tag{A14}$$

Two-dimensional lattice:

We shall take a rectangular lattice with n_1 sites in a row, n_2 rows, so that $N=n_1n_2$. The ith site may be represented by the number pair (p, q) and by the space coordinates (x, y). If a is the spacing, we set

$$x=(p-1)a,\quad y=qa,\quad i=p+qn_1, \tag{A15}$$

where

$$p=1, 2, \cdots, n_1;\quad q=0, 1, \cdots, n_2-1.$$

We then choose

$$c_2=c_{n_1+1}=c_{N-n_1+1}=c_N=1, \tag{A16}$$

and all other c's$=0$. Then,

$$\lambda_p=2\cos\frac{2\pi}{N}(p-1)+2\cos\frac{2\pi n_1}{N}(p-1). \tag{A17}$$

Three-dimensional lattice:

We shall take a lattice with n_1 sites in a row, n_2 rows in a plane, and n_3 planes so that the total number of sites $N=n_1n_2n_3$. The ith site may be represented by the number triple (p, q, s) and by the space coordinates (x, y, z). If a is the spacing, we set

$$x=(p-1)a,\quad y=qa,\quad z=sa,\quad i=p+qn_1+sn_1n_2, \tag{A18}$$

where

$$p=1, 2, \cdots, n_1:\ q=0, 1, \cdots, n_2-1:\ s=0, 1, \cdots, n_3-1.$$

We choose

$$c_2=c_{n_1+1}=c_{n_1n_2+1}=c_{N-n_1n_2+1}=c_{N-n_1+1}=c_N=1, \tag{A19}$$

and all other c's$=0$. Then,

$$\lambda_p=2\cos\frac{2\pi}{N}(p-1)+2\cos\frac{2\pi n_1}{N}(p-1)+2\cos\frac{2\pi n_1n_2}{N}(p-1). \tag{A20}$$

APPENDIX B. ON THE $\lim_{N\to\infty} N^{-1}\sum_{p=1}^{N}\ln[1-2K\lambda_p]$

Consider the general sum

$$S(f)=\lim_{N\to\infty} N^{-1}\sum_{p=1}^{N} f(\lambda_p/2). \tag{B1}$$

The largest characteristic value occurs for $p=1$. We will then assume that the function $f(z)$ is regular when $z>\lambda_1/2$. Consequently, if we write

$$N^{-1}\sum_{p=1}^{N} f(\lambda_p/2)=N^{-1}f(\lambda_1/2)+N^{-1}\sum_{p=2}^{N} f(\lambda_p/2),$$

then

$$S(f)=\lim_{N\to\infty} N^{-1}\sum_{p=2}^{N} f(\lambda_p/2),$$

if $f(\lambda_1/2)$ is finite. This point is mentioned because the significant singularity of the functions to be considered depends on λ_1.

One-dimensional lattice:

From Eq. (A14), we have

$$\frac{\lambda_p}{2}=\cos\frac{2\pi}{N}(p-1).$$

Subdivide the interval $0-2\pi$ into N equal intervals of length $2\pi/N=\Delta\omega_1$. Then set $\omega_1=(p-1)\Delta\omega_1$. Consequently,

$$N^{-1}\sum_{p=2}^{N} f(\lambda_p/2)=\frac{1}{2\pi}\sum_{\omega_1=\Delta\omega_1}^{2\pi-\Delta\omega_1} f(\cos\omega_1)\Delta\omega_1, \quad \text{(B2)}$$

and

$$S(f)=\lim_{\Delta\omega_1\to 0}\frac{1}{2\pi}\sum_{\omega_1=\Delta\omega_1}^{2\pi-\Delta\omega_1} f(\cos\omega_1)\Delta\omega_1 =\frac{1}{2\pi}\int_0^{2\pi} f(\cos\omega_1)d\omega_1. \quad \text{(B3)}$$

It then follows that for $f(\lambda_p/2)=\ln[1-4K(\lambda_p/2)]$,

$$\lim_{N\to\infty} N^{-1}\sum_{p=1}^{N}\ln[1-2K\lambda_p] =\frac{1}{2\pi}\int_0^{2\pi} d\omega_1 \ln[1-4K\cos\omega_1]. \quad \text{(B4)}$$

Two-dimensional lattice:

For this lattice,

$$\frac{\lambda_p}{2}=\cos\frac{2\pi}{N}(p-1)+\cos\frac{2\pi n_1}{N}(p-1), \quad \text{(B5)}$$

with $N=n_1n_2$.

