Ising-Model Reformulation. II. Relation to the Random-External-Field Method

FRANK H. STILLINGER, JR.
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 4 December 1964)

Starting with the previously derived vacuum-state expectation representation of the Ising partition function, an integral transform is applied to part of the Bose field operator arising from pair interactions, generating thereby the effect of random external fields. The remaining pair interaction is treated as a perturbation, whose effect is small in both the high- and the low-temperature extremes. The transformed part of the potential is selected first to generate a Markoff process, and the perturbation equations may then be regarded as conditions that the perturbation have no effect on either the partition function or the long-range order below the transition. In two dimensions, it is shown how the characteristic integral equation of the Markoff process reduces to the matrix eigenvalue problem solved by Onsager, in the limit of just nearest-neighbor interactions.

I. INTRODUCTION

THE first article[1] in this series was devoted to investigating some of the implications of a novel representation for the Ising-model partition function Z, viz., a vacuum-state expectation value of Bose field operators. Although expansion of Z and the spin distribution functions in Feynman diagrams proves useful in recovering the spherical model, and in developing a systematic correction procedure for this approximation, there invariably remains the ever-present many-body-problem embarassment of having to sum graphs of high connectivity for which no general analytical procedure is currently available.

For certain special pair interactions, it is known[2] that the problem of evaluation of Z is equivalent to finding the largest eigenvalue of an integral equation associated with a special Markoff process. One therefore possesses for this class of potentials effectively a means of summing all Feynman diagrams generated in the reformulation of Paper I, at any rate if the characteristic integral equation can be solved.

By now the properties of the integral equation for one-dimensional lattices are well known. We shall show below (Sec. III) the way in which a special case of the class of two-dimensional lattice Markoff processes yields an integral equation that may be precisely reduced to Onsager's eigenvalue problem.[3]

The major objective of this article is to utilize the structure of the reduction to Markoff processes as a starting point in a perturbation theory. Thus, if the original Ising model of interest possessed a spin-pair interaction

$$v(\mathbf{r}_{ij})\mu_i\mu_j,$$

for spins μ_i, $\mu_j=\pm 1$ located respectively at sites at $\mathbf{r}_i$ and $\mathbf{r}_j$, we write

$$v(\mathbf{r})=v_1(\mathbf{r})+v_2(\mathbf{r}), \tag{1}$$

where v_1 leads to the Markoff process, and $v_2=v-v_1$ is the perturbation. Because there is still considerable arbitrariness in the choice of v_1, however, we adopt the point of view (Sec. IV) that the perturbation equations may be used as criteria for selection of an optimum v_1. In particular, it will simultaneously be demanded that v_1 alone yield the same partition function as v, and that the zero-wave-vector susceptibilities for v_1 alone and for v be identical. Below a ferromagnetic transition temperature, this latter condition is equivalent to the demand that v_2 not affect the degree of long-range order.

The reasons for wanting to develop such a "perturbation" theory are twofold. First, we shall see that *both* at very high and at very low temperatures the theory carried only to finite order in v_2 is asymptotically exact. Secondly, the general feeling has developed[4] among students of cooperative phenomena that the analytic character of the extremely interesting critical singularities in various thermodynamic and structural quantities is independent of the finer details of the potential v for a lattice of given dimensionality. Thus, the usual stumbling block in most approximate order-disorder theories is neatly removed by the v_1 Markoff process, and the effect of v_2 on any selected model property is probably a minor elaboration at all temperatures.

Certainly not all Markoff processes generated by the random-external-field interpretation can be solved at present. It seems, however, that since the full range of critical singularities may already be contained in the partition function and spin distribution functions for Markoff v_1's, there is strong additional inducement for extending the list of soluble cases, with a view toward understanding classical phase transitions. By establishing a link to the Feynman-diagram technique developed at length in I, we hope to provide an additional

[1] F. H. Stillinger, Jr., Phys. Rev. 135, A1646 (1964); as is customary, we shall refer to this paper simply as I.
[2] M. Kac and E. Helfand, J. Math. Phys. 4, 1078 (1963); this paper contains references to pertinent related work.
[3] L. Onsager, Phys. Rev. 65, 117 (1944); B. Kaufman, *ibid.* 76, 1232 (1949); B. Kaufman and L. Onsager, *ibid.* 76, 1244 (1949).
[4] M. E. Fisher, in *The Classical Equilibrium Theory of Fluids*, edited by H. L. Frisch and J. L. Lebowitz (W. A. Benjamin Company, New York, 1964). This suspicion is reinforced by the fact that the behavior of certain two-dimensional lattices is rigorously known to undergo no substantial change upon addition of some second-neighbor interactions to the nearest-neighbor case; see: H. S. Green and C. A. Hurst, *Order-Disorder Phenomena* (Interscience Publishers, Inc., New York, 1964), Chap. 7.

weapon useful in the broad theoretical attack on phase transition problems in general, as well as on special Markoff processes in particular.

II. OPERATOR TRANSFORMATION

The partition function Z was expressed in Paper I in the following form[5]:

$$Z(\beta)=\langle 0|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle, \quad \beta=1/kT, \tag{2}$$

for any Ising model on a regular lattice with periodic boundary conditions, regardless of dimensionality or of range of the spin pair interaction potential v. The operators $\mathbf{M}$ (Hermitian) and $\mathbf{D}^\dagger$(non-Hermitian) are constructed from the boson creation ($\mathbf{b}^\dagger$) and annihilation ($\mathbf{b}$) operators for running excitation waves in the lattice[6]:

$$\mathbf{M}=\tfrac{1}{2}\sum_{\mathbf{k}}^{(\tau)} V(\mathbf{k})[\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}^\dagger(-\mathbf{k})+2\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}(\mathbf{k}) +\mathbf{b}(\mathbf{k})\mathbf{b}(-\mathbf{k})+1], \tag{3}$$

$$V(\mathbf{k})=\sum_{\mathbf{r}} v(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r}), \tag{4}$$

$$\mathbf{D}^\dagger=\sum_{n=2}^{\infty} N^{1-n}D_n \sum_{\mathbf{k}_1\cdots\mathbf{k}_{2n}}{}^{(\tau)}{}' \mathbf{b}^\dagger(\mathbf{k}_1)\cdots\mathbf{b}^\dagger(\mathbf{k}_{2n}), \tag{5}$$

$$D_n=\frac{(-1)^{n-1}2^{2n}}{\pi^{2n}(2n)!}\int_0^\infty \frac{y^{2n-1}dy}{\sinh y}. \tag{6}$$

