Ising-Model Reformulation. I. Fundamentals

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The partition function (Z) for the classical Ising model of cooperative phenomena in lattices of arbitrary dimensionality and with interactions of unspecified range is expressed as a vacuum-state expectation value of a product of two operators, each constructed from boson annihilation and creation operators. In the absence of external fields, Z, and similarly the spin-pair correlation function $\psi(\mathbf{r})$, are expanded thereupon into a series of Feynman diagrams. In the case of $\psi(\mathbf{r})$, a formally exact diagram summation (1) shows how the spherical model may be recovered in low-order approximation, (2) suggests a way of introducing systematic corrections to this approximation, and (3) leads to a generalized criterion for suppression of antiferromagnetic order in "nonfitting" lattices. A full topological-diagram reduction to restricted sets of "elementary" subdiagrams is carried out.

I. INTRODUCTION

THIS paper is devoted to the development of a new technique for handling classical order-disorder phenomena. By expressing the partition function for such assemblies as well as the spin-distribution functions in terms of vacuum-state expectation values in quantum field theory, it is possible to draw upon the powerful mathematical tools that have been devised for this latter discipline to effect the necessary evaluations in a systematic way.

The general Ising model treated here has spin $\frac{1}{2}$, but is restricted neither to lattices of specific dimensionality, nor to pair interactions between just nearest neighbors. Inspired by the exact results on the two-dimensional nearest-neighbor Ising model,[1,2] recent sophisticated numerical analyses on three-dimensional models have produced strong conjectures (which, if not exact, are certainly close to correct) about the analytic nature of critical point singularities.[3] These latter analyses, however, are based upon series developments which become intractably difficult to calculate for interaction ranges much beyond nearest neighbors. Since Ising models with extended interactions are of considerable physical interest (for example, in recovering the continuum cooperative gas-liquid-solid molecular assembly as a lattice gas with infinitesimal spacing), one of the strong motivations in presenting this approach has been the desire to understand features common to the set of more general Ising models.

The next section displays the means whereby the original classical statistical problem becomes equivalent to evaluation of a quantum-mechanical matrix element ("vacuum-state expectation value"). The operators originally involved are boson annihilation and creation operators, one attached to each lattice site. Translational symmetry of the problem, however, naturally suggests transformation to running waves of spin excitation.

In the third section, the operators are time ordered, and application of Wick's theorem allows both the partition function (Z) and the singlet (ρ) and pair (ψ) spin-distribution functions to be expressed as linked Feynman cluster diagram sums, where the diagrams have vertices confined essentially to two parallel strips. The ψ series in the absence of external fields is formally summed in Sec. IV in a way which clearly reveals the temperature variation of the wavelength-dependent static susceptibility (essentially the Fourier transform of ψ), as well as the occurrence of long-range order in the assembly. In addition, this way of expressing ψ transparently indicates the procedure for recovering the well-known spherical model,[4] and shows the way for systematic construction of corrections to the spherical model.

A full diagram reduction scheme for the field-free ψ is outlined in the fifth section for isolation of the difficult "elementary" cluster subdiagrams. Although the manipulations are strongly analogous to those that have been applied to the Ursell-Mayer imperfect gas series,[5] the present theory exhibits a richer structure, not only because nontrivial numerical coefficients are associated with diagram vertices of different orders, but also because the number of lines that may terminate at a vertex is necessarily even.

In the final section, the occurrence of long-range order at zero field is discussed in detail, and, in addition, a nonrigorous, but suggestive, criterion is advanced for occurrence of long-range antiferromagnetic order, based upon the extrema of the discrete Fourier transform of the pair interaction.

Generalization of most of the present theory to finite fields is reserved for a later communication.

II. INITIAL TRANSFORMATIONS

Let the positions of the sites of a regular lattice (in any number of dimensions) be $\mathbf{r}_1 \cdots \mathbf{r}_N$. The site at $\mathbf{r}_i$ will possess a classical spin μ_i which may have the values ± 1. If these spins interact in pairs by means of a potential

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] C. N. Yang, Phys. Rev. **85**, 808 (1952).
[3] A compilation of results may be found in M. E. Fisher, J. Math. Phys. 4, 278 (1963).
[4] T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).
[5] J. M. J. van Leeuwen, J. Groeneveld, and J. deBoer, Physica **25**, 792 (1959).

$v(\mathbf{r}_{ij})\mu_i\mu_j$, and with an external field equal to $H(\mathbf{r}_i)$ at site i, the partition function is

$$Z(\beta,H)=2^{-N}\sum_{\mu_1\cdots\mu_N=\pm1}\exp\{-\beta\sum_{i=1}^{N}H(\mathbf{r}_i)\mu_i-\beta\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\mu_i\mu_j\}, \quad (1)$$

$$\beta=(kT)^{-1}.$$

In the following it will be supposed that cyclic Born-von Karman boundary conditions apply to the lattice. For convenience, Z has been normalized to unity in the high-temperature limit in Eq. (1).

The multiple summation in (1) may trivially be converted to multiple-integral form.

$$Z(\beta,H)=\int_{-\infty}^{+\infty}d\mu_1\cdots\int_{-\infty}^{+\infty}d\mu_N\exp\{-\beta\sum_{i=1}^{N}H(\mathbf{r}_i)\mu_i-\beta\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\mu_i\mu_j\}p(\mu_1)\cdots p(\mu_N) \quad (2)$$

by means of suitable weight functions involving Dirac deltas.

$$p(\mu)=\tfrac{1}{2}[\delta(\mu-1)+\delta(\mu+1)]. \quad (3)$$

Since the weight-function product vanishes unless the absolute value of each μ_i is unity, Z will be unchanged if any function $F(\mu_1\cdots\mu_N)$ is inserted in the integrand of Eq. (2) if it has the property that it equals unity for these same spin values.

$$Z(\beta,H)=\int_{-\infty}^{+\infty}d\mu_1\cdots\int_{-\infty}^{+\infty}d\mu_N F(\mu_1\cdots\mu_N)\times\exp\{-\beta\sum_{i=1}^{N}H(\mathbf{r}_i)\mu_i-\beta\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\mu_i\mu_j\} \quad (4)$$

$$\times p(\mu_1)\cdots p(\mu_N),$$

$$F(\pm1,\pm1,\cdots,\pm1)=1.$$

We shall presently choose a specific form for F.

Each function $p(\mu_i)$ may formally be expanded in terms of some orthonormal set of functions $\{\varphi_n\}$ complete on the entire real axis. In particular, we choose this set to be the eigenfunctions of the one-dimensional Schrödinger wave equation for the harmonic oscillator.[6]

$$\varphi_n(x)=[\pi^{1/2}2^n n!]^{-1/2}\exp(-x^2/2)H_n(x), \quad (5)$$

where the H_n are the Hermite polynomials.

$$H_0(x)=1,\quad H_1(x)=2x,\quad H_2(x)=4x^2-2,\quad H_3(x)=8x^3-12x,\ \text{etc.} \quad (6)$$

[6] L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1935), p. 80.

Consequently, one may write

$$p(\mu_i)=\alpha\sum_{m=0}^{\infty}\varphi_{2m}(\alpha)\varphi_{2m}(\alpha\mu_i), \quad (7)$$

where α is a temporarily arbitrary scaling parameter. Only even-order terms appear in Eq. (7) due to the evenness of the function p.

The operators

$$\mathbf{a}_i^\dagger=[(\alpha\mu_i)-d/d(\alpha\mu_i)]/2^{1/2},\quad \mathbf{a}_i=[(\alpha\mu_i)+d/d(\alpha\mu_i)]/2^{1/2}, \quad (8)$$

act, respectively, as creation and annihilation operators for the scaled set $\varphi_n(\alpha\mu_i)$.

$$\mathbf{a}_i^\dagger\varphi_n(\alpha\mu_i)=(n+1)^{1/2}\varphi_{n+1}(\alpha\mu_i),\quad \mathbf{a}_i\varphi_n(\alpha\mu_i)=n^{1/2}\varphi_{n-1}(\alpha\mu_i). \quad (9)$$

In addition, they satisfy the boson commutation relations

$$[\mathbf{a}_i,\mathbf{a}_j]=0,\quad [\mathbf{a}_i^\dagger,\mathbf{a}_j^\dagger]=0,\quad [\mathbf{a}_i,\mathbf{a}_j^\dagger]=\delta_{ij}, \quad (10)$$

where $[\mathbf{A},\mathbf{B}]=\mathbf{AB}-\mathbf{BA}$. Specifically, we note the identity

$$\mu_i=(\mathbf{a}_i^\dagger+\mathbf{a}_i)/2^{1/2}\alpha. \quad (11)$$

On account of the first relation (9), it is possible to express each weight function p as the result of allowing a non-Hermitian operator $\mathbf{d}^\dagger$ to operate on φ_0.

$$p(\mu_i)/\alpha\varphi_0(\alpha)=\mathbf{d}_i^\dagger\varphi_0(\alpha\mu_i),\quad \mathbf{d}_i^\dagger=1+\sum_{m=1}^{\infty}\frac{H_{2m}(\alpha)}{2^m(2m)!}(\mathbf{a}_i^\dagger)^{2m}. \quad (12)$$

At this point, $F(\mu_1\cdots\mu_N)$ is chosen to be

$$F(\mu_1\cdots\mu_N)=\frac{\varphi_0(\alpha\mu_1)}{\varphi_0(\alpha)}\frac{\varphi_0(\alpha\mu_2)}{\varphi_0(\alpha)}\cdots\frac{\varphi_0(\alpha\mu_N)}{\varphi_0(\alpha)}. \quad (13)$$

Substitution of Eqs. (11), (12), and (13) into (4) yields the result

$$Z(\beta,H)=\int_{-\infty}^{+\infty}d(\alpha\mu_1)\cdots\times\int_{-\infty}^{+\infty}d(\alpha\mu_N)\varphi_0(\alpha\mu_1)\cdots\varphi_0(\alpha\mu_N)\exp(-\beta\mathbf{M})\cdot\mathbf{d}_1^\dagger\mathbf{d}_2^\dagger\cdots\mathbf{d}_N^\dagger\varphi_0(\alpha\mu_1)\cdots\varphi_0(\alpha\mu_N)$$

$$=\langle0|\exp(-\beta\mathbf{M})\mathbf{d}_1^\dagger\cdots\mathbf{d}_N^\dagger|0\rangle; \quad (14)$$

$$\mathbf{M}=\frac{1}{2^{1/2}\alpha}\sum_{i=1}^{N}H(\mathbf{r}_i)(\mathbf{a}_i^\dagger+\mathbf{a}_i)+\frac{1}{2\alpha^2}\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})(\mathbf{a}_i^\dagger+\mathbf{a}_i)(\mathbf{a}_j^\dagger+\mathbf{a}_j). \quad (15)$$

We have therefore succeeded in transforming the classical Ising partition function by means of elementary manipulations into a quantum-mechanical vacuum-state expectation value of certain field operators; the "vacuum," denoted by $|0\rangle$, consists of linear harmonic oscillators in their ground states at each lattice site.