Let us write

$$p-1=p_2+p_1n_2, \quad p_1=0, 1, \cdots, n_1-1;\quad p_2=0, 1, \cdots, n_2-1. \quad \text{(B6)}$$

Then

$$\frac{2\pi}{N}(p-1)=\frac{2\pi}{n_1n_2}p_2+\frac{2\pi}{n_1}p_1,\quad \frac{2\pi n_1}{N}(p-1)=\frac{2\pi}{n_2}p_2+2\pi p_1,$$

and

$$\frac{\lambda_p}{2}=\cos\left(\frac{2\pi}{n_1n_2}p_2+\frac{2\pi}{n_1}p_1\right)+\cos\left(\frac{2\pi}{n_2}p_2\right), \quad \text{(B7)}$$

since p_1 is an integer.

Hence,

$$N^{-1}\sum_{p=2}^{N} f(\lambda_p/2)=N^{-1}\sum_{\substack{p_2=1\\p_1=0}}^{n_1-1} f(\lambda_{p_1+1}/2) +N^{-1}\sum_{p_1=1}^{n_1-1}\sum_{p_2=0}^{n_2-1} f(\lambda_{p_2+p_1n_2+1}/2). \quad \text{(B8)}$$

Now let

$$\Delta\omega_2=2\pi/n_2,\quad \omega_2=(2\pi/n_2)p_2.$$

$$\frac{\lambda_{p_2+p_1n_2+1}}{2}=\cos\left(\frac{\omega_2}{n_1}+\frac{2\pi}{n_1}p_1\right)+\cos\omega_2. \quad \text{(B9)}$$

Since ω_2 always ranges between 0 and 2π, ω_1/n_1 vanishes in the limit n_1. We then may write, as $n_2\to\infty$,

$$\sum_{p_2=0}^{n_2-1} f\left(\frac{\lambda_{p_2+p_1n_2+1}}{2}\right)\to\frac{n_2}{2\pi}\int_0^{2\pi} d\omega_2 f \times f\left(\cos\frac{2\pi}{n_1}p_1+\cos\omega_2\right), \quad \text{(B10)}$$

and

$$N^{-1}\sum_{p=2}^{N} f\left(\frac{\lambda_p}{2}\right)\to\frac{1}{2\pi n_1}\int_0^{2\pi} d\omega_2 f(1+\cos\omega_2) +\frac{n_2}{2\pi N}\sum_{p_1=1}^{n_1-1}\int_0^{2\pi} d\omega_2 f\left(\cos\frac{2\pi}{n_1}p_1+\cos\omega_2\right). \quad \text{(B11)}$$

The summation over p_1 leads to a second independent integral. Letting $\Delta\omega_1=2\pi/n_1$, $\omega_1=(2\pi/n_1)p_1$, then

$$S(f)=\frac{1}{(2\pi)^2}\int_0^{2\pi}\int_0^{2\pi} d\omega_1 d\omega_2 f(\cos\omega_1+\cos\omega_2). \quad \text{(B12)}$$

In the case that $f(\lambda_p/2)=\ln[1-4K(\lambda_p/2)]$,

$$\lim_{N\to\infty} N^{-1}\sum_{p=1}^{N}\ln[1-2K\lambda_p]=\frac{1}{(2\pi)^2}\int_0^{2\pi}\int_0^{2\pi} d\omega_1 d\omega_2 \times\ln[1-4K(\cos\omega_1+\cos\omega_2)]. \quad \text{(B13)}$$

Three-dimensional lattice:

For this lattice

$$\frac{\lambda_p}{2}=\cos\frac{2\pi}{N}(p-1)+\cos\frac{2\pi n_1}{N}(p-1)+\cos\frac{2\pi n_1 n_2}{N}(p-1)$$

with $N=n_1n_2n_3$.