The $\mathbf{k}$'s are the reciprocal lattice vectors inside the first Brillouin zone τ. The primed summation in (5) is further restricted by momentum conservation:

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

The spin-pair correlation function, which plays a central role in the statistical thermodynamics of cooperative phenomena, may similarly be expressed in terms of matrix elements of boson operators. For a translationally invariant system one has

$$\langle\mu_i\mu_j\rangle=\psi(r_{ij}) =\delta_{ij}+(NZ)^{-1}\sum_{\mathbf{k}}^{(\tau)}\exp(i\mathbf{k}\cdot\mathbf{r}_{ij}) \times\langle\mathbf{k},-\mathbf{k}|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle, \tag{7}$$

where δ_{ij} is the Kronecker delta. The states $\langle\mathbf{k},-\mathbf{k}|$ in Eq. (7) involve single excitations in states $\mathbf{k}$ and $-\mathbf{k}$, but none in any of the others. The higher order correlation functions have similar, but more complicated, matrix-element representations.

An integral transform may now be applied to the operator $\exp(-\beta\mathbf{M})$, which appears in both the Z and ψ expressions, (2) and (7). First write $\mathbf{M}=\mathbf{M}_1+\mathbf{M}_2$, in accord with the potential split-up of Eq. (1), where $\mathbf{M}_1$ and $\mathbf{M}_2$ have the same form as shown in Eq. (3) for $\mathbf{M}$, but with the transforms V_1 and V_2 of v_1 and v_2 replacing V. Since $\mathbf{M}_1$ and $\mathbf{M}_2$ commute,

$$\exp(-\beta\mathbf{M})=\exp(-\beta\mathbf{M}_2)\exp(-\beta\mathbf{M}_1). \tag{8}$$

An $N\times N$ matrix $(\mathbf{B})_{ij}$ may now be introduced, whose inverse is the cyclic matrix

$$(\mathbf{B}^{-1})_{ij}=-\beta v_1(\mathbf{r}_j-\mathbf{r}_i). \tag{9}$$

We assume that $-\beta v_1(0)$ is sufficiently large that $\mathbf{B}^{-1}$ will be positive definite. Then since the set of numbers $T(\mathbf{k})=-\beta V_1(\mathbf{k})$ for $\mathbf{k}$ in τ are precisely the N eigenvalues of $\mathbf{B}^{-1}$, the eigenvalues of the necessarily cyclic matrix $\mathbf{B}$ are $1/T(\mathbf{k})$. Accordingly, one may write the multiple Gaussian integral

$$\exp(-\beta\mathbf{M}_1)=\int d\mathbf{\Phi}P(\mathbf{\Phi})\exp(-\beta\mathbf{M}_0), \tag{10}$$

$$P(\mathbf{\Phi})=(2\pi)^{-N/2}|\mathbf{B}|^{1/2} \times\exp\{-\tfrac{1}{2}\sum_{\mathbf{k}}^{(\tau)}[T(\mathbf{k})]^{-1}\Phi_{\mathbf{k}}{}^*\Phi_{\mathbf{k}}\}, \tag{11}$$

$$\mathbf{M}_0=\sum_{\mathbf{k}}^{(\tau)}[(\Phi_{\mathbf{k}}{}^*/\beta)\mathbf{b}^\dagger(\mathbf{k})+(\Phi_{\mathbf{k}}/\beta)\mathbf{b}(\mathbf{k})], \tag{12}$$

$$\Phi_{\mathbf{k}}{}^*=\Phi_{-\mathbf{k}}.$$

The integrals $\int d\mathbf{\Phi}$ in Eq. (10) are over the N independent real and imaginary parts of the complex parameters $\Phi_{\mathbf{k}}$.

The new operator $\mathbf{M}_0$ is linear in the field operators, rather than bilinear as is $\mathbf{M}_1$, and it has exactly the same form as an $\mathbf{M}$ operator for an Ising model with independent spins interacting only with an external field.[1] The value of the external field corresponding to the set of $\Phi_{\mathbf{k}}$ which acts on the site at $\mathbf{r}_j$ is the real number φ_j/β, where

$$\varphi_j=N^{-1/2}\sum_{\mathbf{k}}^{(\tau)}\Phi_{\mathbf{k}}\exp(-i\mathbf{k}\cdot\mathbf{r}_j), \qquad \Phi_{\mathbf{k}}=N^{-1/2}\sum_{\mathbf{r}_j}\varphi_j\exp(i\mathbf{k}\cdot\mathbf{r}_j), \tag{13}$$

so that aside from a factor β the $\Phi_{\mathbf{k}}$ may be interpreted as the Fourier coefficients of an inhomogeneous external field acting on the set of spins. If we let the brackets $\langle\cdots\rangle$ denote averaging over the $\Phi_{\mathbf{k}}$'s with the normalized weight function $P(\mathbf{\Phi})$, Eq. (10) reads

$$\exp(-\beta\mathbf{M}_1)=\langle\exp(-\beta\mathbf{M}_0)\rangle, \tag{10'}$$

[5] For notational simplicity we disregard real external fields, though their inclusion would cause no fundamental problem.

[6] Unlike the case in I, we will allow the spin-pair potential $v(\mathbf{r})$ to be possibly nonvanishing at the origin. This requires retention of unity in the bracket of Eq. (3), which did not appear in the corresponding Eq. (20) of I.