On account of the translational symmetry assumed for the lattice, it is natural to seek a description of the cooperative assembly in terms of running excitation waves. Accordingly, new boson operators are introduced for each vector $\mathbf{k}$ in the first Brillouin zone (τ) of the space reciprocal to the lattice.

$$\begin{aligned}\mathbf{b}^\dagger(\mathbf{k})&=N^{-1/2}\sum_{j=1}^{N}\exp(i\mathbf{k}\cdot\mathbf{r}_j)\mathbf{a}_j^\dagger,\\ \mathbf{b}(\mathbf{k})&=N^{-1/2}\sum_{j=1}^{N}\exp(-i\mathbf{k}\cdot\mathbf{r}_j)\mathbf{a}_j.\end{aligned}\tag{16}$$

The inverse relations are

$$\begin{aligned}\mathbf{a}_j^\dagger&=N^{-1/2}\sum_{k}^{(\tau)}\exp(-i\mathbf{k}\cdot\mathbf{r}_j)\mathbf{b}^\dagger(\mathbf{k}),\\ \mathbf{a}_j&=N^{-1/2}\sum_{k}^{(\tau)}\exp(i\mathbf{k}\cdot\mathbf{r}_j)\mathbf{b}(\mathbf{k}),\end{aligned}\tag{17}$$

where the $\mathbf{k}$ summations are restricted to the zone τ. These new operators satisfy the same boson commutation relations as the previous set, Eq. (9)

$$\begin{aligned}[\mathbf{b}(\mathbf{k}),\mathbf{b}(\mathbf{k}')]&=0,\\ [\mathbf{b}^\dagger(\mathbf{k}),\mathbf{b}^\dagger(\mathbf{k}')]&=0,\\ [\mathbf{b}(\mathbf{k}),\mathbf{b}^\dagger(\mathbf{k}')]&=\delta(\mathbf{k}-\mathbf{k}').\end{aligned}\tag{18}$$

After defining the following discrete Fourier transforms,

$$\begin{aligned}H_k&=N^{-1/2}\sum_{j=1}^{N}H(\mathbf{r}_j)\exp(i\mathbf{k}\cdot\mathbf{r}_j),\\ V(\mathbf{k})&=\sum_{r}v(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r}),\end{aligned}\tag{19}$$

the interaction operator $\mathbf{M}$ may readily be expressed in terms of the $\mathbf{b}$'s

$$\begin{aligned}\mathbf{M}=&\frac{1}{2^{1/2}\alpha}\sum_{k}^{(\tau)}[H_{-k}\mathbf{b}^\dagger(\mathbf{k})+H_k\mathbf{b}(\mathbf{k})]+\frac{1}{4\alpha^2}\sum_{k}^{(\tau)}V(\mathbf{k})\\ &\times[\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}^\dagger(-\mathbf{k})+2n(\mathbf{k})+\mathbf{b}(\mathbf{k})\mathbf{b}(-\mathbf{k})],\end{aligned}\tag{20}$$

$$n(\mathbf{k})=\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}(\mathbf{k}).$$

In obtaining this result, we have used reflection invariance of V

$$V(\mathbf{k})=V(-\mathbf{k}),$$

and the vanishing of the spin self-interaction

$$Nv(\mathbf{r}=0)=\sum_{k}^{(\tau)}V(\mathbf{k})=0.$$

For most cases of interest, only one term of the external field sum in $\mathbf{M}$ will appear, i.e., H_0, corresponding to the homogeneous field.

In a similar way, the product $\mathbf{d}_1^\dagger\cdots\mathbf{d}_N^\dagger$ may be rewritten in terms of the $\mathbf{b}^\dagger$'s alone. First, one has

$$\begin{aligned}\mathbf{d}_1^\dagger\cdots\mathbf{d}_N^\dagger&=\prod_{j=1}^{N}\left\{1+\sum_{m=1}^{\infty}\frac{H_{2m}(\alpha)}{2^m(2m)!}(\mathbf{a}_j^\dagger)^{2m}\right\}\\ &=\exp\{\sum_{j=1}^{N}\sum_{n=1}^{\infty}D_n(\alpha)(\mathbf{a}_j^\dagger)^{2n}\};\end{aligned}\tag{21}$$

the numerical coefficients $D_n(\alpha)$ are the semi-invariants of the set $H_{2m}(\alpha)/2^m(2m)!$, and are calculated explicitly in Appendix A. If the heretofore arbitrary scaling parameter α is now set equal to $2^{-1/2}$, the leading coefficient in Eq. (21), $D_1(\alpha)$, can be made to vanish, so that in the following it will be supposed that this choice has been made. Under this circumstance, reference to Eq. (A5) of the Appendix A shows that the surviving coefficients are equal to

$$D_n=\frac{(-1)^{n-1}2^{2n-1}(2^{2n}-1)B_{2n-1}}{n(2n)!}\quad(n=2,3,\cdots),\tag{22}$$

and the B_{2n-1} are the Bernoulli numbers[7]

$$\begin{aligned}B_1&=1/6,\\ B_3&=1/30,\\ B_5&=1/42,\\ B_7&=1/30,\ \text{etc.}\end{aligned}\tag{23}$$

Finally, eliminating the $\mathbf{a}_j^\dagger$ from expression (21) by means of the first of Eqs. (17), one has

$$\begin{aligned}&\mathbf{d}_1^\dagger\cdots\mathbf{d}_N^\dagger=\exp(\mathbf{D}^\dagger),\\ &\mathbf{D}^\dagger=\sum_{n=2}^{\infty}N^{1-n}D_n\sum_{k_1\cdots k_{2n}}^{(\tau)\prime}\mathbf{b}^\dagger(\mathbf{k}_1)\cdots\mathbf{b}^\dagger(\mathbf{k}_{2n}),\end{aligned}\tag{24}$$

where the multiple-$\mathbf{k}$ summations in $\mathbf{D}^\dagger$ are constrained to conserve "momentum,"

$$\mathbf{k}_1+\cdots+\mathbf{k}_{2n}=0,$$

as indicated by the primed summation symbol. The general Ising partition function may thus be written

$$Z(\beta,H)=\langle 0|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle.\tag{25}$$

The special choice for α is such that the leading term

[7] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, 1952), pp. 125–6. In this reference, our B_{2n-1} is denoted by B_n.

in the weight function expansion (7) provides the correct second moment for $p(\mu)$ (the succeeding terms contribute nothing to this second moment). Retention of only this leading term (remembering that φ_0 is a Gaussian function) is equivalent to neglect of $\mathbf{D}^\dagger$ in Eq. (25). The resulting approximate partition function is known as the "Gaussian model," which diverges below a certain characteristic temperature.[4] In spite of the fact that $\mathbf{D}^\dagger$ contains no physical parameters, such as temperature, one therefore sees that its effects on the partition function of interest are even qualitatively important. When viewed from the present point of view, the difficulty in solving Ising problems rests in taking proper account of this non-Hermitian operator. The remainder of this paper is concerned with precisely this problem.

The singlet spin average $\rho(\mathbf{r}_i)$ and the spin-pair correlation function $\psi(\mathbf{r}_i,\mathbf{r}_j)$ may similarly be expressed in terms of quantum-mechanical matrix elements in the same vacuum state. One finds for the former, using exactly the same manipulations as before,

$$\begin{aligned}\rho(r_i)&=\langle\mu_i\rangle\\&=2^{-N}Z^{-1}\sum_{\mu_1\cdots\mu_N=\pm1}\mu_i\exp\{-\beta\sum_{i=1}^{N}H(\mathbf{r}_i)\mu_i-\beta\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\mu_i\mu_j\}\\&=\frac{\langle 0|N^{-1/2}\sum_{k}^{(\tau)}[\exp(-i\mathbf{k}\cdot\mathbf{r}_i)\mathbf{b}^\dagger(\mathbf{k})+\exp(i\mathbf{k}\cdot\mathbf{r}_i)\mathbf{b}(\mathbf{k})]\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle}{\langle 0|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle}.\end{aligned}\tag{26}$$

Since the square-bracketed creation operators appear to the left of all other operators in (26), they may be dropped.

$$\rho(\mathbf{r}_i)=\frac{\langle 0|N^{-1/2}\sum_{k}^{(\tau)}\exp(i\mathbf{k}\cdot\mathbf{r}_i)\mathbf{b}(\mathbf{k})\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle}{\langle 0|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle}.\tag{27}$$

Analogously, the pair correlation expression is

$$\begin{aligned}\psi(\mathbf{r}_i,\mathbf{r}_j)+\rho(\mathbf{r}_i)\rho(\mathbf{r}_j)&=\langle\mu_i\mu_j\rangle\\&=Z^{-1}\langle 0|N^{-1}\sum_{k,k'}^{(\tau)}[\exp(-i\mathbf{k}\cdot\mathbf{r}_i)\mathbf{b}^\dagger(\mathbf{k})+\exp(i\mathbf{k}\cdot\mathbf{r}_i)\mathbf{b}(\mathbf{k})]\\&\qquad\times[\exp(-i\mathbf{k}'\cdot\mathbf{r}_j)\mathbf{b}^\dagger(\mathbf{k}')+\exp(i\mathbf{k}'\cdot\mathbf{r}_j)\mathbf{b}(\mathbf{k}')]\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle.\end{aligned}\tag{28}$$

Again, the creation operators $\mathbf{b}^\dagger(\mathbf{k})$ may be dropped; also, $b^\dagger(\mathbf{k}')$ can combine only with $\mathbf{b}(\mathbf{k})$ when $\mathbf{k}'=\mathbf{k}$ to give δ_{ij}.

$$\psi(\mathbf{r}_i,\mathbf{r}_j)+\rho(\mathbf{r}_i)\rho(\mathbf{r}_j)=\delta_{ij}+Z^{-1}\langle 0|N^{-1}\sum_{k,k'}^{(\tau)}\exp[i(\mathbf{k}\cdot\mathbf{r}_i+\mathbf{k}'\cdot\mathbf{r}_j)]\mathbf{b}(\mathbf{k})\mathbf{b}(\mathbf{k}')\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle.\tag{29}$$

III. GENERATION OF DIAGRAMS

In order to begin devising a scheme for evaluating Z as the vacuum-state expectation value shown in Eq. (25), it is convenient to make use of Feynman's operator-ordering calculus.[8] Thus, we formally write

$$Z(\beta,H)=\left\langle 0\left|\exp\left[-\int_0^\beta\mathbf{M}(s)ds\right]\exp\left[\int_{-1}^{0}\mathbf{D}^\dagger(t)dt\right]\right|0\right\rangle.\tag{30}$$

The variables s and t which now index the operators $\mathbf{M}$ and $\mathbf{D}^\dagger$ may be considered as "times" at which the operators act. After expanding the exponentials, the operators are always to be "time-ordered," so that operators with smaller s or t appear to the right of those with larger values. As was shown in the previous section, both $\mathbf{M}$ and $\mathbf{D}^\dagger$ are constructed out of running-wave creation $\mathbf{b}^\dagger$ and annihilation $\mathbf{b}$ operators, so that in expression (30) the time indexing amounts to assigning times to these creation and annihilation operations; as examples:

$$\mathbf{b}^\dagger(\mathbf{k},t),\quad\mathbf{b}(\mathbf{k}',s).\tag{31}$$

[8] R. P. Feymnan, Phys. Rev. 84, 108 (1951).