There is no need to repeat the analysis, as it follows the two-dimensional analysis closely. The result is that

$$S(f)=\frac{1}{(2\pi)^3}\iiint_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times f(\cos\omega_1+\cos\omega_2+\cos\omega_3). \quad \text{(B14)}$$

If $f(\lambda_p/2)=\ln[1-4K(\lambda_p/2)]$, then

$$\lim_{N\to\infty} N^{-1}\sum_{p=1}^{N}\ln[1-2K\lambda_p]=\frac{1}{(2\pi)^3}\iiint_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times\ln[1-4K(\cos\omega_1+\cos\omega_2+\cos\omega_3)]. \quad \text{(B15)}$$

Consider now a function

$$F_{jk}(f)=\sum_{p=1}^{N} V_{jp}V_{kp}f(\lambda_p/2), \quad \text{(B16)}$$

with

$$V_{jp}V_{kp}=N^{-1}\left[\cos\frac{2\pi}{N}(j-k)(p-1)+\sin\frac{2\pi}{N}(j+k-2)(p-1)\right].$$

$$F_{jk}(f)=N^{-1}f\left(\frac{\lambda_1}{2}\right)+N^{-1}\sum_{p=2}^{N}f\left(\frac{\lambda_p}{2}\right)\times\left[\cos\frac{2\pi}{N}(j-k)(p-1)+\sin\frac{2\pi}{N}(j+k-2)(p-1)\right].$$

Therefore, let us consider

$$G_{jk}(f)=N^{-1}\sum_{p=2}^{N}f(\lambda_p/2)\exp\left[in_{jk}\frac{2\pi}{N}(p-1)\right],\quad\text{(B17)}$$

where n_{jk} is an integer depending linearly on j and k, that is,

$$n_{jk}=A+Bj+Ck,$$

with A, B, C as integers.

From before,

$$\frac{\lambda_p}{2}=\cos\frac{2\pi}{N}(p-1)+\cos\frac{2\pi n_1}{N}(p-1)+\cos\frac{2\pi n_1n_2}{N}(p-1),$$

$N=n_1n_2n_3$, where we are supposing the three-dimensional lattice.

Let us now write

$$p-1=rn_3+q;\ r=0,1,\cdots,n_1n_2-1;\ q=0,1,\cdots,n_3-1.$$

Now

$$\sum_{p=2}^{N}=\sum_{r=0}^{n_1n_2-1}\sum_{q=1}^{n_3-1},$$

so that

$$G_{jk}(f)=N^{-1}\sum_{r=0}^{n_1n_2-1}\sum_{q=1}^{n_3-1}f(\lambda_p/2)\times\exp\left[in_{jk}\left(\frac{2\pi r}{n_1n_2}+\frac{2\pi q}{n_1n_2n_3}\right)\right],$$

and

$$\frac{\lambda_p}{2}=\cos\left(\frac{2\pi r}{n_1n_2}+\frac{2\pi q}{n_1n_2n_3}\right)+\cos\left(\frac{2\pi r}{n_2}+\frac{2\pi q}{n_2n_3}\right)+\cos\left(2\pi r+\frac{2\pi q}{n_3}\right).$$

Let

$$\Delta\omega_3=2\pi/n_3,\quad \omega_3=(2\pi/n_3)q.$$

Since r is an integer, $\cos(2\pi r+2\pi q/n_3)=\cos\omega_3$. Also as n_1, n_2, n_3 become large,

$$\lambda_p/2=\cos\frac{2\pi r}{n_1n_2}+\cos\frac{2\pi r}{n_2}+\cos\omega_3.$$

Furthermore,

$$\sum_{q=1}^{n_3-1}=\frac{n_3}{2\pi}\sum_{2\pi/n_3}^{2\pi-2\pi/n_3}\Delta\omega_3\to\frac{n_3}{2\pi}\int_0^{2\pi}d\omega_3.$$

Hence,

$$G_{jk}(f)=\frac{n_3}{2\pi N}\int_0^{2\pi}d\omega_3\sum_{r=0}^{n_1n_2-1}f(\lambda_p/2)\times\exp\left[in_{jk}\left(\frac{2\pi r}{n_1n_2}+\frac{\omega_3}{n_1n_2}\right)\right].$$

Now let

$$r=tn_2+U,\quad t=0,1,\cdots,n_1-1;\quad U=0,1,\cdots,n_2-1.$$

$$\frac{\lambda_p}{2}=\cos\left(\frac{2\pi t}{n_1}+\frac{2\pi u}{n_1n_2}\right)+\cos\left(2\pi t+\frac{2\pi u}{n_2}\right)+\cos\omega_3.$$