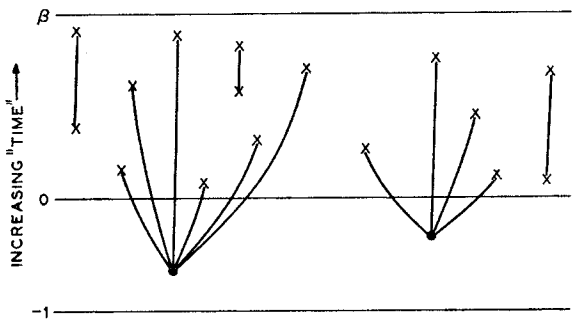

FIG. 1. Typical contribution to the partition function Z, which is expressed in the random-external-field notation of Eq. (14′), for the case of vanishing $\mathbf{M}_2$.

and partition function expression (2) becomes

$$Z(\beta)=\langle\langle 0|\exp(-\beta\mathbf{M}_2)\exp(-\beta\mathbf{M}_0)\exp(\mathbf{D}^\dagger)|0\rangle\rangle. \quad (14)$$

The external field averaging operation $\langle\cdots\rangle$ may equally well be carried out in terms of $\varphi_1\cdots\varphi_N$.[7] Substituting the second of Eqs. (13) into Eq. (11) yields

$$P(\mathbf{\Phi})=p(\boldsymbol{\varphi})=(2\pi)^{-N/2}|\mathbf{B}|^{1/2}\times\exp\{-\tfrac{1}{2}\sum_{j,l=1}^{N}(\mathbf{B})_{jl}\varphi_j\varphi_l\}; \quad (15)$$

upon recognizing the expression for the cyclic matrix $\mathbf{B}$ in terms of its eigenvalues and eigenfunctions,[8]

$$(\mathbf{B})_{jl}=\sum_{\mathbf{k}}^{(\tau)}[NT(\mathbf{k})]^{-1}\exp[i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_j)]. \quad (16)$$

The advantage of using the variables $\mathbf{\Phi}$ is of course the diagonal character of $P(\mathbf{\Phi})$.

We shall initially proceed to examine the character of the Feynman diagrams generated by the operators in Eq. (14), in the special circumstance of vanishing v_2 and $\mathbf{M}_2$ (which case will be denoted by subscript "one"),

$$Z_1(\beta)=\langle\langle 0|\exp(-\beta\mathbf{M}_0)\exp(\mathbf{D}^\dagger)|0\rangle\rangle. \quad (14')$$

In the final section we take up again the more general case of nonzero $\mathbf{M}_2$. As was demonstrated in I, application of Wick's theorem to "time-ordered" field operators in a representation such as (14′) permits one to draw Feynman diagrams on a pair of parallel strips of width unity [for $\exp(\mathbf{D}^\dagger)$] and of width β [for $\exp(-\beta\mathbf{M}_0)$].

Figure 1 illustrates a typical contribution to Z_1 for the case in hand.[9] One notices that the graph may consist of several disconnected parts (as determined by the manner in which the application of Wick's theory has contracted pairs of operators) which are either of two types: (1) "bursts" of four or a larger even number of excitations originating in the lower strip [see Eq. (5) for $\mathbf{D}^\dagger$], or (2) disconnected line segments confined wholly to the upper strip. The crosses in the upper strip will be called "external field vertices" since each arises from either a destruction (upper graph-line terminus) or creation (lower graph-line terminus) operator from $\mathbf{M}_0$ in Eq. (12), and therefore carries with it a Φ_k or Φ_k^* factor. The lower strip bursts carry factors D_n.

One can now proceed to sum up the contributions of all graphs of $Z_1(\beta)$. Besides the upper strip factors already mentioned for each graph, it is necessary to include:

(1) $(-\beta)^{2m}/(2m)!$ from expansion of $\exp(-\beta\mathbf{M}_0)$, where $2m$ is the (necessarily even) number of $\mathbf{M}_0$ operators;

(2) $\prod_{j=2}^{\infty}(N^{1-j}D_j)^{n_j}/n_j!$ from a term in expansion of $\exp(\mathbf{D}^\dagger)$ involving n_2 bursts of 2×2 excitations, $\cdots$, n_j burst of $2j$, $\cdots$;

(3) $(2m)!/(2\sum jn_j)!(2m-2\sum jn_j)!$ ways of dividing $\mathbf{M}_0$'s between contractions with themselves and with $\mathbf{D}^\dagger$'s;

(4) $(2m-2\sum jn_j)!/(2!)^{m-\sum jn_j}(m-\sum jn_j)!$ ways of contracting $2m-2\sum jn_j$ $\mathbf{M}_0$'s among themselves to give the simple line segments in the upper region;

(5) $(2\sum jn_j)!/\prod_{j=2}^{\infty}[(2j)!]^{n_j}$ ways of partitioning $2\sum jn_j$ $\mathbf{M}_0$'s among bursts for contractions;

(6) $\prod_{j=2}^{\infty}[(2j)!]^{n_j}$ ways of actually contracting the $\mathbf{M}_0$'s within already-assigned bursts. The result is found straightforwardly to be

$$Z_1(\beta)=\langle\exp\{\tfrac{1}{2}\sum_{\mathbf{k}}^{(\tau)}\Phi_k^*\Phi_k+\sum_{j=2}^{\infty}N^{1-j}D_j\times\sum_{\mathbf{k}_1\cdots\mathbf{k}_{2j}}^{(\tau)\prime}\Phi_{\mathbf{k}_1}\cdots\Phi_{\mathbf{k}_{2j}}\}\rangle. \quad (17)$$

This may easily be converted to a more familiar expression in Gaussian random variable theory[2] by eliminating the Φ's with the second Eq. (13):

$$Z_1(\beta)=\langle\prod_{l=1}^{N}\cosh\varphi_l\rangle. \quad (18)$$

To obtain this result, it is necessary to utilize an identity satisfied by the coefficients D_j[10]:

$$\sum_{j=2}^{\infty}D_jx^j=-\tfrac{1}{2}x+\ln\cosh\sqrt{x}. \quad (19)$$

Precisely the same type of diagram summation may be carried out for the nondiagonal matrix element appearing in the pair correlation function of Eq. (7) after application of the same integral transform to $\mathbf{M}_1$,

[7] The transformation Jacobian for $\mathbf{\Phi}\to\boldsymbol{\varphi}$ is unity.