The expansion of Eq. (30) may be written

$$Z(\beta,H)=\sum_{m,n=0}^{\infty}\frac{(-1)^m}{m!n!}\int_0^{\beta}ds_1\cdots ds_m\int_{-1}^{0}dt_1\cdots dt_n\langle 0|\,\mathbf{T}[\mathbf{M}(s_1)\cdots\mathbf{M}(s_m)\mathbf{D}^{\dagger}(t_1)\cdots\mathbf{D}^{\dagger}(t_n)]\,|0\rangle\,, \tag{32}$$

in which $\mathbf{T}$ is the time-ordering operator, and

$$\mathbf{M}(s)=\sum_{\mathbf{k}}^{(\tau)}[H_{-k}b^{\dagger}(\mathbf{k},s)+H_k\mathbf{b}(\mathbf{k},s)]+\tfrac{1}{2}\sum_{\mathbf{k}}^{(\tau)}V(\mathbf{k})[\mathbf{b}^{\dagger}(\mathbf{k},s)\mathbf{b}^{\dagger}(-\mathbf{k},s)+2\mathbf{b}^{\dagger}(\mathbf{k},s)\mathbf{b}(\mathbf{k},s)+\mathbf{b}(\mathbf{k},s)\mathbf{b}(-\mathbf{k},s)]\,,$$

$$\mathbf{D}^{\dagger}(t)=\sum_{n=2}^{\infty}N^{1-n}D_n\sum_{\mathbf{k}_1\cdots\mathbf{k}_{2n}}^{(\tau)\prime}\mathbf{b}^{\dagger}(\mathbf{k}_1,t)\cdots\mathbf{b}^{\dagger}(\mathbf{k}_{2n},t)\,. \tag{33}$$

Insertion of these expressions into Eq. (32) generates time-ordered operator products.

$$\mathbf{T}[\mathbf{A},\mathbf{B}\cdots\mathbf{Y},\mathbf{Z}], \tag{34}$$

in which $\mathbf{A}$, $\mathbf{B},\cdots$, $\mathbf{Y}$, $\mathbf{Z}$ are operators just of type (31).

The classification and calculation of the various contributions to Z are now enormously facilitated by application of Wick's theorem.[9] The only terms from the expansion of (34) into normal products which can give nonvanishing contributions to the vacuum-state expectation value are those which are completely contracted.[9] A graphical interpretation of the various modes of contraction may now be provided. Figure 1 exhibits a typical term. The two parallel strips represent the "time" intervals during which the $\mathbf{D}^{\dagger}$'s (lower strip) and $\mathbf{M}$'s (upper strip) operate. The dark circles represent sets of $\mathbf{b}$'s and $\mathbf{b}^{\dagger}$'s with the same "time" indices [one sees from (33) that they occur in pairs in the upper strip, and in sets of four or a larger even number in the lower strip]. The crosses, occurring only in the upper strip, are external field vertices provided by the leading terms in $\mathbf{M}$, which are linear in the field operators. The lines connecting vertices specify which sets of field operators have their members jointly contracted. The "time" integrations have the effect of moving vertices up or down within a strip. A line emanating upward from a vertex represents an excitation created at that vertex; a vertex at the upper end of a line destroys that excitation.

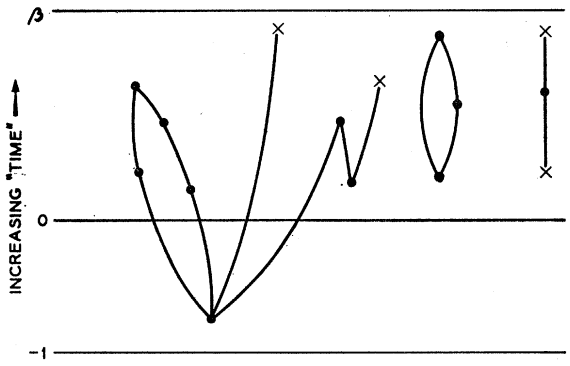

FIG. 1. A diagram of a typical term contributing to the general Ising partition function. The "time" coordinate is the Feynman index whereby the operators are ordered within the vacuum-state expectation value.

It may be seen from Fig. 1 that moving vertices about in the upper strip changes their annihilation or creation character, and therefore changes whichever of the specific terms in $\mathbf{M}$ the vertices represent. By freely performing the time integrations, however, all possibilities are neatly collected once and only once. It is clear that only even numbers (greater than two) of upward-radiated lines are permitted in the lower strip.

The operation of Wick's theorem allows contraction only of field operators with the same $\mathbf{k}$, so the final set of independent $\mathbf{k}$ summations in a given diagram is generally less than the number from which the contributing field operators came. Aside from these summations and time integrations (which give only trivial factors 1 or β for lower and upper strips, respectively), the value of a specific diagram is just the product of H_k's, $V(k)$'s, and $N^{1-n}D_n$'s for the vertices it contains.

Figure 1 shows by example that the general diagram consists of several disconnected parts. Suppose that in the m,n term in sum (32), Wick's theorem has, by contractions, linked up the $\mathbf{M}$'s and $\mathbf{D}^{\dagger}$'s in such a way that there are $\omega(\mu,\nu)$ linked sets consisting of μ $\mathbf{M}$'s and ν $\mathbf{D}^{\dagger}$'s. We must have the conditions

$$m=\sum_{\mu,\nu=0}^{\infty}\mu\omega(\mu,\nu)\,,\qquad n=\sum_{\mu,\nu=0}^{\infty}\nu\omega(\mu,\nu)\,. \tag{35}$$

The number of ways of dividing the m distinguishable $\mathbf{M}$'s and n distinguishable $\mathbf{D}^{\dagger}$'s into these subsets is

$$m!n!/\prod_{\mu,\nu=0}^{\infty}[\omega(\mu,\nu)]![\mu!\nu!]^{\omega(\mu,\nu)}\,. \tag{36}$$

If this combinatorial factor is inserted in Eq. (32), we

[9] D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961), pp. 38–40.

find

$$\ln Z(\beta,H)=\sum_{\mu,\nu}\frac{(-1)^{\mu}}{\mu!\nu!}\int_0^{\beta}ds_1\cdots ds_{\mu}\times\int_{-1}^{0}dt_1\cdots dt_{\nu}S_{\mu\nu}(s_1\cdots s_{\mu},t_1\cdots t_{\nu}),\quad(37)$$

where $S_{\mu\nu}(s_1\cdots t_{\nu})$ stands for the sum of terms from the Wick contractions of

$$\langle 0|\mathbf{T}[\mathbf{M}(s_1)\cdots\mathbf{M}(s_{\mu})\mathbf{D}^{\dagger}(t_1)\cdots\mathbf{D}^{\dagger}(t_{\nu})]|0\rangle,$$

which have *connected* graphs. We have thus obtained a "linked-cluster" expansion of the general Ising model free energy, which is required by the thermodynamic condition that this be an extensive quantity.

The diagrams allow one to visualize the details in a physical picture of the field-theoretic calculation of the partition function. For times less than -1, the system of harmonic oscillators on the lattice remains in the vacuum state. Between -1 and 0, it is subject to an agency which generates bursts of four, or a larger even number, of boson running-wave "excitons." During the interval 0 to β, these bosons are subject to forward scattering, annihilation, and further creation. $Z(\beta,H)$ is the probability that the system coincidentally finds itself in the vacuum state after all this agitation.

Since, as shown in Eqs. (27) and (29), the expectation value formulas for singlet and pair spin averages contain extra destruction operators, some diagrams that will arise in their evaluation require a slight modification. Because these extra field operators have been placed to the left of the other operators, they will be regarded as acting at a "time" later than β, and so must be represented by vertices above the upper strip.

Figure 2 illustrates the type of diagrams that arise in the evaluation of the numerator of the $\rho(\mathbf{r}_i)$ expression, Eq. (27). The diagrams consist of connected portions of precisely the same type encountered in evaluation of Z, as well as one connected portion including the new vertex above the upper strip. If one takes account of the number of ways in which $\mathbf{M}$'s and $\mathbf{D}^{\dagger}$'s may be distributed between connected portions of the new and old types, it is easy to see that the denominator of Eq. (27), which is Z itself, exactly cancels the old type, so $\rho(\mathbf{r}_i)$ is equal to the sum of all graphs connected to a single external vertex.

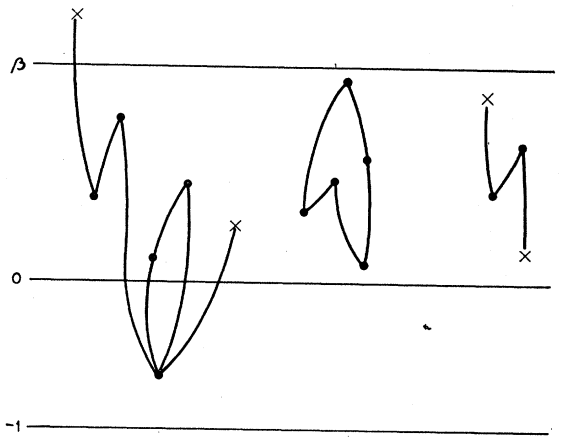

FIG. 2. The types of connected diagram portions encountered in evaluation of the numerator of the $\rho(\mathbf{r}_i)$ expression, (27). All but that part connected to the uppermost vertex are cancelled by the denominator.

In the case of the pair correlation function, there are two vertices above the upper strip, and the factor Z^{-1} again cancels all portions unconnected to either of these extra vertices. The remainder may consist, in any particular case, either of (A) two unconnected portions, one attached to each of the upper vertices, or (B) a singly connected structure bridging the two upper vertices. Since the two in case (A) are each exactly the types of diagrams contributing to $\rho(\mathbf{r}_i)$, and since $\psi(\mathbf{r}_i,\mathbf{r}_j)$ in Eq. (29) is defined to have $\rho(\mathbf{r}_i)\rho(\mathbf{r}_j)$ subtracted off, it is easy to see that only the doubly rooted graphs of case (B) contribute to $\psi(\mathbf{r}_i,\mathbf{r}_j)$.

IV. THE FIELD-FREE PAIR CORRELATION FUNCTION

For the remainder of this article, we shall suppose that no external fields act on the lattice, so the first set of terms in $\mathbf{M}(s)$ vanish [Eq. (33)] as well as each $\rho(\mathbf{r}_i)$. The partition function $Z(\beta)$ then may be obtained just from $\psi(\mathbf{r}_{ij})$, now a function of relative distance, through the intermediary of the average energy per spin, $E(\beta)/N$.

$$\ln Z(\beta)=-\int_0^{\beta}E(\beta')d\beta',\qquad E(\beta)=\tfrac{1}{2}N\sum_{r_{ij}}v(\mathbf{r}_{ij})\psi(\mathbf{r}_{ij},\beta).\quad(38)$$

Since the requisite combinatorial analysis to follow is simpler in the case of ψ than for Z itself, we elect to work primarily with this pair function.

Analogously to Eq. (37), the spin-pair correlation function may be expressed.

$$\psi(\mathbf{r}_{ij})=\delta_{ij}+\sum_{\mu,\nu}\frac{(-1)^{\mu}}{\mu!\nu!}\int_0^{\beta}ds_1\cdots ds_{\mu}\times\int_{-1}^{0}dt_1\cdots dt_{\nu}S_{\mu\nu}^{(2)}(s,s',s_1\cdots s_{\mu},t_1\cdots t_{\nu}),\quad(39)$$

where $S^{(2)}$ is the sum of the class (B) diagrams of the previous section, which are obtained by Wick's theorem contractions from

$$\langle 0|\mathbf{T}\{N^{-1}\sum_{k,k'}^{(\tau)}\exp[i(\mathbf{k}\cdot\mathbf{r}_i+\mathbf{k}'\cdot\mathbf{r}_j)]\mathbf{b}(\mathbf{k},s)\mathbf{b}(\mathbf{k}',s')\times\mathbf{M}(s_1)\cdots\mathbf{M}(s_{\mu})\mathbf{D}^{\dagger}(t_1)\cdots\mathbf{D}^{\dagger}(t_{\nu})\}|0\rangle.\quad(40)$$

One possible diagram is illustrated in Fig. 3.