Let $\Delta\omega_2=2\pi/n_2$, $\omega_2=(2\pi/n_2)U$. Then

$$\sum_{r=0}^{n_1n_2-1}=\sum_{t=0}^{n_1-1}\sum_{u=0}^{n_2-1}=\sum_{t=0}^{n_1-1}\frac{n_2}{2\pi}\sum_{0}^{2\pi-2\pi/n_2}\Delta\omega_2\to\sum_{t=0}^{n_1-1}\frac{n_2}{2\pi}\int_0^{2\pi}d\omega_2.$$

Then $\cos(2\pi t+2\pi U/n_2)=\cos\omega_2$, and

$$\lambda_p/2=\cos(2\pi t/n_1)+\cos\omega_2+\cos\omega_3,$$

$$G_{jk}(f)\to\frac{n_2n_3}{(2\pi)^2N}\int\int_0^{2\pi}d\omega_2d\omega_3\sum_{t=0}^{n_1-1}f\left(\frac{\lambda_p}{2}\right)\times\exp\left[in_{jk}\left(\frac{2\pi t}{n_1}+\frac{\omega_2}{n_1}+\frac{\omega_3}{n_1n_2}\right)\right].$$

Now set $\Delta\omega_1=2\pi/n_1$, $\omega_1=2\pi t/n_1$. Hence,

$$G_{jk}(f)\to\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi}d\omega_1d\omega_2d\omega_3f\left(\frac{\lambda}{2}\right)\times\exp\left[in_{jk}\left(\omega_1+\frac{\omega_2}{n_1}+\frac{\omega_3}{n_1n_2}\right)\right],\quad\text{(B18)}$$

with $\lambda/2=\cos\omega_1+\cos\omega_2+\cos\omega_3$.

The numbers j, k denote lattice sites, and these numbers will change as N changes. We must now use the one invariant property of the lattice site—its distance from a fixed origin. Let $j=p_1+q_1n_1+s_1n_1n_2$ as defined in Appendix A, Eq. (A18). Then $x_1=(p_1-1)a$, $y_1=q_1a$, $z_1=s_1a$. Thus, we write

$$n_{jk}=A+B(p_1+q_1n_1+s_1n_1n_2)+C(p_2+q_2n_1+s_2n_1n_2),$$

or (B19)

$$n_{jk}=(A+Bp_1+Cp_2)+(Bq_1+Cq_2)n_1+(Bs_1+Cs_2)n_1n_2,$$

where only n_1, n_2, n_3 change as N changes.

Consequently,

$$n_{jk}(\omega_1+\omega_2/n_1+\omega_3/n_1n_2)=(A+Bp_1+Cp_2)\omega_1+(Bq_1+Cq_2)n_1\omega_1+(Bs_1+Cs_2)n_1n_2\omega_1+(Bq_1+Cq_2)\omega_2+(Bs_1+Cs_2)n_1n_2\omega_2+(Bs_1+Cs_2)\omega_3.$$

We now note that

$$(Bq_1+Cq_2)n_1\omega_1=(Bq_1+Cq_2)2\pi t;$$
$$(Bs_1+Cs_2)n_1n_2\omega_1=(Bs_1+Cs_2)n_2 2\pi t;$$
$$(Bs_1+Cs_2)n_1n_2\omega_2=(Bs_1+Cs_2)n_1 2\pi U;$$

that is, these quantities are integral multiples of 2π, and they can be neglected in the exponential. Thus,

$$n_{jk}\left(\omega_1+\frac{\omega_2}{n_1}+\frac{\omega_3}{n_1n_2}\right)\approx(A+Bp_1+Cp_2)\omega_1+(Bq_1+Cq_2)\omega_2+(Bs_1+Cs_2)\omega_3$$
$$=\left[A+B\left(\frac{x_1}{a}+1\right)+C\left(\frac{x_2}{a}+1\right)\right]\omega_1+\left[B\frac{y_1}{a}+C\frac{y_2}{a}\right]\omega_2+\left[B\frac{z_1}{a}+C\frac{z_2}{a}\right]\omega_3\equiv\theta. \quad \text{(B20)}$$

Finally,

$$G_{jk}(f)=\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi}d\omega_1d\omega_2d\omega_3f(\lambda/2)\exp[i\theta], \quad \text{(B21)}$$

with θ defined in Eq. (B20).