[8] P. O. Löwdin, R. Pauncz, and J. de Heer, J. Math. Phys. **1**, 461 (1960); J.-L. Calais and K. Appel, *ibid.* **5**, 1001 (1964).

[9] It should be borne in mind here that the outer bracket ($\langle\langle\cdots\rangle\rangle$) averaging operation is to be carried out *after* summation over diagrams has been performed; we temporarily suppose therefore that the Φ_k are a fixed set of quantities.

[10] See Eq. (A4) of Paper I and the text immediately following.

again assuming $\mathbf{M}_2=0$,

$$\psi_1(\mathbf{r}_{ij})=\delta_{ij}+N^{-1}\sum_{\mathbf{k}}^{(\tau)}\exp(i\mathbf{k}\cdot\mathbf{r}_{ij}) \times\frac{\langle\langle\mathbf{k},-\mathbf{k}|\exp(-\beta\mathbf{M}_0)\exp(\mathbf{D}^\dagger)|0\rangle\rangle}{\langle\langle 0|\exp(-\beta\mathbf{M}_0)\exp(\mathbf{D}^\dagger)|0\rangle\rangle}. \quad (20)$$

Figures 2(a) and 2(b) show that the two remaining excitations in $\langle\mathbf{k},-\mathbf{k}|$, the state above the upper strip, may be indicated by bringing two lines upward out of the upper strip. As exhibited in Fig. 2, the two "external" vertices terminating this pair of special lines either may or may not be internally connected to one another.

The graphs generated by the numerator of Eq. (20) therefore consist of the same parts as encountered already in evaluation of Z_1, *plus* the new parts connected to the upper vertices. Graph summation will thus yield (inside the averaging brackets for the numerator) a product of two factors; the first appears in Eq. (17) or (18), and the second is the sum over parts connected to the two external vertices. We shall not repeat the lengthy but uninstructive algebra here; one finds

$$\psi_1(\mathbf{r}_{ij})=\delta_{ij}+(NZ_1)^{-1}\sum_{\mathbf{s}}\langle\{\prod_{l=1}^{N}\cosh\varphi(r_l)\} \times\{\tanh\varphi(\mathbf{r}_j+\mathbf{s})\tanh\varphi(\mathbf{r}_i+\mathbf{s}) -\delta_{ij}\tanh^2\varphi(\mathbf{r}_i+\mathbf{s})\}\rangle. \quad (21)$$

Owing to the translational invariance of the lattice system, each of the N terms in the $\mathbf{s}$ sum in Eq. (21) will be equal. Therefore, when the sites i and j are distinct,

$$\psi_1(r_{ij})=Z_1^{-1}\langle\{\prod_{l=1}^{N}\cosh\varphi_l\}\tanh\varphi_i\tanh\varphi_j\rangle. \quad (22)$$

This result is a standard form in the extant theory of random external fields.[11] In a similar way, one could sum Feynman diagrams for higher order spin-correlation functions $\langle\mu_i\mu_j\cdots\mu_t\rangle$ for larger numbers of discrete sites, with the resulting insertion of the requisite larger number of tanh factors in an expression of type (22).

III. ONSAGER'S EIGENVALUE PROBLEM

The interactions $v_1(\mathbf{r})$ of interest here are those inducing an especially simple product representation for $p(\boldsymbol{\varphi})$, which will depend upon the lattice under consideration. Thus, for the linear lattice, p will be supposed to split into factors for each nearest-neighbor bond[2]

$$p(\boldsymbol{\varphi})=(2\pi)^{-N/2}|\mathbf{B}|^{1/2}q(\varphi_1;\varphi_2)q(\varphi_2;\varphi_3)\cdots q(\varphi_{N-1};\varphi_N)q(\varphi_N;\varphi_1), \quad (23)$$

[11] See Eq. (5.1) of Ref. 2.

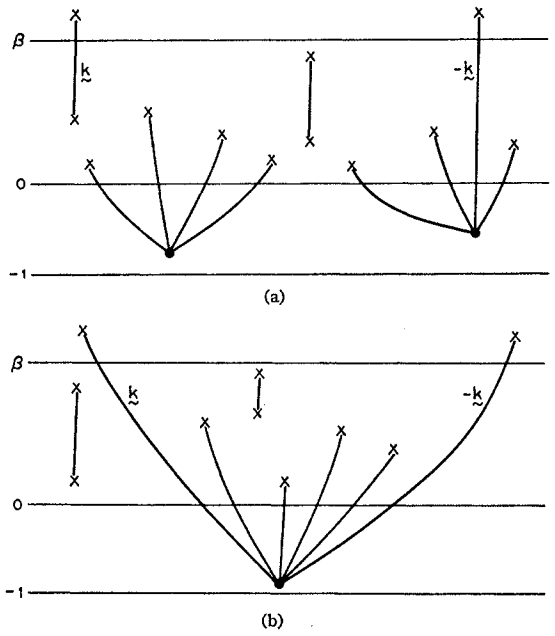

FIG. 2. Diagrams arising in evaluation of the $\mathbf{M}_2=0$ pair-correlation-function numerator, Eq. (19). The lines terminating in vertices above the upper strip, and labeled $\mathbf{k}$ and $-\mathbf{k}$, are the two excitations in the final state $\langle\mathbf{k},-\mathbf{k}|$. Cases (a) and (b) exhibit, respectively, the possibilities that these external vertices may either be disconnected or connected.