In general, it is possible to distinguish a "primary" path between the two uppermost vertices, regardless of how complicated the diagram may be. As Fig. 3 shows, this primary path may dip down into the lower strip and return immediately to the upper strip, or else, by means of two or more of the lower strip creation processes, the primary path temporarily splits into alternate routes. Thus, the set of diagrams giving ψ may be characterized as set of vertices in the upper strip, which are connected in a linear sequence, but that this sequence may be interrupted by lower region processes.

It has already been remarked that the Gaussian model is equivalent to neglect of $\mathbf{D}^\dagger$, or what amounts to the same thing in graphical terms, to neglect of the lower region processes. A typical diagram for the Gaussian model ψ therefore consists of an *uninterrupted* sequence of upper region vertices, the set of which may easily be summed. For this latter purpose we note first that contractions can arrange μ $\mathbf{M}$'s in $\mu!$ distinct ways along the primary path. Furthermore, contractions between field operators in $\mathbf{M}(s_1)$ and $\mathbf{M}(s_2)$ require that the summation indices $\mathbf{k}$ in

$$\mathbf{M}(s_i)=\sum_k^{(\tau)} V(\mathbf{k})[\tfrac{1}{2}\mathbf{b}^\dagger(\mathbf{k},s_i)b^\dagger(-\mathbf{k},s_i) +n(\mathbf{k},s_i)+\tfrac{1}{2}\mathbf{b}(\mathbf{k},s_i)b(-\mathbf{k},s_i)]$$

from the two must either be equal, or the negatives of one another [only equality is allowed for $n(\mathbf{k},s_1)$],[9] so all possibilities may be handled with a *single* $\mathbf{k}$ summation for a complete diagram, with a factor $V(\mathbf{k})$ from each vertex. Thus, the Gaussian model pair correlation function ψ_G is

$$\begin{aligned}\psi_G(\mathbf{r}_{ij})&=\delta(\mathbf{r}_{ij})+\sum_{\mu=1}^{\infty}\frac{(-1)^\mu}{\mu!}\mu!\int_0^\beta ds_1\cdots ds_\mu \times N^{-1}\sum_k^{(\tau)}\exp[i(\mathbf{k}\cdot\mathbf{r}_i-\mathbf{k}\cdot\mathbf{r}_j)][V(\mathbf{k})]^\mu\\ &=\delta(\mathbf{r}_{ij})+N^{-1}\sum_k^{(\tau)}\frac{-\beta V(\mathbf{k})}{1+\beta V(\mathbf{k})}\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})\\ &=N^{-1}\sum_k^{(\tau)}\frac{1}{1+\beta V(\mathbf{k})}\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij}).\end{aligned}\tag{41}$$

Here it has been recognized that $\mathbf{k}'=-\mathbf{k}$, in obtaining this last result from Eq. (40), on account of the fact that any diagram must have an odd total number of pair creation (both lines up) and pair annihilation vertices (both lines down), each of which induces a $\mathbf{k}$ sign change along the primary path.

Since only macroscopic lattices will be of concern, the Brillouin zone sum in Eq. (41) passes into an integral

$$N^{-1}\sum_k^{(\tau)}\to\frac{1}{\tau}\int_\tau d\mathbf{k},$$

$$\psi_G(\mathbf{r}_{ij})=\frac{1}{\tau}\int_\tau\frac{\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})}{1+\beta V(\mathbf{k})}d\mathbf{k}.\tag{42}$$

Also, from (38), the Gaussian model partition function becomes

$$\ln Z_G(\beta)=-\frac{N}{2\tau}\int_\tau\ln[1+\beta V(\mathbf{k})]d\mathbf{k}.\tag{43}$$

One can clearly see from either Eq. (42) or (43) that the rather trivial Gaussian model diverges below the temperature at which $1+\beta V(\mathbf{k})$ first develops a zero in τ.[10] It is hence essential to put back into ψ the lower region processes. Any diagram including a lower region process (three are shown in Fig. 3) may be converted to another acceptable ψ diagram by putting in any other lower region process in its place. Consequently, it is convenient to consider a partial summation over all such conceivable lower region processes to have taken place in ψ diagrams at each position where the primary path dips into the lower strip. The result of this summation will be essentially a new lower region vertex, the analog of those in the upper strip giving factors $V(\mathbf{k})$, each of which will contribute some factor $W(\mathbf{k},\beta)$ to the graph.[11]

It is necessary next to write down an exact version of the Gaussian pair function, Eq. (42), which incorporates $W(\mathbf{k},\beta)$, giving the correct ψ for our original general

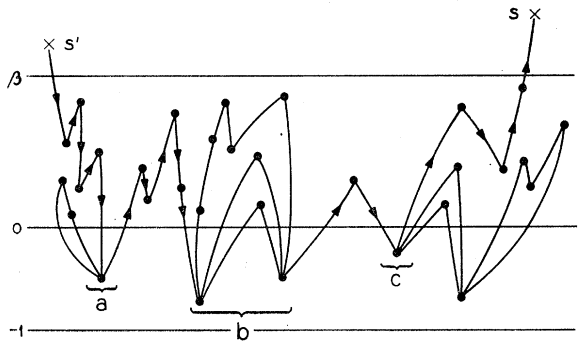

FIG. 3. A typical diagram contributing to the zero-external-field pair correlation function. The primary path connecting the two uppermost vertices ("times" s and s') has been indicated by arrows. The distinct lower region processes interrupting this primary path have each been emphasized by curly brackets. The middle one of these three lower region processes (b) in effect temporarily splits the fundamental path into several alternate routes, though these latter converge again to the single primary path.

[10] This temperature may readily be identified as the transition temperature predicted by the mean field theory.

[11] The β dependence of W arises out of the "time" integrations for V vertices included along paths within the lower region processes.

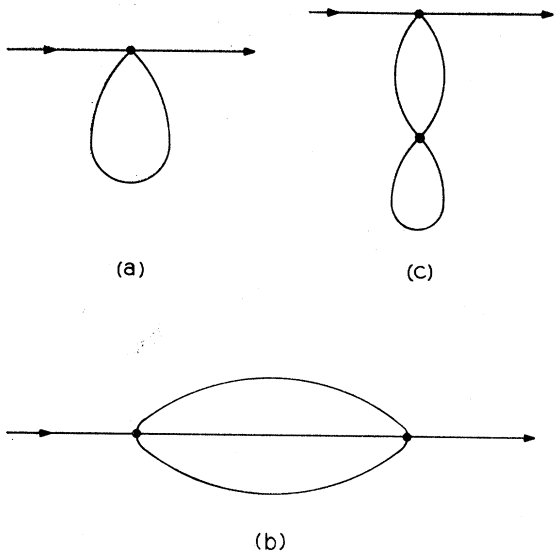

FIG. 4. Simplified drawings of the three lower region processes appearing in Fig. 3. As before, the primary path is indicated by arrows.

Ising problem. Re-expansion of the integrand of (42) yields a geometric series in $-\beta V(\mathbf{k})$, the separate factors of whose terms are isomorphic to the linear sequences of V vertices in the corresponding diagrams. Likewise, the complete Ising problem requires an expression, each of whose expansion terms contain factors that may be put into one-to-one correspondence with the linear sequences of V and W vertices in the complete set of ψ graphs. Recognizing that no two W vertices may occur next to one another (an intervening V vertex is required to turn the primary path downward between them), but that all other possibilities are allowed, one immediately verifies that the generating expression

$$\frac{1}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}[1+W(\mathbf{k},\beta)]-1 \qquad (44)$$

reproduces the correct set of sequences of $[-\beta V(\mathbf{k})]$ and $[W(\mathbf{k},\beta)]$. It is a direct consequence that

$$\psi(\mathbf{r}_{ij},\beta)=\delta(\mathbf{r}_{ij})+\frac{1}{\tau}\int_\tau\left\{\frac{1+W(\mathbf{k},\beta)}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}-1\right\}\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})d\mathbf{k}$$

$$=\frac{1}{\tau}\int_\tau\frac{[1+W(\mathbf{k},\beta)]\exp(-ik\cdot\mathbf{r}_{ij})}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}d\mathbf{k}; \qquad (45)$$

this is the exact version of simple result (42). In addition, the exact Ising partition function may be displayed in a form similar to Z_G in Eq. (43).

$$\ln Z(\beta)=-\frac{N}{2\tau}\int_\tau\ln[1+\beta V(\mathbf{k},\beta)]d\mathbf{k} \qquad (46)$$

when one sets

$$\beta V(\mathbf{k},\beta)=\exp\left\{\int_0^\beta d\beta'\times\frac{[1+W(\mathbf{k},\beta')]V(\mathbf{k})}{1+[1+W(\mathbf{k},\beta')]\beta' V(\mathbf{k})}\right\}-1. \qquad (47)$$

Appendix B deduces the relation between W and the "direct" correlation function.

To be of any use whatever, our formally correct expression (45) for ψ must naturally be supplemented by a means of determining $W(\mathbf{k},\beta)$. Toward this end, it is useful to introduce a simplified convention for drawing lower region processes summed in $W(\mathbf{k},\beta)$. Only the lower region vertices are explicitly indicated, along with the incoming and outgoing sections of the primary path, and each internal path (regardless of how many V vertices originally appeared along it) connecting lower region vertices is drawn as a simple line. Figure 4 displays the reduced representations of the three W processes appearing in Fig. 3.

A much more complicated W process is shown in part (a) of Fig. 5, which would be exceedingly difficult to visualize in its original graphical form on the two "time" strips. In this diagram, there are several occurrences of W processes along otherwise simple, single internal paths. For each of these internal paths the situation is therefore very similar to the entire set of possibilities

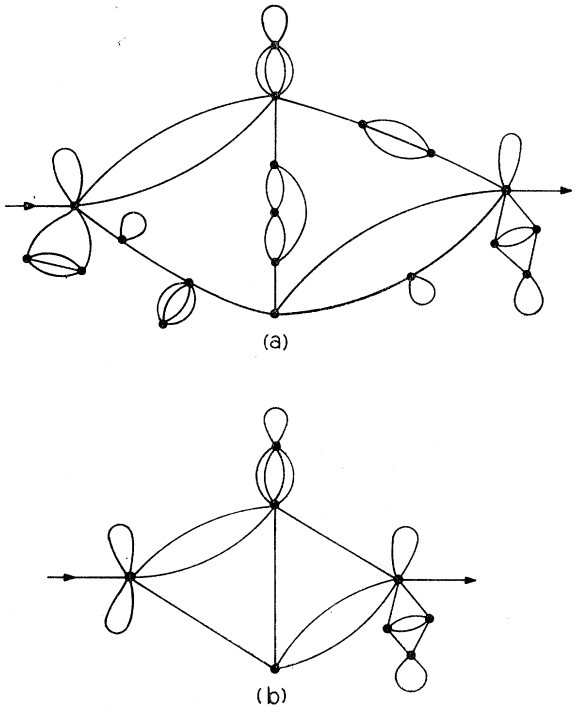

FIG. 5. (a) A complicated W process along whose internal lines further W processes occur; (b) reduced diagram for (a) in which the new bonds are given in Eq. (48).

for ψ itself, the very quantity we wish to calculate. This fact suggests a redefinition of the bond to be drawn henceforth as a simple line, so that the resultant diagrams of W processes themselves contain no W processes which may be removed by snipping two simple lines, the resulting ends of which then get tied together to form a single uninterrupted line. Part (b) of Fig. 5 indicates this latter reduction for Fig. 5(a). The remaining possible set of W processes may be called "reduced."