If we assume that one of the spins is located at the origin, it is very easy to see that

$$\lim_{N\to\infty}N^{-1}\sum_{p=2}^{N}f(\lambda_p/2)\cos\frac{2\pi}{N}(j-k)(p-1)=\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi}d\omega_1d\omega_2d\omega_3f(\lambda/2)\times\cos\left(\frac{x_1\omega_1}{a}+\frac{y_1\omega_2}{a}+\frac{z_1\omega_3}{a}\right),$$

$$\lim_{N\to\infty}N^{-1}\sum_{p=2}^{N}f(\lambda_p/2)\sin\frac{2\pi}{N}(j+k-2)(p-1)=\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi}d\omega_1d\omega_2d\omega_3f(\lambda/2)\times\sin\left(\frac{x_1\omega_1}{a}+\frac{y_1\omega_2}{a}+\frac{z_1\omega_3}{a}\right),$$

where it is understood that x_1, y_1, z_1 are multiples of a.

Hence, we have

$$F_{jk}(f)=\frac{f(3)}{N}+\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi}d\omega_1d\omega_2d\omega_3f\left(\sum_{j=1}^{3}\cos\omega_j\right)\times\cos\left(\frac{x_1\omega_1}{a}+\frac{y_1\omega_2}{a}+\frac{z_1\omega_3}{a}\right), \quad \text{(B22)}$$

because the integral having the sine in the integrand is zero since λ is an even function of ω_1, ω_2, ω_3.

APPENDIX C. THE EVALUATION OF THE PARTITION FUNCTION OF THE SPHERICAL MODEL

$$Q_N(S)=A_N^{-1}\int\cdots\int_{\sum_{j=1}^{N}\epsilon_j^2=N}d\epsilon_1\cdots d\epsilon_N\exp[K\sum_{i,j}{}'\epsilon_i\epsilon_j]. \quad \text{(C1)}$$

We may also write

$$Q_N(S)=A_N^{-1}\int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N\times\exp[K\sum_{i,j}{}'\epsilon_i\epsilon_j]\delta(N-\sum_{j=1}^{N}\epsilon_j^2),$$

or

$$Q_N(S)=A_N^{-1}\int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N\times\exp[K\sum_{i,j}{}'\epsilon_i\epsilon_j]\frac{1}{2\pi i}\int_{-i\infty}^{+i\infty}ds\times\exp[s(N-\sum_{j=1}^{N}\epsilon_j^2)]. \quad \text{(C2)}$$

For our next step, we wish to interchange the integration over the $\{\epsilon_j\}$ with the integration over s. This can not be done because the form $K\sum_{i,j}{}'\epsilon_i\epsilon_j$ is not negative definite. However, we may write

$$K\sum_{i,j}{}'\epsilon_i\epsilon_j=N\alpha_0-N\alpha_0+K\sum_{i,j}{}'\epsilon_i\epsilon_j=N\alpha_0-\alpha_0\sum_{j=1}^{N}\epsilon_j^2+K\sum_{i,j}{}'\epsilon_i\epsilon_j,$$

because of the spherical condition. By choosing α_0 real, positive, and sufficiently large, the form can be made negative definite. Then we have

$$Q_N(S)=\frac{A_N^{-1}}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty}ds\exp[Ns]\int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N \times\exp[-s\sum_{j=1}^{N}\epsilon_j^2+K\sum_{i,j}{}'\epsilon_i\epsilon_j], \quad \text{(C3)}$$

where $s=\alpha_0$ is a line to the right of the singularities of the integrand as a function of s.

Making use of the orthogonal transformation of the variables $\{\epsilon_j\}$ discussed in Appendix A, the integration over the $\{\epsilon_j\}$ may be written

$$\int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_N\exp[-s\sum_{j=1}^{N}y_j^2+K\sum_{j=1}^{N}\lambda_jy_j^2] =\pi^{N/2}[\prod_{j=1}^{N}(s-K\lambda_j)]^{-\frac{1}{2}} =\pi^{N/2}\exp[-\tfrac{1}{2}\sum_{j=1}^{N}\ln(s-K\lambda_j)], \quad \text{(C4)}$$

and

$$Q_N(S)=\frac{A_N^{-1}\pi^{N/2}}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty}ds \times\exp[Ns-\tfrac{1}{2}\sum_{j=1}^{N}\ln(s-K\lambda_j)]. \quad \text{(C5)}$$

It is clear that we require $\alpha_0>K|\lambda_{\max}|$.