in which the function q depends only on the two external fields acting on adjacent sites. In the case of a two-dimensional lattice (we choose the rectangular lattice for definiteness) we again assume that p consists of factors corresponding to the nearest-neighbor links ($N=mn$):

$$p(\boldsymbol{\varphi})=(2\pi)^{-mn/2}|\mathbf{B}|^{1/2}\prod_{j=1}^{m}\prod_{l=1}^{n}q_x(\varphi_{jl};\varphi_{j+1,l}) \times q_y(\varphi_{jl};\varphi_{j,l+1}) =(2\pi)^{-mn/2}|\mathbf{B}|^{1/2}\prod_{l=1}^{m}Q(\boldsymbol{\varphi}_l,\boldsymbol{\varphi}_{l+1}), \quad (24)$$

$$Q(\boldsymbol{\varphi}_l,\boldsymbol{\varphi}_{l+1})=\prod_{j=1}^{n}q_x^{1/2}(\varphi_{jl};\varphi_{j+1,l})q_y(\varphi_{jl};\varphi_{j,l+1}) \times q_x^{1/2}(\varphi_{j,l+1};\varphi_{j+1,l+1}).$$

The last form shown for p in (24) has been written as the same linear sequence of factors as in (23), but now the variables $\boldsymbol{\varphi}_l$ and $\boldsymbol{\varphi}_{l+1}$ in each factor Q are a pair of sets of n external fields in vertical columns next to one another, columns l and $l+1$. In exactly the same way, p for a three-dimensional lattice would be taken as a linear sequence of Q's whose variables were the spins in successive *layers* of the lattice.

In the case of the planar rectangular lattice to which Eq. (24) applies, one sees from Eq. (15) that $\mathbf{B}$ will have nonvanishing matrix elements only for nearest neigh-

bors,

$$\begin{aligned} B_{kl}&=0 \quad k,\, l \text{ not neighbors or the same site;}\\ &=b_x \quad k,\, l \text{ horizontal neighbors;}\\ &=b_y \quad k,\, l \text{ vertical neighbors;}\\ &=a \quad k=l. \end{aligned} \tag{25}$$

Given these matrix elements it is easy to obtain the eigenvalues $\lambda(\mathbf{k})$ of the cyclic matrix $\mathbf{B}$ [8]:

$$\lambda(\mathbf{k})=a+2b_x\cos k_x+2b_y\cos k_y. \tag{26}$$

Here k_x and k_y are the x and y components of the vectors $\mathbf{k}$ inside τ.

It has already been remarked that $\lambda(\mathbf{k})=1/T(\mathbf{k})$, and we invert Eq. (16) to find

$$\begin{aligned} -\beta v_1(\mathbf{r}_l-\mathbf{r}_j)&=(\mathbf{B}^{-1})_{jl}\\ &=(mn)^{-1}\sum_{\mathbf{k}}^{(\tau)}\frac{\exp[-i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_j)]}{a+2b_x\cos k_x+2b_y\cos k_y}\\ &=\frac{1}{\tau}\int_\tau\frac{\exp[-i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_j)]}{a+2b_x\cos k_x+2b_y\cos k_y}d\mathbf{k}. \end{aligned} \tag{27}$$

The last expression is the permissible integral limit for the Brillouin zone sum, and the resulting set of admissible v_1's following from the assumed form (24) for $p(\varphi)$ are proportional to the Green's function for the finite difference version of the Laplacian operator in two dimensions. Similarly, the linear and simple cubic lattices would permit v_1's proportional to their own Green's functions, which would involve one and three cosine functions, respectively, in their integral denominators, instead of the two in Eq. (27).[12]

The reason for desiring a $p(\varphi)$ which is a linear sequence of factors is that Z_1 in Eq. (14′) becomes an m-fold iterated kernel, and so

$$\ln Z_1\sim\ln[(2\pi)^{-mn/2}|\mathbf{B}|^{1/2}\lambda_{\max}{}^m], \tag{28}$$

where $\lambda_{\max}$ is the largest eigenvalue of the integral equation,

$$\lambda f(\varphi)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}d\varphi' K(\varphi,\varphi')f(\varphi'), \tag{29}$$

$$K(\varphi,\varphi')=Q(\varphi,\varphi')\prod_{j=1}^{n}\cosh^{1/2}(\varphi_j)\cosh^{1/2}(\varphi_j'). \tag{30}$$

Equation (29) may be regarded as the characteristic integral equation of a Markoff process. The process is one-dimensional for the linear lattices, but is n-dimensional for the rectangular lattice which we shall continue to examine at some length for the remainder of this section.

[12] The Green's functions for the linear lattice may be integrated by elementary means, and those for the simple cubic lattice have been tabulated in: A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman, and H. W. Milnes, Royal Belgian Academy 14, Part 7, 15 (1960).

If b_x and b_y are much smaller than a in Eq. (27), the two denominator cosine terms represent small variations, and so one has

$$-\beta v_1(\mathbf{r}_l-\mathbf{r}_j)\cong\frac{1}{(2\pi)^2 a}\int_\tau\left[1-\frac{2b_x}{a}\cos k_x-\frac{2b_y}{a}\cos k_y\right]\times\exp(-i\mathbf{k}\cdot\mathbf{r}_{lk})d\mathbf{k}, \tag{31}$$

where we recall that τ is a $2\pi\times2\pi$ square in k space. The integral in Eq. (31) vanishes unless $\mathbf{r}_{lk}$ is either zero or equal to a nearest-neighbor distance.

$$\begin{aligned} -\beta v_1(0)&=1/a,\\ -\beta v_1(\mathbf{u}_x)&=-b_x/a^2,\\ -\beta v_1(\mathbf{u}_y)&=-b_y/a^2; \end{aligned} \tag{32}$$