By considerations of the sort that led to formula (44), we can also write down an expression whose expansion terms yield in a one-to-one fashion the possible sequences of $[-\beta V]$'s and W's along this new type of renormalized bond. Since there must again be at least one V between each two lower region vertices along the bond, as well as those at the endpoints of the bond, one finds the bond function to be

$$L(\mathbf{k},\beta)=\frac{-\beta V(\mathbf{k})}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}, \tag{48}$$

since the expanded form contains all orderings of any number of $[-\beta V]$'s and W's except those which have either W's at the ends, or contiguous pairs of W's.

We are now in a position to write down a formal expression for $W(\mathbf{k},\beta)$ as a sum over the entire set of "reduced" diagrams. In doing so, it is necessary to be careful to consider the number of distinct ways that the even number of creation operators in each lower region vertex still remaining in any given reduced diagram might have been contracted with operators along the bonds. The general result may be written

$$\begin{aligned} W(\mathbf{k},\beta)&=\sum_{\{\mathbf{R}\}}\frac{1}{\sigma(\mathbf{R})}\left(\frac{4!D_2}{N}\right)^{n_2(\mathbf{R})}\cdots\left(\frac{(2l)!D_l}{N^{l-1}}\right)^{n_l(\mathbf{R})}\cdots \\ &\qquad\times\sum_{k_1\cdots k_{\gamma(\mathbf{R})}}{}'\prod_{\alpha=1}^{\gamma(\mathbf{R})}L(\mathbf{k}_\alpha,\beta) \\ &=\sum_{\{\mathbf{R}\}}W_{\mathbf{R}}(\mathbf{k},\beta). \end{aligned} \tag{49}$$

$\{\mathbf{R}\}$ is the entire set of reduced diagrams which must be summed to yield W, and any given diagram $\mathbf{R}$ possesses $\gamma(\mathbf{R})$ internal bonds, and $n_l(\mathbf{R})$ vertices terminating $2l$ lines (possibly including the primary path portions indicated by arrows). The $(2l)!$ associated with D_l in Eq. (49) is the number of ways of distributing the $2l$ creation operators among the bonds emanating from that particular vertex, under contractions. $\sigma(\mathbf{R})$ is a symmetry number for diagram $\mathbf{R}$, equal to the number of ways that relabelings of labeled vertices *and* internal bonds leads to basically the same arrangement. The $\mathbf{k}$ summation in (49) has been primed to show that the $\mathbf{k}$'s for all internal bonds are not independent, but the sum of $\mathbf{k}$'s at each vertex must vanish.[12]

The reduced diagrams $\mathbf{R}$ naturally fall into two classes according to whether or not the primary path enters and leaves the same vertex, as exemplified respectively by Figs. 4(a) and (b). Since these entering and leaving segments in the case of the former type must have opposite momenta, the rest of the momenta for the internal lines converging on this vertex must separately satisfy conservation of momentum, unlike the situation for the second $\mathbf{R}$ set. Since it is only through these momentum conservation restrictions that the value of a given $W_{\mathbf{R}}$ can depend on $\mathbf{k}$, the primary path momentum, the first class of $W_{\mathbf{R}}$'s must be independent of $\mathbf{k}$.

Any $W_{\mathbf{R}}(\mathbf{k},\beta)$ may be written as an average constant value over τ, plus a part which fluctuates across τ with average value zero; thus,

$$W_{\mathbf{R}}(\mathbf{k},\beta)=\bar{W}_{\mathbf{R}}(\beta)+\delta W_{\mathbf{R}}(\mathbf{k},\beta), \tag{50}$$

where

$$\begin{aligned} \bar{W}_{\mathbf{R}}(\beta)&=\frac{1}{\tau}\int_\tau W_{\mathbf{R}}(\mathbf{k},\beta)d\mathbf{k}, \\ \int\delta W_{\mathbf{R}}(\mathbf{k},\beta)d\mathbf{k}&=0. \end{aligned} \tag{51}$$

We have just concluded that $\delta W_{\mathbf{R}}$ identically vanishes for $\mathbf{R}$'s with a single entering and leaving primary path vertex. If the fluctuations are tentatively neglected for the remaining $W_{\mathbf{R}}$'s, the pair correlation function expression (45) reduces to

$$\psi(\mathbf{r}_{ij},\beta)\cong\frac{1}{\tau}\int_\tau\frac{[1+W(\beta)]\exp(-i\mathbf{r}_{ij}\cdot\mathbf{k})}{1+[1+W(\beta)]\beta V(\mathbf{k})}d\mathbf{k}. \tag{52}$$

Using Eqs. (38), the partition function in the $\mathbf{k}$-independent W approximation is found to be

$$\begin{aligned} \ln Z(\beta)&\cong-\frac{N}{2}\sum_{\mathbf{r}ij}v(r_{ij})\int_0^\beta\psi(r_{ij},\beta')d\beta' \\ &=-\frac{N}{2\tau}\int_0^\beta d\beta'\int_\tau\frac{[1+W(\beta')]V(\mathbf{k})}{1+[1+W(\beta')]\beta' V(\mathbf{k})}. \end{aligned} \tag{53}$$

Since the value of ψ is known for $\mathbf{r}_{ij}=0$,

$$\psi(0,\beta)=\langle\mu_i^2\rangle=1=\frac{1}{\tau}\int_\tau\frac{1+W(\mathbf{k},\beta)}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}d\mathbf{k}. \tag{54}$$

Equation (52) immediately leads to determination of a $\mathbf{k}$-independent W without any need to calculate cluster

[12] In the case of the vertex or vertices which terminate the primary path segments, the extra momenta for these latter must be included in the conservation conditions.

diagrams.

$$[1+W(\beta)]^{-1}=\frac{1}{\tau}\int_{\tau}\frac{d\mathbf{k}}{1+[1+W(\beta)]\beta V(\mathbf{k})}. \quad (55)$$

This approximate Ising model calculation may be identified as the spherical model.[13] Therefore, the assumption of no fluctuations in W across τ is equivalent to "smearing out" the discrete spin density $p(\mu_1)\cdots p(\mu_N)$ uniformly over the hypersphere in N space which passes through its 2^N points of nonvanishing probability. The major deficiencies in a spherical model approximation to the Ising problem are well known. (1) No phase transition is predicted in two-dimensional lattices with short-range interactions; (2) in the three-dimensional nearest-neighbor case, the specific heat is bounded, and the temperature dependence of magnetization is incorrect near the critical temperature; (3) the magnetization approaches unity linearly with temperature T as $T\rightarrow 0$, rather than as $A\exp(-B/T)$; (4) the predicted critical point pair correlation function is not correct. By taking account, even approximately, of the fluctuations of the $W_{\mathbf{R}}(\mathbf{k},\beta)$ across τ, one begins a systematic correction of the spherical model, and presumably begins to "unsmear" the spin distribution of the hypersphere.

V. THE STRUCTURE OF REDUCED W DIAGRAMS

Since the first class of W diagrams are constant over τ, their $\mathbf{r}$-space transforms $w_{\mathbf{R}}$ are lattice Kronecker delta functions:

$$W_{\mathbf{R}}(\beta)=\sum_{\mathbf{r}}\exp(i\mathbf{k}\cdot\mathbf{r})w_{\mathbf{R}}(\mathbf{r},\beta),$$

$$w_{\mathbf{R}}(\mathbf{r},\beta)=\frac{1}{\tau}\int_{\tau}W_{\mathbf{R}}(\beta)\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{k} \quad (56)$$

$$=W_{\mathbf{R}}(\beta)\delta(\mathbf{r}).$$

Although we shall not reproduce the tedious and uninformative details here, it may be shown that the constant $W_{\mathbf{R}}(\beta)$ may each be evaluated as a cluster sum on the original lattice. The term corresponding to graph $\mathbf{R}$ in Eq. (49) equals the product of bonds $l(\mathbf{r}_\alpha,\beta)$, one for each internal line of $\mathbf{R}$, where

$$l(\mathbf{r}_\alpha,\beta)=\frac{1}{\tau}\int_{\tau}L(\mathbf{k}_\alpha,\beta)\exp(-i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha)d\mathbf{k}_\alpha \quad (57)$$

is the transform of L, and position summations are to be taken over all vertices of $\mathbf{R}$ excepting the single one along the primary path. Note that closed loop internal lines beginning and ending at the same vertex are to be interpreted as $l(0,\beta)$.

[13] In Ref. 4, only the case of nearest-neighbor interactions of strength $-J$ [for which $V(\mathbf{k})$ is a sum of cosines] was explicitly worked out, though the generalization is straightforward. One may identify $\{2\beta J[1+W(\beta)]\}^{-1}$ as the saddle-point parameter z_s introduced by Berlin and Kac. See, also, R. Brout, Phys. Rev. 118, 1009 (1960).

In a similar way, the second class of W diagrams may also be interpreted as clusters on the original lattice:

$$W_{\mathbf{R}}(\mathbf{k},\beta)=\sum_{\mathbf{r}}\exp(i\mathbf{k}\cdot\mathbf{r})w_{\mathbf{R}}(\mathbf{r},\beta),$$

$$w_{\mathbf{R}}(\mathbf{r},\beta)=\frac{1}{\tau}\int_{\tau}W_{\mathbf{R}}(\mathbf{k},\beta)\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}, \quad (58)$$

where again the bonds are functions $l(\mathbf{r}_\alpha,\beta)$. The distance variable $\mathbf{r}$ in $w_{\mathbf{R}}(\mathbf{r},\beta)$ is the distance between the two vertices which, respectively, receive and discharge the primary path, and which are to be regarded as fixed. Other vertices are summed over the lattice.

We may now commence a program for analyzing the structure of the contributions to $W(\mathbf{k},\beta)$ which must be taken into account in proceeding beyond the spherical model. As a first consideration, the lower region vertex coefficients D_n, given explicitly in Eq. (22), are rather cumbersome to work with in that form. Rather, it will be convenient to use an integral representation of the Bernoulli numbers,[7] which leads to the following alternative expression:

$$D_n=\frac{(-1)^{n-1}2^{2n}}{\pi^{2n}(2n)!}\int_0^{\infty}\frac{y^{2n-1}dy}{\sinh y}. \quad (59)$$

Since we shall be working with cluster integrals in their $\mathbf{r}$-space interpretation, each free field point will be subject not only to a spatial summation, but a y integration as well to generate the correct multiplicative coefficient for that vertex.

This new vertex coefficient representation makes it especially easy to carry out a vertex renormalization. Reference to Fig. 5(b), an already bond-renormalized W diagram, illustrates the possibility of each remaining vertex acting as articulation point (single point of attachment) for certain portions of the diagram, such as simple loops. It is clear that any number of such distinct portions may be attached at any given vertex. The usual combinatorial arguments suffice to show that when account is taken of the distinct ways in which lines emanating from a point could be assigned to portions with this single attachment point (root), and to paths in the remaining diagram, that partial summation over singly rooted portions yields a renormalized vertex coefficient in the form

$$\bar{D}_n(\beta)=\frac{(-1)^{n-1}2^{2n}}{\pi^{2n}(2n)!}\int_0^{\infty}\frac{y^{2n-1}\exp[F(y,\beta)]dy}{\sinh y}, \quad (60)$$

which is now temperature-dependent. Here, $F(y,\beta)$ stands for a sum over all singly rooted portions, and the successive terms in expansion of $\exp[F]$ cover the cases of zero, one, two, $\cdots$, such portions attached to the vertex in question. Though we shall return to the problem of determination of F at this section's end, we shall temporarily proceed with formal use of the $\bar{D}_n$'s.