It is somewhat convenient to let $s=2Kz$. Then

$$Q_N(S)=A_N^{-1}\pi^{N/2}2Ke^{-\frac{1}{2}N\ln 2K}\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty}dz \times\exp[N2Kz-\tfrac{1}{2}\sum_{j=1}^{N}\ln(z-\tfrac{1}{2}\lambda_j)], \quad \text{(C6)}$$

where $z_0>\frac{1}{2}|\lambda_{\max}|=\frac{1}{2}\lambda_1$.

Since we are interested in the limit $N\to\infty$, let

$$f(z)=\lim_{N\to\infty}N^{-1}\sum_{j=2}^{N}\ln(z-\tfrac{1}{2}\lambda_j), \quad \text{(C7)}$$

$$g(z)=2Kz-\tfrac{1}{2}f(z).$$

Therefore,

$$Q_N(S)=A_N^{-1}\pi^{N/2}2Ke^{-\frac{1}{2}N\ln 2K}\frac{1}{2\pi i} \times\int_{z_0-i\infty}^{z_0+i\infty}dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{+Ng(z)}. \quad \text{(C8)}$$

Evaluating the complex integral by the method of steepest descent,

$$Q_N(S)\cong\frac{2K\pi^{N/2}e^{-\frac{1}{2}N\ln 2K+Ng(z_s)}}{A_N(z_s-\frac{1}{2}\lambda_1)^{\frac{1}{2}}[2\pi N(\partial^2g/\partial z^2)_{z_s}]^{\frac{1}{2}}}, \quad \text{(C9)}$$

where the saddle point z_s is determined by

$$(\partial g/\partial z)_{z_s}=0,\quad\text{and}\quad(\partial^2g/\partial z^2)_{z_s}>0. \quad \text{(C10)}$$

If the saddle point exists, then, with

$$A_N=2\pi^{N/2}N^{\frac{1}{2}(N-1)}/\Gamma(N/2),$$

$$-\psi/kT=\lim_{N\to\infty}N^{-1}\ln Q_N(S)=-\tfrac{1}{2}-\tfrac{1}{2}\ln 4K+g(z_s),$$

or

$$-\psi/kT=-\tfrac{1}{2}-\tfrac{1}{2}\ln 4K+2Kz_s-\tfrac{1}{2}f(z_s). \quad \text{(C11)}$$

We now proceed to investigate the existence of a saddle point.

If we let n denote the dimensionality of the simple lattices, let us denote $f(z)$ by $f_n(z)$. From Appendix B we have

$$f_n(z)=\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int d\omega_1\cdots d\omega_n\ln[z-\sum_{j=1}^{n}\cos\omega_j]. \quad \text{(C12)}$$

Then

$$\frac{\partial g_n}{\partial z}=2K-\frac{1}{2}\frac{\partial f_n}{\partial z}=2K-\frac{1}{2}\cdot\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int d\omega_1\cdots d\omega_n \times[z-\sum_{j=1}^{n}\cos\omega_j]^{-1}, \quad \text{(C13)}$$

and

$$\frac{\partial^2g_n}{\partial z^2}=-\frac{1}{2}\frac{\partial^2f_n}{\partial z^2}=\frac{1}{2}\cdot\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int d\omega_1\cdots d\omega_n \times\left[z-\sum_{j=1}^{n}\cos\omega_j\right]^{-2}. \quad \text{(C14)}$$

The equation for the saddle point is

$$4K=\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int d\omega_1\cdots d\omega_n[z_s-\sum_{j=1}^{n}\cos\omega_j]^{-1}. \quad \text{(C15)}$$

The only possible value for z_s is real and positive. If z_s exists, then Eq. (C14) shows that $(\partial^2g_n/\partial z^2)_{z_s}>0$.

If T is very large, K is very small. Therefore, z_s must be large, and in first approximation $4Kz_s=1$. As T decreases, z_s decreases.

Let us consider the one-dimensional lattice.