($\mathbf{u}_x$ and $\mathbf{u}_y$ here stand for the primitive lattice vectors). If we therefore write in the general case

$$\begin{aligned} a(\gamma)&=\exp(-\gamma)/\beta J_x{}^{1/2}J_y{}^{1/2},\\ b_x(\gamma)&=-\exp(-2\gamma)/\beta J_y,\\ b_y(\gamma)&=-\exp(-2\gamma)/\beta J_x, \end{aligned} \tag{33}$$

then allowing γ to become very large yields in the limit an interaction which vanishes beyond nearest neighbors, and for them

$$\begin{aligned} v_1(\mathbf{u}_x)&=-J_x,\\ v_1(\mathbf{u}_y)&=-J_y. \end{aligned} \tag{34}$$

Therefore [aside from the trivial shift in energy due to spin self-interactions $v_1(0)$], we have recovered the nearest-neighbor Ising model in two dimensions. For arbitrary values of γ the interaction v_1 will tend to spread out beyond the nearest neighbors, but will always decay to zero with increasing distance.[13]

Written out explicitly, the kernel K in Eq. (30) is seen to have the following form:

$$\begin{aligned} K(\varphi,\varphi')=\prod_{j=1}^{n}&\cosh^{1/2}(\varphi_j)\exp[-\tfrac{1}{4}[a(\gamma)](\varphi_j{}^2+\varphi_j'{}^2)\\ &-\tfrac{1}{2}[b_y(\gamma)](\varphi_j\varphi_{j+1}+\varphi_j'\varphi_{j+1}')-b_x(\gamma)\varphi_j\varphi_j']\\ &\times\cosh^{1/2}(\varphi_j'). \end{aligned} \tag{35}$$

Having just noticed that nearest-neighbor Ising models correspond to b's very much smaller than a, we examine the kernel K_0 resulting from neglect of the b's in Eq. (35)

$$\begin{aligned} K_0(\varphi,\varphi')=\prod_{j=1}^{n}&\cosh^{1/2}(\varphi_j)\exp[-\tfrac{1}{4}[a(\gamma)]\\ &\times(\varphi_j{}^2+\varphi_j'{}^2)]\cosh^{1/2}(\varphi_j'), \end{aligned} \tag{36}$$

[13] We must always have $a>2b_x+2b_y$ to have insured the positive-definiteness of $\mathbf{B}^{-1}$, and hence the convergence of integral (27).

and its associated integral equation,

$$\lambda_0 f_0(\varphi)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}d\varphi' K_0(\varphi,\varphi')f_0(\varphi'). \quad (37)$$

A nodeless eigenfunction belongs to the maximum eigenvalue according to Perron's theorem,[14] and one easily verifies that the corresponding f_0 and λ_0 are

$$f_0(\varphi_1\cdots\varphi_n)=C\prod_{j=1}^{n}\cosh^{1/2}(\varphi_j)\exp(-(\tfrac{1}{4}a)\varphi_j^2), \quad (38)$$

$$\lambda_0=\int_{-\infty}^{+\infty}d\varphi_1'\cdots\int_{-\infty}^{+\infty}d\varphi_n'\prod_{j=1}^{n}\cosh(\varphi_j')\times\exp(-(\tfrac{1}{2}a)\varphi_j'^2)$$
$$=[(2\pi/a)^{1/2}\exp(1/2a)]^n; \quad (39)$$

C is a suitable normalizing constant. When it is recognized that $|\mathbf{B}|=a^{mn}$ for this case of negligible b's, substitution of λ_0 into the partition-function expression (28) yields

$$\ln Z_0\sim mn/2a=-\tfrac{1}{2}mn\beta v_1(0). \quad (40)$$

This is the correct result for the mn spins subject only to their self-interaction.

One therefore concludes, even in the $\gamma\to\infty$ limit of nearest-neighbor interactions, where the b's become very much smaller than a, that b_x and b_y are nevertheless still the source of the pair interactions. Their role may be clarified as follows. It may first be recognized that for very large γ, and hence small $a(\gamma)$, that $f_0(\varphi_1\cdots\varphi_n)$ has sharp maxima near the 2^n points

$$\varphi_1=\pm 1/a,\quad \varphi_2=\pm 1/a,\cdots,\varphi_n=\pm 1/a. \quad (41)$$

Therefore we introduce new variables,

$$\bar\varphi_j=a\varphi_j,\quad \bar\varphi_j'=a\varphi_j', \quad (42)$$

so that in terms of the new variables, the maxima occur very close to $(\pm 1,\pm 1,\cdots,\pm 1)$. Let

$$\Delta(\bar\varphi)=\exp(-\bar\varphi^2/4a); \quad (43)$$

then one has indeed that

$$f_0(\varphi_1\cdots\varphi_n)=f_0(\bar\varphi_1\cdots\bar\varphi_n)$$
$$=C'\sum_{\mu_1\cdots\mu_n=\pm 1}\prod_{j=1}^{n}\Delta[\bar\varphi_j-(-1)^{\frac{1}{2}(1+\mu_j)}] \quad (44)$$

with C' a normalizing constant), to within terms of negligible order. By making the same variable change (42) in the integral Eq. (36) one obtains

$$\lambda_0 f_0(\bar\varphi)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}d\bar\varphi'\bar K_0(\bar\varphi,\bar\varphi')f_0(\bar\varphi'), \quad (45)$$

in which the transformed kernel $\bar K_0$ may be written with sufficient accuracy as

$$\bar K_0(\bar\varphi,\bar\varphi')=[\exp(1/2a)/2a]^n\prod_{j=1}^{n}[\Delta(\bar\varphi_j+1)+\Delta(\bar\varphi_j-1)][\Delta(\bar\varphi_j'+1)+\Delta(\bar\varphi_j'-1)]$$
$$=[\exp(1/2a)/2a]^n\sum_{\mu_1\cdots\mu_n=\pm 1}\sum_{\mu_1'\cdots\mu_n'=\pm 1}\prod_{j=1}^{n}\Delta[\bar\varphi_j-(-1)^{\frac{1}{2}(1+\mu_j)}]\Delta[\bar\varphi_j'-(-1)^{\frac{1}{2}(1+\mu_j')}]. \quad (46)$$

In the nearest-neighbor limit, then, both f_0 and $\bar K_0$ are characterized by extremely sharp and narrow maxima.