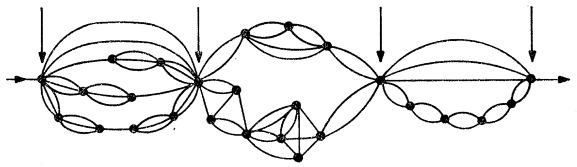

FIG. 6. A diagram remaining after both bond and vertex renormalizations have been effected. Such diagrams typically consist of a series of links (in this case to be separated at the vertical arrows) whose two end points terminate an odd number of lines.

The entire set of diagrams which gave $\mathbf{k}$-independent contributions to $W(\mathbf{k},\beta)$ have now contracted just to a single vertex.

Remembering that at least one singly rooted portion must have originally been connected at this vertex, one sees that the sum over all such diagrams must be [formally using the integrals (59) and (60) for $n=1$]

$$\bar{D}_1(\beta)-D_1=\frac{2}{\pi^2}\int_0^\infty \frac{y}{\sinh y}\{\exp[F(y,\beta)]-1\}dy. \quad (61)$$

Of course, if one uses condition (54) to fix the sum of $\bar{W}_R$'s for the *entire* set of W diagrams, this last expression need not be used.

Having thus removed singly rooted portions from the W-diagram vertices, the typical remaining structure for the nontrivial k-dependent diagrams is illustrated by Fig. 6. One sees that these diagrams consist of a series of one or more non-nodal links. Since the vertex renormalization does not alter the fact that an even number of lines must terminate at a vertex, it is obvious that the end points of each link must terminate an *odd* number of lines. Therefore, the remaining diagrams may be said to form *odd nodal chains*.

Let us examine for the moment two vertices in a diagram which are directly connected by j lines. Suppose that their coefficients are $\bar{D}_m$ and $\bar{D}_n$, containing, respectively, $(2m)!$ and $(2n)!$ as denominators. There are first the factors

$$\frac{(2m)!}{j!(2m-j)!} \quad \text{and} \quad \frac{(2n)!}{j!(2n-j)!}$$

to be taken into account, for the number of ways of choosing j paths out of the total number at each vertex to form the "bundle" between them. Also, there are $j!$ ways of matching up beginnings and ends of lines. Hence, so far as factorials are concerned, one must consider the factor

$$\frac{1}{j!}\times\frac{1}{(2m-j)!(2n-j)!}, \quad (62)$$

with just a single $j!$ for the bundle of j lines. Of course the remaining $(2m-j)!(2n-j)!$ gets cancelled as one proceeds to account for the total ways of forming other bundles in the diagram, until one ends up with comparable factorials for each bundle in the diagram. Thus, the factorials may, in effect, be removed from the *vertices*, and associated, at least in part, with parallel sets of *paths*.

It is most convenient to carry out our combinatorial analysis under the y integrals, and in doing so, the two ends of each l bond may be regarded as having absorbed some of the factors from the right side of (60); thus, we take the bond factor to be

$$\frac{i\times 2}{\pi}y_1 l(\mathbf{r},\beta)\frac{i\times 2}{\pi}y_2=-\frac{4y_1y_2}{\pi^2}l(\mathbf{r},\beta), \quad (63)$$

between a pair of vertices whose auxiliary integration variables are y_1 and y_2, leaving behind the operation

$$-\int_0^\infty \frac{\exp[F(y_1,\beta)]}{y_1\sinh y_1}dy_1\cdots$$

and its y_2 partner to remain associated with the vertices. In this spirit, we can therefore write the nontrivial part of $w(\mathbf{r}_{12},\beta)$ as the effect of two such integral operations (corresponding to the left-most and right-most vertices in a diagram) operating on a "nodal odd" function u

$$w(\mathbf{r}_{12},\beta)=[\bar{D}_1(\beta)-D_1]\delta(\mathbf{r})+\int_0^\infty \frac{\exp[F(y_1,\beta)]dy_1}{y_1\sinh y_1}$$
$$\times\int_0^\infty \frac{\exp[F(y_2,\beta)]dy_2}{y_2\sinh y_2}u(\mathbf{r}_{12},\beta,y_1,y_2). \quad (64)$$

Next, let $U(\mathbf{r}_{12},\beta,y_1,y_2)$ be the sum over all non-nodal links whose chains (including the one-link chain) form u, as previously noted. One has

$$u(\mathbf{r}_{12},\beta,y_1,y_2)=U(\mathbf{r}_{12},\beta,y_1,y_2)-\sum_{\mathbf{r}_3}\int_0^\infty dy_3$$
$$\times U(\mathbf{r}_{13},\beta,y_1,y_3)\frac{\exp[F(y_3,\beta)]}{y_3\sinh y_3}u(\mathbf{r}_{32},\beta,y_3,y_2), \quad (65)$$

since iteration of the right-hand side reproduces the chains. Symbolically, we write

$$u=U-U*u, \quad (66)$$

since, aside from the auxiliary integration, this would be a lattice convolution. Figure 6 shows that chains can also occur as parts of diagrams in which the links terminate at both ends in *even* numbers of lines. Therefore, we need also to define an even nodal chain function, $g(\mathbf{r}_{12},\beta,y_1,y_2)$, and an even non-nodal link function, $G(\mathbf{r}_{12},\beta,y_1,y_2)$, which are related in the same way as their odd analogs.

$$g=G-G*g. \quad (67)$$

One can now attempt to analyze the bond- and vertex-renormalized W diagrams into parts consisting of examples of even and odd nodal chains, and thereby seek to establish a closed set of functional equations for u, U, g, and G in terms of l, and hence the original interaction. One immediate complication is the fact that our previous bond renormalization did not allow l itself to be included as a permissible non-nodal link in sum U. However, not only can isolated l's occur as parts of diagrams (which cannot otherwise be identified as parts of g or u chains), but as the left-most link in Fig. 6 illustrates, we can still have paths between a pair of nodes also consisting of (1) a single bond and a u chain in series (in both orders), (2) a single bond separating two u-chain sequences. So, to simplify appearances in following equations, we introduce a "modified" odd-chain function $\tilde{u}$ to include not only the original u, but l and cases (1) and (2).

$$\tilde{u}(\mathbf{r}_{12},\beta,y_1,y_2)=u(\mathbf{r}_{12},\beta,y_1,y_2)-\frac{4y_1y_2}{\pi^2}l(\mathbf{r}_{12},\beta)$$
$$+\left[-\frac{4y_1y_3}{\pi^2}l(\mathbf{r}_{13},\beta)\right]*u(\mathbf{r}_{32},\beta,y_3,y_2)$$
$$+u(\mathbf{r}_{13},\beta,y_1,y_3)*\left[-\frac{4y_3y_2}{\pi^2}l(\mathbf{r}_{32},\beta)\right]$$
$$+u(\mathbf{r}_{13},\beta,y_1,y_3)*\left[-\frac{4y_3y_4}{\pi^2}l(\mathbf{r}_{34},\beta)\right]*u(\mathbf{r}_{42},\beta,y_4,y_2). \quad (68)$$

The next step is to define even ($\mathcal{G}$) and odd ($\mathcal{U}$) elementary diagram functionals. An even (odd) elementary diagram consists of two end points (denoted by 1 and 2, say), and $n\geq 2$ field points which are connected by lines such that (1) the two end points terminate an even (odd) number of lines greater than one; (2) each field point terminates an even number of lines greater than or equal to four; (3) there are only one or two lines connecting each pair of points directly (no loops are allowed); (4) there are no subdiagrams involving one or more vertices which may be removed by cuts at two other vertices; (5) no bonds directly connect the end points.

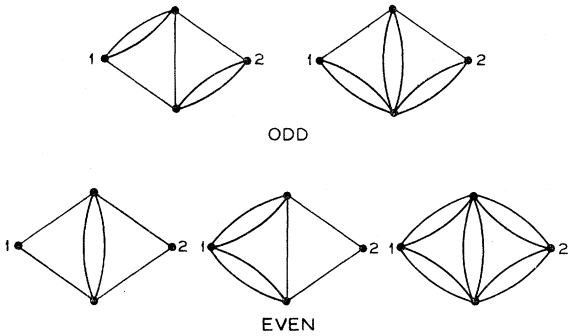

FIG. 7. The five basic types of elementary diagrams with two field points. The second of the three "even" diagrams may be turned end-for-end to yield an additional contribution to the even elementary diagram sum.

The five basically different types of even and odd elementary diagrams for $n=2$ are shown in Fig. 7. The number of possibilities increases enormously as n increases.

Not only can any elementary diagram itself (as drawn in Fig. 7) serve as an acceptable part of a W diagram, but replacement of each single bond by a $\tilde{u}$ link or any parallel pair of bonds between two vertices by a g diagram also leads to valid possibilities. Let $\mathfrak{D}_{gn}$ and $\mathfrak{D}_{un}$, respectively, stand for even and odd elementary diagrams with n field points, and also let $\eta(\mathfrak{D}_{gn})$ or $\eta(\mathfrak{D}_{un})$ be the number of essentially different ways of distributing n field point labels over the graphs. The even and odd elementary diagram sums are

$$\mathcal{G}(\mathbf{r}_{12},\beta,y_1,y_2)=\sum_{n=2}^{\infty}\sum_{\{\mathfrak{D}_{gn}\}}\frac{(-1)^n\eta(\mathfrak{D}_{gn})}{n!}\sum_{\mathbf{r}_3\cdots\mathbf{r}_{n+2}}\int_0^\infty\frac{\exp[F(y_3,\beta)]dy_3}{y_3\sinh y_3}\cdots\int_0^\infty\frac{\exp[F(y_{n+2},\beta)]dy_{n+2}}{y_{n+2}\sinh y_{n+2}}$$
$$\times\prod_{\mu=1}^{n_g(\mathfrak{D}_{gn})}g(\mathbf{r}_\mu,\beta,y_{i(\mu)},y_{j(\mu)})\prod_{\nu=1}^{n_u(\mathfrak{D}_{gn})}\tilde{u}(\mathbf{r}_\nu,\beta,y_{i(\nu)},y_{j(\nu)}); \quad (69)$$

$$\mathcal{U}(\mathbf{r}_{12},\beta,y_1,y_2)=\sum_{n=2}^{\infty}\sum_{\{\mathfrak{D}_{un}\}}\frac{(-1)^n\eta(\mathfrak{D}_{un})}{n!}\sum_{\mathbf{r}_3\cdots\mathbf{r}_{n+2}}\int_0^\infty\frac{\exp[F(y_3,\beta)]dy_3}{y_3\sinh y_3}\cdots\int_0^\infty\frac{\exp[F(y_{n+2},\beta)]dy_{n+2}}{y_{n+2}\sinh y_{n+2}}$$
$$\times\prod_{\mu=1}^{n_g(\mathfrak{D}_{un})}g(\mathbf{r}_\mu,\beta,y_{i(\mu)},y_{j(\mu)})\prod_{\nu=1}^{n_u(\mathfrak{D}_{un})}\tilde{u}(\mathbf{r}_\nu,\beta,y_{i(\nu)},y_{j(\nu)}). \quad (70)$$

The numbers of single bonds, and of pairs of parallel bonds between pairs of vertices have been denoted by n_u and n_g.