The saddle point equation is

$$4K=\frac{1}{2\pi}\int_0^{2\pi}d\omega_1[z_s-\cos\omega_1]^{-1}=(z_s^2-1)^{-\frac{1}{2}}, \quad \text{(C16)}$$

and

$$z_s=[1+(4K)^{-2}]^{\frac{1}{2}}.$$

Furthermore,

$$f_1(z_s)=\frac{1}{2\pi}\int_0^{2\pi} d\omega_1 \ln[z_s-\cos\omega_1] = \ln\tfrac{1}{2}[z_s+(z_s^2-1)^{\frac{1}{2}}]. \quad \text{(C17)}$$

Hence,

$$-\psi_1/kT=-\tfrac{1}{2}+\tfrac{1}{2}[1+(4K)^2]^{\frac{1}{2}} -\tfrac{1}{2}\ln\tfrac{1}{2}\{1+[1+(4K)^2]^{\frac{1}{2}}\}. \quad \text{(C18)}$$

In this case, as $T\rightarrow 0$, $K\rightarrow\infty$ so that $z_s\rightarrow 1$. The singularity of $f_1(z)$, $z=1$, is never reached. The steepest descent technique improves in accuracy insofar as $(\partial^2 g_1/\partial z^2)_{z_s}$ approaches ∞ as z_s approaches 1. The conclusion is that ψ_1 is a regular function of T in the range $0<T<\infty$.

Continuing with the two-dimensional lattice, the saddle point equation is

$$4K=\frac{1}{(2\pi)^2}\int\int_0^{2\pi} d\omega_1 d\omega_2[z_s-\cos\omega_1-\cos\omega_2]^{-1}. \quad \text{(C19)}$$

This equation may be written

$$4K=(2/\pi z_s)K(2/z_s), \quad \text{(C20)}$$

with $K(u)$ the complete elliptic integral

$$K(u)=\int_0^1 dt[(1-t^2)(1-u^2t^2)]^{-\frac{1}{2}}. \quad \text{(C21)}$$

As T decreases, z_s decreases and approaches the singularity $z=2$ of $f_2(z)$. In the neighborhood of $z=2$ we can use the expansion[6]

$$K\left(\frac{2}{z}\right)=-\frac{1}{2\pi}\sum_{n=0}^{\infty}\left\{\frac{\Gamma(\frac{1}{2}+n)}{n!}\right\}^2\left(1-\frac{4}{z^2}\right)^n \times\left\{\ln\left(1-\frac{4}{z^2}\right)-4\ln 2+\left(\frac{1}{1}-\frac{1}{2}+\cdots-\frac{1}{2n}\right)\right\}. \quad \text{(C22)}$$

Consequently, we see that $K(2/z_s)$ approaches infinity as $z_s\rightarrow 2$, and so z_s will exist for all allowed K. The singularity is not reached for a finite temperature. For this lattice, ψ_2 is again a regular function of T in the range $0<T<\infty$.

Finally, we take up the three-dimensional lattice for which the saddle point equation is

$$4K=\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times[z_s-\cos\omega_1-\cos\omega_2-\cos\omega_3]^{-1}. \quad \text{(C23)}$$

[6] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, London, England, 1927), fourth edition, p. 299.

The singularity of $f_3(z)$ occurs at $z=3$. As T decreases, z_s decreases and approaches the value 3. It is easy to show that for $z_s=3$ the integral converges. In fact, the integral has been evaluated by Watson[7] with the result that

$$4K_c\equiv\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times[3-\cos\omega_1-\cos\omega_2-\cos\omega_3]^{-1}=0.50546. \quad \text{(C24)}$$

This means that a saddle point exists down to a critical temperature $T_c=(3.9568)J/k$. Therefore, we have:

$T>T_c(K<K_c)$

$$-\psi_3/kT=-\tfrac{1}{2}-(\tfrac{1}{2})\ln(4K)+2Kz_s-(\tfrac{1}{2})f_3(z_s), \quad \text{(C25)}$$

where z_s is defined through Eq. (C23).