How do b_x and b_y modify this simple picture? We shall now write integral Eq. (29) as

$$\lambda f(\bar\varphi)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}d\bar\varphi'\bar K(\bar\varphi,\varphi')f(\bar\varphi'), \quad (47)$$

with

$$\bar K(\bar\varphi,\bar\varphi')=\bar K_0(\varphi,\bar\varphi')\prod_{j=1}^{n}\exp\left[-\frac{b_y}{2a^2}(\bar\varphi_j\bar\varphi_{j+1}+\bar\varphi_j'\bar\varphi_{j+1}')-\frac{b_x}{a^2}\bar\varphi_j\bar\varphi_j'\right]. \quad (48)$$

Since b_x/a^2 and b_y/a^2 are of order unity in the $\gamma\to\infty$ limit, the factors multiplying $\bar K_0$ on the right-hand side of Eq. (48) act essentially as constants over the narrow width of each of the peaks of K_0. Hence $\bar K$ has the same behavior as $\bar K_0$, except the newly inserted factors change the magnitudes of its maxima; unlike $\bar K_0$ they are now not all the same height. Therefore

$$\bar K(\bar\varphi,\bar\varphi')=[\exp(1/2a)/2a]^n\sum_{\mu_1\cdots\mu_n=\pm 1}\sum_{\mu_1'\cdots\mu_n'=\pm 1}L(\mathfrak{y},\mathfrak{y}')\prod_{j=1}^{n}\Delta[\bar\varphi_j-(-1)^{\frac{1}{2}(1+\mu_j)}]\Delta[\bar\varphi_j'-(-1)^{\frac{1}{2}(1+\mu_j')}], \quad (49)$$
$$L(\mu,\mu')=\exp[\tfrac{1}{2}(\beta J_y)(\mu_j\mu_{j+1}+\mu_j'\mu_{j+1}')+\beta J_x\mu_j\mu_j'].$$

[14] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill Book Company, Inc., New York, 1960), p. 278.

On account of the differing peak heights exhibited by $\bar{K}$, one expects similar behavior for the eigenfunctions $\bar{f}(\bar{\varphi})$. Noting that

$$\int_{-\infty}^{+\infty} d\bar{\varphi}'\Delta^2[\bar{\varphi}'-(-1)^S]=(2\pi a)^{1/2}, \tag{50}$$

one finds by substitution of

$$f(\varphi)=\sum_{\mu_1\cdots\mu_n=\pm 1} C(\mu_1\cdots\mu_n) \times\prod_{j=1}^{n}\Delta[\bar{\varphi}_j-(-1)^{\frac{1}{2}(1+\mu_j)}] \tag{51}$$

and kernel (49) into integral Eq. (47) that a solution will be obtained, provided that the set of 2^n constants $C(\mu_1\cdots\mu_n)$ satisfy the matrix equation

$$\bar{\lambda}\mathbf{C}=\mathbf{L}\mathbf{C}. \tag{52}$$

Here the function $L(\mathfrak{y},\mathfrak{y}')$ is represented by a $2^n\times 2^n$ matrix, and the set of constants $C(\mathfrak{y})$ by a 2^n-component column vector. In Eq. (52) the $\bar{\lambda}$ is simply related to λ by

$$\bar{\lambda}=(2a/\pi)^{n/2}\exp(-n/2a)\lambda. \tag{53}$$

The matrix eigenvalue problem (52) is precisely the one solved originally for the rectangular Ising model by Onsager.[3] In view of Eqs. (28) and (53),

$$(mn)^{-1}\ln Z_1\sim-\ln 2-\tfrac{1}{2}\beta v_1(0)+n^{-1}\ln\bar{\lambda}_{\max}; \tag{54}$$

the $-\ln 2$ is required by the high-temperature normalization of Z_1:

$$\lim_{\beta\to 0} Z_1(\beta)=1, \tag{55}$$

since

$$\lim_{\beta\to 0}\lambda_{\max}=2^n. \tag{56}$$

IV. PERTURBATION THEORY

Although the criteria for selection of the optimum Markoff process potential v_1 may readily be carried out by means of Feynman diagram summations, we choose here to work in the more conventional and direct space of the spins themselves. One has

$$\exp[N\beta v_2(0)/2]Z(\beta) =\Big\langle\sum_{\mu_1\cdots\mu_N=\pm 1}\exp\{-\sum_{i=1}^{N}\varphi_i\mu_i-\beta\sum_{i<j=1}^{N}v_2(\mathbf{r}_{ij})\mu_i\mu_j\}\Big\rangle \tag{57}$$

for the partition function, excluding the v_2 part of the spin self-energies. This expression may be rewritten

$$\exp[N\beta v_2(0)/2]Z_1(\beta)\cdot\Big\langle\sum_{\mu_1\cdots\mu_N=\pm 1}\exp\{-\sum_{i=1}^{N}\varphi_i\mu_i-\beta\sum_{i<j=1}^{N}v_2(\mathbf{r}_{ij})\mu_i\mu_j\}\Big\rangle/Z_1(\beta)$$

$$=\exp[N\beta v_2(0)/2]Z_1(\beta)[Z_1(\beta)]^{-1}\Big\langle\sum_{\mu_1\cdots\mu_N=\pm 1}\exp\{-\sum_{i=1}^{N}\varphi_i\mu_i\}\{1-\beta\sum_{i<j=1}^{N}v_2(\mathbf{r}_{ij})\mu_i\mu_j+\cdots\}\Big\rangle$$

$$=\exp[N\beta v_2(0)/2]Z_1(\beta)\{1-\beta\sum_{i<j=1}^{N}v_2(\mathbf{r}_{ij})\psi_1(r_{ij})+\cdots\}, \tag{58}$$

where the exponential has been expanded under the assumption that successive terms are negligibly small, and Z_1 and ψ_1 are the previously introduced partition function and pair-correlation function for v_1 alone.