Aside from determination of F, the cluster analysis may now be completed by writing down two further relations, one for U and one for G. These may be derived by noting that sums of even and odd "simple" diagrams (all field points connected among themselves by paths

not through the end points) are, respectively, equal to[5]

$$S_g(\mathbf{r}_{12})=g(\mathbf{r}_{12})-G(\mathbf{r}_{12})+\mathcal{G}(\mathbf{r}_{12}),$$
$$S_u(\mathbf{r}_{12})=\tilde{u}(\mathbf{r}_{12})-U(\mathbf{r}_{12})+\mathcal{U}(\mathbf{r}_{12}). \tag{71}$$

The non-nodal even sum G may be built up out of any number of even simple diagrams, and an even number of odd simple diagrams in parallel, *excepting* the case of just a single even simple chain, which must then be elementary.

$$G=\exp(S_g)\cosh(S_u)-1-S_g+\mathcal{G}. \tag{72}$$

Similarly, U consists of any number of S_g's, and an odd number of S_u's, *except* that a single S_u diagram standing alone must be elementary.

$$U=\exp(S_g)\sinh(S_u)-S_u+\mathcal{U}. \tag{73}$$

Substitute from Eqs. (71) to obtain

$$g(\mathbf{r}_{12})=\exp[g(\mathbf{r}_{12})-G(\mathbf{r}_{12})+\mathcal{G}(\mathbf{r}_{12})]\times\cosh[\tilde{u}(r_{12})-U(\mathbf{r}_{12})+\mathcal{U}(\mathbf{r}_{12})]-1, \tag{74}$$
$$\tilde{u}(\mathbf{r}_{12})=\exp[g(\mathbf{r}_{12})-G(\mathbf{r}_{12})+\mathcal{G}(\mathbf{r}_{12})]\times\sinh[\tilde{u}(\mathbf{r}_{12})-U(\mathbf{r}_{12})+\mathcal{U}(\mathbf{r}_{12})].$$

Once one is given $F(y,\beta)$, Eqs. (66), (67), (69), and (70), along with the definition of $\tilde{u}$, Eq. (68), in principle constitute solution to the Ising problem (though one is up against the typical difficulty of having to evaluate complicated elementary diagram sums, which is the real deterrent to obtaining exact results).

Some of the possible singly articulated diagram parts which contribute to F were shown in Fig. 5(b). The F sum may be obtained by providing a second root for these parts by introducing a parameter λ which is allowed to vary continuously in the range $0\leq\lambda\leq1$. Then, if a factor λ has been appended to each of the originally drawn vertices (including all V vertices and lower region vertices that were suppressed in drawing bond- and vertex-renormalized diagrams) of that part,

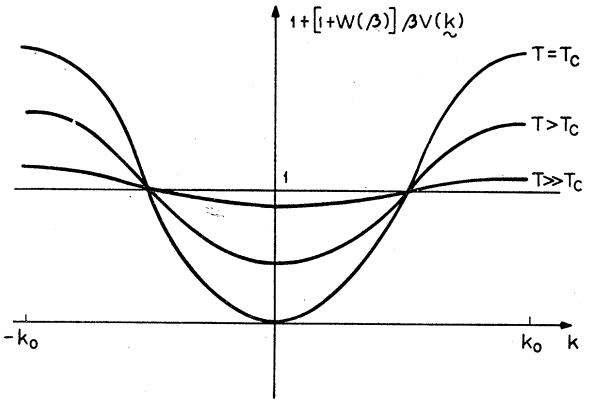

FIG. 8. Temperature variation of the pair correlation function integrand denominator for the three-dimensional spherical ferromagnet. The values are shown only along an arbitrary ray through the $\mathbf{k}$-space origin, which intersects the Brillouin zone boundaries at $\pm k_0$.

a λ differentiation effectively makes each vertex in turn a second root, and adds the results. But we see that both a new vertex and the old root vertex terminate even numbers of lines, and the resulting doubly rooted diagrams are precisely those of the nodal even chain sum. It is therefore possible to repeat essentially the same diagram reductions for the F determination as have just been completed for $\lambda=1$, but retaining an explicit λ dependence.

The effective partition function in the presence of variable λ is

$$Z_\lambda(\beta)=\langle 0|\exp(-\lambda\beta\mathbf{M})\exp(\lambda\mathbf{D}^\dagger)|0\rangle, \tag{75}$$

and the corresponding pair correlation function reads

$$\psi_\lambda(\mathbf{r}_{ij})=\delta(\mathbf{r}_{ij})+\frac{1}{\lambda\tau}\int_\tau\left\{\frac{1+W_\lambda(\mathbf{k},\beta)\lambda}{1+[1+W_\lambda(\mathbf{k},\beta)\lambda]\beta V(\mathbf{k})\lambda}-1\right\}\times\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})d\mathbf{k},$$
$$\psi_\lambda(\mathbf{r}_{ij}=0)=1, \tag{76}$$

which are the generalizations of Eqs. (25), (45), and (54). Next, the renormalized bond function, Eq. (48), becomes

$$L_\lambda(\mathbf{k},\beta)=\frac{-\beta V(\mathbf{k})}{1+[1+W_\lambda(\mathbf{k},\beta)\lambda]\beta V(\mathbf{k})\lambda}, \tag{77}$$

where one λ factor has been excluded to simplify the following. The function F itself must also be λ indexed so that the expression (64) relating w to a nodal odd-chain sum now appears

$$w_\lambda(\mathbf{r}_{12},\beta)=-\frac{2}{\pi^2}\int_0^\infty\frac{ydy}{\sinh y}\times\{\exp[F_\lambda(y,\beta)]-1\}\delta(\mathbf{r}_{12})+\int_0^\infty\frac{\exp[F_\lambda(y_1,\beta)]dy_1}{y_1\sinh y_1}\times\int_0^\infty\frac{\exp[F_\lambda(y_2,\beta)]dy_2}{y_2\sinh y_2}u_\lambda(\mathbf{r}_{12},\beta,y_1,y_2). \tag{78}$$

Equations (66) and (67) become

$$u_\lambda=U_\lambda-\lambda U_\lambda(*)_\lambda u_\lambda, \tag{79}$$
$$g_\lambda=G_\lambda-\lambda G_\lambda(*)_\lambda g_\nu,$$

in which $(*)_\lambda$ is the same operation as $*$, but with F_λ replacing F. Also, the $\tilde{u}_\lambda$ generalization of Eq. (68) is

$$\tilde{u}_\lambda=u_\lambda-\frac{4y_1y_2}{\pi^2}l_\lambda+\lambda\left[-\frac{4y_1y_3}{\pi^2}l_\lambda\right](*)_\lambda u_\lambda+\lambda u_\lambda(*)_\lambda\left[-\frac{4y_3y_2}{\pi^2}l_\lambda\right]+\lambda^2\left[-\frac{4y_1y_3}{\pi^2}l_\lambda\right](*)_\lambda u_\lambda(*)_\lambda\left[-\frac{4y_4y_2}{\pi^2}l_\lambda\right]. \tag{80}$$

The even and odd elementary diagram sums have λ subscripts on each F, $\tilde{u}$, and g that appear in (69) and (70), as well as extra factors λ^n:

$$\mathcal{G}_\lambda=\sum_{n=2}^{\infty}\lambda^n\sum_{\{\mathcal{D}_{gn}\}}\cdots,$$
$$\mathcal{U}_\lambda=\sum_{n=2}^{\infty}\lambda^n\sum_{\{\mathcal{D}_{un}\}}\cdots. \tag{81}$$

Equations (74) remain valid after each function receives a λ subscript. Finally, we determine F_λ by reintegrating the doubly rooted diagram sum over λ:

$$F_\lambda(y_1,\beta)=-\sum_{\mathbf{r}_2}\int_0^\lambda d\lambda'\int_0^\infty dy_2 \times\frac{\exp[F_{\lambda'}(y_2,\beta)]}{y_2\sinh y_2}g_{\lambda'}(\mathbf{r}_{12},\beta,y_1,y_2). \tag{82}$$

This completes the formal cluster analysis.

VI. THE OCCURRENCE OF LONG-RANGE ORDER

In order to see how the occurrence of long-range order in an Ising model, as T is lowered below T_c, is reflected in the central quantity $W(\mathbf{k},\beta)$, we first review the behavior of the three-dimensional spherical model ferromagnet. For definiteness, a simple cubic lattice with nearest-neighbor interaction J will be assumed, so

$$V(\mathbf{k})=-2J[\cos k_x+\cos k_y+\cos k_z] \tag{83}$$

(distances will be measured in lattice spacing units). At very high temperature (β small), the exact $W(\mathbf{k},\beta)$, as well as its spherical model constant analog $W(\beta)$ determined by (55), are negligibly small. As a result, the integrand denominator of the spherical model

$$1+[1+W(\beta)]\beta V(\mathbf{k}) \tag{84}$$

will have a shallow positive minimum at $\mathbf{k}=0$, which tends to get deeper as the temperature is lowered. This behavior is shown in Fig. 8.

If the spherical model $W(\beta)$ remained zero as T was lowered, the integral on the right-hand side of Eq. (55) would increase above its $\beta=0$ limit, unity, so that this equation could not be satisfied. The equation can, however, be satisfied if $W(\beta)$ becomes negative for $\beta>0$, since then $[1+W(\beta)]^{-1}>1$. In the integrals' denominator, $[1+W(\beta)]\beta$ acts as an effective inverse temperature less than β, so the unique solution $W(\beta)$ (which goes to zero as $\beta\to 0$) represents a balance between the two members.

In this three-dimensional example, a sufficiently large value of β is eventually reached where (84) becomes zero at $\mathbf{k}=0$, though the $\mathbf{k}$-space differential volume element $4\pi k^2dk$ is sufficient to maintain integrability in Eqs. (52) and (55). This is the spherical model critical point,[4] $\beta=\beta_c$. When β exceeds β_c, it is necessary to treat separately the $\mathbf{k}=0$ term in the $\mathbf{k}$-sum precursor of integrals such as (52) and (55), exactly as is done in treatment of Bose-Einstein condensation of the ideal gas.[14] Then in this low-temperature region $W(\beta)$ varies in such a way as precisely to maintain the root of (84) at $k=0$, namely

$$W(\beta)=-1-[1/\beta V(0)]\ (\beta\geq\beta_c). \tag{85}$$

The pair correlation function in the spherical model becomes

$$\psi(\mathbf{r}_{ij},\beta)=m^2(\beta)+\frac{1}{\beta\tau}\int_\tau\frac{\exp(i\mathbf{k}\cdot\mathbf{r}_{ij})d\mathbf{k}}{V(\mathbf{k})-V(0)}, \tag{86}$$

and Eq. (55) becomes replaced by

$$1=m^2(\beta)+\frac{1}{\beta\tau}\int_\tau\frac{d\mathbf{k}}{V(\mathbf{k})-V(0)}, \tag{87}$$

which is now a relation for determination of the long-range order $m(\beta)=\lim_{r\to\infty}\psi^{1/2}(r,\beta)$.