Since the partition function is defined for all positive T, we must investigate the range $T<T_c$. This requires consideration of the complex integral in the neighborhood of the branch point, $z=3$, of $f_3(z)$. The integral to consider is

$$\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-3)^{-\frac{1}{2}}e^{+Ng_3(z)}. \quad \text{(C26)}$$

If we cut the z-plane from $z=3$ to $z=-\infty$ along the real axis, then the integrand is analytic in the cut plane. Since $f_3(z)$ is analytic in the cut plane, we shall consider the behavior of df_3/dz in the neighborhood of $z=3$ and obtain $f_3(z)$ by integration. Now

$$\frac{df_3}{dz}=\frac{1}{(2\pi)^3}\int\int\int_0^{2\pi} d\omega_1 d\omega_2 d\omega_3 \times[z-\cos\omega_1-\cos\omega_2-\cos\omega_3]^{-1} =\frac{1}{\pi^2}\int_0^{\pi} d\omega_3\frac{2}{q}K\left(\frac{2}{q}\right), \quad \text{(C27)}$$

where $q=z-\cos\omega_3$. Using the expansion for $K(2/q)$ given in Eq. (C22), it is found by analytic continuation that

$$df_3/dz=4K_c-(2\pi^2)^{-\frac{1}{2}}(z-3)^{\frac{1}{2}}+O(z-3), \quad \text{(C28)}$$

and, therefore,

$$f_3(z)=f_3(3)+4K_c(z-3) -(2^{\frac{1}{2}}/3\pi)(z-3)^{\frac{3}{2}}+O([z-3]^2). \quad \text{(C29)}$$

We then have

$$g_3(z)=g_3(3)+2(K-K_c)(z-3) +(2^{-\frac{1}{2}}/3\pi)(z-3)^{\frac{3}{2}}+O([z-3]^2). \quad \text{(C30)}$$

Consequently, the integrand always has a saddle point

[7] G. N. Watson, Quart. J. Math. **10**, 266 (1939).

at $z=3$ if $K>K_c$ $(T<T_c)$.[8] The path of steepest descent has a cusp at $z=3$ and the path is shown in Fig. 3.

Evaluating the complex integral, we find that

$$\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-3)^{-\frac{1}{2}}e^{+Ng_3(z)} \cong [N2\pi(K-K_c)]^{-\frac{1}{2}}e^{+Ng_3(z)}. \quad \text{(C31)}$$

Hence, for $T<T_c(K>K_c)$

$$-\psi_3/kT=-\tfrac{1}{2}-(\tfrac{1}{2})\ln(4K)+6K-(\tfrac{1}{2})f_3(3). \quad \text{(C32)}$$

The discontinuity that is involved can also be seen from the following consideration. Dropping the subscript s, the saddle point is the solution of the equation

$$4K=df_3(z)/dz,$$

which defines z as a function of K. From this equation, it follows that for $T>T_c$,

$$\frac{dz}{dK}=4\bigg/\frac{d^2f_3}{dz^2}, \quad \text{(C33)}$$

and

$$\frac{d^2z}{dK^2}=-\left(\frac{dz}{dK}\right)^2\frac{d^3f_3}{dz^3}\bigg/\frac{d^2f_3}{dz^2}. \quad \text{(C34)}$$

[8] The mathematical reason for the transition in the three-dimensional lattice is the "sticking" of the saddle point. This same phenomenon has been found by Kramers. [H. A. Kramers, Commun. Kamerlingh Onnes Lab., Leiden, Suppl. No. 83 (1936).]

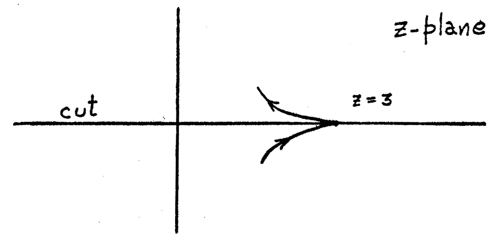

FIG. 3. Path of steepest descent for $T<T_c$.

In the neighborhood of the branch point $z=3$, we have from Eq. (C29)

$$\begin{aligned} d^2f_3/dz^2 &\simeq -(2^{-\frac{3}{2}}/\pi)(z-3)^{-\frac{1}{2}}; \\ d^3f_3/dz^3 &\simeq (2^{-5/2}/\pi)(z-3)^{-\frac{3}{2}}. \end{aligned} \quad \text{(C35)}$$

Consequently,

$$\lim_{z\to 3}\frac{dz}{dK}=\lim_{z\to 3}\{-\pi 2^{7/2}(z-3)^{\frac{1}{2}}\}=0,$$

and

$$\lim_{z\to 3}\frac{d^2z}{dK^2}=64\pi^2.$$

On the other hand, for $T<T_c$, $z=\text{constant}$, so that $dz/dK=d^2z/dK^2=0$. The discontinuity occurs in the second derivative, and this causes a discontinuity in slope of the specific heat *vs* temperature curve at T_c.