Assuming that only the term linear in v_2 in Eq. (58) need be retained, the invariance of $\exp[N\beta v_2(0)/2]Z$ to the presence of v_2 obviously demands

$$\sum_{r>0} v_2(\mathbf{r})\psi_1(\mathbf{r})=0. \tag{59}$$

Thus the pair-correlation function in the unperturbed system may be considered a weight function such that the correspondingly weighted sum of v_2 over all positive pair distances is to vanish. This is our first criterion. It could straightforwardly be extended to higher orders in v_2 if desired, involving higher order distribution functions in the v_1 system.

The pair-correlation function in the perturbed system may be written in the following form [equivalent to Eq. (22)]:

$$\psi(\mathbf{r}_{ij})=\frac{\sum_{\mu_1\cdots\mu_N=\pm 1}\langle\mu_i\mu_j\exp\{-\sum_{k=1}^{N}\varphi_k\mu_k-(\beta/2)\sum_{k\neq l=1}^{N}v_2(\mathbf{r}_{kl})\mu_k\mu_l\}\rangle}{\sum_{\mu_1\cdots\mu_N=\pm 1}\langle\exp\{-\sum_{k=1}^{N}\varphi_k\mu_k-(\beta/2)\sum_{k\neq l=1}^{N}v_2(\mathbf{r}_{kl})\mu_k\mu_l\}\rangle}. \tag{60}$$

The first criterion, Eq. (59), ensures invariance of the denominator, so v_2 may be dropped from it. If the numerator then is expanded through terms linear in v_2 one obtains formally ($\mathbf{r}_{ij}>0$)

$$\psi(ij)=\psi_1(ij)-(\beta/2)\sum_{\substack{k,l=1\\(k\neq l;\,k,l\neq i,\,j)}}^{N} v_2(kl)\eta_1(ijkl)$$

$$-2\beta\sum_{\substack{l=1\\(\neq i,\,j)}}^{N} v_2(il)\psi_1(jl)-\beta v_2(ij). \quad (61)$$

$\eta_1(ijkl)$ is the mean value of the product $\mu_i\mu_j\mu_k\mu_l$ in the unperturbed system; it is given by an expression of type (60), with this quadruplet product in the numerator summand replacing the pair product. Our second criterion will demand that the sum

$$\sum_{r>0}\psi(\mathbf{r})$$

be invariant to the perturbing potential v_2. This requires that the last three terms on the right side of Eq. (61), when summed over all $\mathbf{r}_{ij}>0$, give zero,

$$0=\sum_{\mathbf{r}_{ij}>0}\{\tfrac{1}{2}\sum_{\substack{k,l=1\\(k\neq l;\,k,l\neq i,\,j)}}^{N} v_2(kl)\eta_1(ijkl)$$

$$+2\sum_{\substack{l=1\\(\neq i,\,j)}}^{N} v_2(il)\psi_1(jl)+2v_2(ij)\}. \quad (62)$$

At temperatures sufficiently high that the unperturbed lattice of spins exhibits no long-range order, $\eta_1(ijkl)$ vanishes if the four spins indicated are separated from one another by more than a few lattice spacings. Below a ferromagnetic transition temperature T_c, though, η_1 approaches the fourth power of the degree of long-range order for mutually separated configurations. To eliminate the apparent $T<T_c$ divergence of the first sum in Eq. (62), we may use the first criterion, Eq. (59), to subtract the vanishing quantity

$$\tfrac{1}{2}\psi_1(ij)\sum_{k\neq l}v_2(kl)\psi_1(kl),$$

with the resulting second criterion

$$0=\sum_{\mathbf{r}_{ij}>0}\{\tfrac{1}{2}\sum_{\substack{k,l=1\\(k\neq l;\,k,l\neq i,\,j)}}^{N} v_2(kl)[\eta_1(ijkl)$$

$$-\psi_1(ij)\psi_1(kl)]+2\sum_{\substack{l=1\\(\neq i,\,j)}}^{N} v_2(il)\psi_1(lj)$$

$$+v_2(ij)[1-2\psi_1^2(ij)]\}. \quad (63)$$

Below T_c, the unperturbed pair-correlation function $\psi_1(\mathbf{r})$ likewise fails to approach zero as $r\to\infty$. Consequently, the middle term in Eq. (63) also will diverge. But no use of the first criterion can eliminate this divergence. As a result, one is forced to the conclusion that for $T<T_c$ the second criterion, Eq. (63), reduces to

$$\sum_{r>0}v_2(\mathbf{r})=0, \quad (64)$$

to within order N^{-1}, since this is the only way that the more complicated expression (63) could vanish. Since $\psi_1(\mathbf{r})$ continuously develops a long-range tail as T is lowered through T_c, one sees that the simple form (64) for the more complex condition (63) is attained in a smooth, continuous fashion.

Equations (59) and (63) are implicit relations (through ψ_1 and η_1) for the optimum v_1 choice, which are valid through first order in the perturbing potential v_2. Clearly our criteria could be extended to higher order in v_2, but at the expense of involving correlation functions for more than four spins in the unperturbed system. At very high temperature, the first-order results always suffice, since v_2 appears divided by kT. Also, at the low-temperature extreme the perturbing effect of v_2 is small due to the "stiffness" of the nearly complete long-range order. In this latter regime $\psi_1(\mathbf{r})$ is, for all practical purposes, the constant unity, so Eqs. (59) and (64) become identical to one another and to the result of the mean field theory (asymptotically exact at low temperature) under the invariant long-range order condition.

As a final comment, we note that when our two basic criteria are applied to some initial interaction $v(\mathbf{r})$ the optimum Markoff potential v_1 will not be the same at all temperatures. Rather, $Z_1(\beta)$ and the unperturbed correlation functions of various orders will be determined by a potential $v_1(\mathbf{r},\beta)$ containing an implicit temperature variation. In taking derivatives of Z_1 to obtain the mean energy and specific heat, one must remember to account for these implicit variations.