In the case of the two-dimensional square-lattice analog, the spherical model condition (55) does not allow the denominator (84) to develop a zero for finite β, for if it did (the $\mathbf{k}$-space differential volume element is now $2\pi kdk$), the right-member integral would diverge logarithmically. The condition could then only be satisfied if $[1+W(\beta)]^{-1}$ were infinite, $1+W(\beta)=0$, but this would contradict the assumption of a denominator zero. It is known, of course, that the two-dimensional nearest-neighbor ferromagnet really does exhibit a phase transition with long-range order below a finite β_c.[1]

The difficulty evidently is that the spherical model use of a constant W forces the denominator expression (84) always to be parabolic in the neighborhood of $\mathbf{k}=0$. The exact two-dimensional Ising model must have a $\mathbf{k}$-dependent W which "sharpens" the minimum to the extent that at β_c the corresponding infinite singularity produced by the denominator's vanishing is sufficiently weaker that $2\pi k\,dk$ converts it to an integrable function. This tendency toward minimum sharpening is already heralded by examining the simplest contribution to W which has a $\mathbf{k}$ dependence; it corresponds to graph 4(b), and provides the dominant $\mathbf{k}$ dependence at high temperature (since it can contain the smallest number of V vertices). For small β it equals

$$\tfrac{4}{3}(\beta J)^3[\cos k_x+\cos k_y+\cos k_z],$$

introducing a "second harmonic" into the previously pure sinusoidal expression (84), with a sign that accentuates (sharpens) the minimum. One may safely presume that in three dimensions also, the correct $W(\mathbf{k},\beta)$ somesomewhat sharpens the minimum behavior at β_c. This

[14] C. Kittel, *Elementary Statistical Physics* (John Wiley & Sons, Inc., New York, 1958), p. 98.

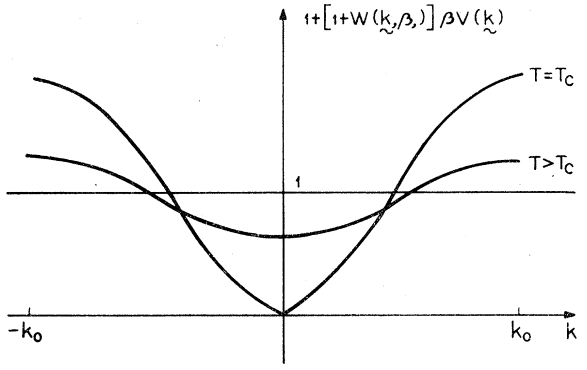

FIG. 9. Pair correlation function integrand denominator for the correct Ising model. At the critical temperature, the curve touches the axis with a sharper bend than the parabolic shape predicted by the spherical model.

modified denominator behavior, as β approaches β_c from below, is schematically illustrated in Fig. 9.

Again, when β exceeds β_c, the $\mathbf{k}=0$ term must receive special consideration, giving rise to extra $m^2(\beta)$ terms in Eqs. (52) and (54). However, there is no reason (in an exact evaluation) for the $\mathbf{k}\neq 0$ values of (84) to be β-independent, as for the spherical model. Indeed, since $m^2(\beta)$ approaches 1 faster with increasing β than the spherically model predicts (so the "gas" of overturned spins rapidly becomes very dilute and uncorrelated except as nearest neighbors) it seems certain that the denominator recedes from the axis to again approach the constancy shown at high temperature, with the single exception of the isolated point at $\mathbf{k}=0$. This is shown in Fig. 10. Apparently, when $\beta>\beta_c$,

$$\lim_{k\to 0}[W(k,\beta)-W(0,\beta)]>0\,, \tag{88}$$

so that $w(\mathbf{r},\beta)$ will have a long-ranged constant part proportional to N^{-1}.

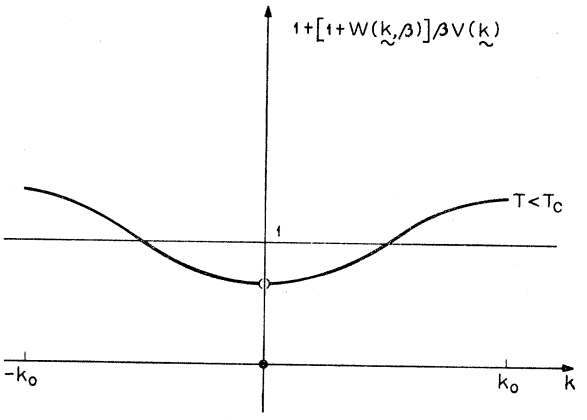

FIG. 10. ψ integrand denominator below the transition temperature. The function is similar to the $T>T_c$ case of Fig. 9. with the exception of the single isolated point at $\mathbf{k}=0$, which sits on the k axis.

We turn finally to a consideration of antiferromagnetic order. A change in the sign of J for the square and simple cubic lattices has the effect of making $\mathbf{k}=0$ a maximum of denominator (84), and placing minima at the vertices of τ. It is at these vertices that the Ising two- and three-dimensional models develop denominator zeros at a Néel temperature greater than zero, but for the same reason as before, the spherical antiferromagnet can exhibit similar behavior only in the three-dimensional case.

It is rigorously known that the plane triangular lattice with nearest-neighbor antiferromagnetic interaction cannot exhibit long-range order.[15] The reason may be traced to the fact that in this case

$$V(\mathbf{k})=2J[\cos(k_x)+\cos(\tfrac{1}{2}k_x+\tfrac{1}{2}\sqrt{3}k_y)+\cos(\tfrac{1}{2}k_x-\tfrac{1}{2}\sqrt{3}k_y)]\,, \tag{89}$$

[and therefore (84) as well] has its absolute minimum value along the entire boundary of the Brillouin zone τ (it is hexagonal), rather than just at a finite set of points. Thus, in spite of the fact that a "sharpening" mechanism for (84) apparently exists in the full Ising model cluster theory, it is not sufficiently effective to produce an integrable integrand with denominator zeros all along this boundary, at finite β.

We tentatively propose, therefore, a nonrigorous criterion for the nonoccurrence of antiferromagnetic order, for interactions not necessarily restricted to nearest neighbors: If $V(\mathbf{k})$ possesses a locus of absolute minima in τ or on the boundary of τ which consists at least in part of arcs of curves in two-dimensional systems, or surfaces for three-dimensional systems, then no long-range order should arise at finite temperature. $V(\mathbf{k})$'s with minima just at distinct points in two dimentsions, or, at worst, along space curves in three dimensions presumably can display a generalized sort of antiferromagnetic order, with a period possibly incommensurate with the underlying lattice.[16]

APPENDIX A

The coefficients $D_n(\alpha)$ may be obtained from the generating expression

$$1+\sum_{m=1}^{\infty}\frac{H_{2m}(\alpha)}{2^m(2m)!}x^m=\exp[\sum_{n=1}^{\infty}D_n(\alpha)x^n] \tag{A1}$$

by expanding the right-hand side, and equating coefficients of the same power of x. To accomplish the same end, we note first the Cauchy integral formula for the Hermite polynomials[17]

$$H_n(\alpha)=\frac{(-1)^n n!}{2\pi i}e^{\alpha^2}\oint\frac{e^{-z^2}dz}{(z-\alpha)^{n+1}}\,. \tag{A2}$$

[15] G. H. Wannier, Phys. Rev. **79**, 357 (1950).
[16] F. H. Stillinger, Jr., Phys. Rev. **126**, 1239 (1962).
[17] This integral formula follows immediately from the generating expression $H_n(x)=(-1)^n\exp(x)^2(d/dx)^n\exp(-x^2)$.

The contour of integration circles the pole once in the counterclockwise direction. If (A2) is substituted into each term on the left-hand side of (A1), and the resulting geometric series summed, one obtains

$$\exp[\sum_{n=1}^{\infty} D_n(\alpha)x^n]=1+\frac{e^{\alpha^2}x}{2(2\pi i)} \times \oint \frac{e^{-z^2}dz}{(z-\alpha)[z-\alpha+(x/2)^{1/2}][z-\alpha-(x/2)^{1/2}]}. \quad \text{(A3)}$$

To have insured the validity of the transformation leading to (A3), the contour necessarily must circumscribe the three roots of the denominator in this last expression.

The integral occurring in (A3) may easily be evaluated by residues. The result is

$$\sum_{n=1}^{\infty} D_n(\alpha)x^n=-\tfrac{1}{2}x+\ln\cosh[\alpha(2x)^{1/2}]. \quad \text{(A4)}$$

Comparison with the known power-series expansion of the right-hand side[18] provides the desired result

$$D_n(\alpha)=-\tfrac{1}{2}\delta_{1n}+(-1)^{n-1}\frac{2^{3n-1}(2^{2n}-1)B_{2n-1}}{n(2n)!}\alpha^{2n}. \quad \text{(A5)}$$

The B's are the Bernoulli numbers listed previously in Eq. (23). Because the Kronecker delta function δ_{1n} is nonvanishing only for $D_1(\alpha)$, only this one coefficient can be eliminated by proper choice of $\alpha>0$. From (A5) one finds that α must be set equal to $2^{-1/2}$ for this purpose. The D_n values quoted in Eq. (22) thereupon follow.

APPENDIX B

In the lattice gas interpretation of an Ising model, sites with spin $+1$ are regarded as occupied by molecules, and those with spin -1 are empty.[19] The lattice gas pair correlation function $\gamma(\mathbf{r}_{ij})$ for sites i and j is defined by

$$\gamma(\mathbf{r}_{ij})=\langle\nu_i\nu_j\rangle/\langle\nu_i\rangle\langle\nu_j\rangle-2\delta_{ij}, \quad \text{(B1)}$$

where the molecular occupation parameters ν have been introduced:

$$\nu_i=\tfrac{1}{2}(1+\mu_i), \text{ etc.} \quad \text{(B2)}$$

The Ornstein-Zernike direct correlation function $x(\mathbf{r}_{12})$ is implicitly defined in terms of γ by means of the convolution sum equation (integral equation for the continuum model)[20]

$$\gamma(\mathbf{r}_{ij})-1=x(\mathbf{r}_{ij})+\sum_{rl} x(\mathbf{r}_{il})\langle\nu_l\rangle[\gamma(\mathbf{r}_{lj})-1], \quad \text{(B3)}$$

where density is measured on a per-site basis.

For our field-free Ising models, each $\langle\nu_l\rangle=\frac{1}{2}$, and a Fourier transformation of (B3) allows the transform of x to be expressed in terms of the transform of $\gamma-1$.

$$X(\mathbf{k})=\Gamma(\mathbf{k})/[1+\tfrac{1}{2}\Gamma(\mathbf{k})]; \quad \text{(B4)}$$

we have set

$$\{X(\mathbf{k}),\Gamma(\mathbf{k})\}=\sum_{r}\exp(i\mathbf{k}\cdot\mathbf{r})\{x(\mathbf{r}),\gamma(\mathbf{r})-1\}. \quad \text{(B5)}$$

Also, $\gamma-1$ may be identified as our Ising model spin-pair correlation function ψ by inserting (B2) into (B1). Therefore, examination of Eq. (45) allows one to conclude:

$$\Gamma(\mathbf{k})=\frac{1+W(\mathbf{k},\beta)}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}-2. \quad \text{(B6)}$$

Insertion of this last expression into (B4) finally leads to a relation between the $\mathbf{k}$-space version of the direct correlation function and $W(\mathbf{k},\beta)$.

$$X(\mathbf{k},\beta)=2[1-2\beta V(\mathbf{k})]-4[1+W(\mathbf{k},\beta)]^{-1}. \quad \text{(B7)}$$

From this last result, we can immediately conclude that $x(\mathbf{r})$ for the spherical model ($\mathbf{k}$-independent W) is everywhere proportional to the pair interaction except at the origin.

[18] B. O. Pierce, *A Short Table of Integrals* (Ginn and Company, New York, 1929), 3rd ed., p. 92.

[19] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).

[20] L. S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam **17**, 193 (1914).