Journal of Statistical Physics, Vol. 7, No. 3, 1973

Generating Functionals and the Ising Model

Clas Blomberg[1]

Received April 21, 1972

The Ising model is studied by the generating functional approach in order to provide a better understanding of that method. It is shown how to derive a general solution of a functional equation in terms of infinite-dimensional integrals. This solution is not unique; the different possibilities are characterized by different paths of integration. Further, the saddle point approximation is used for the integrals in order to obtain second-order correlation functions. It is shown that besides the "normal" solution, one obtains several anomalous ones, which correspond directly to the nonphysical solutions of the transfer matrix method for treating the partition function. It is also shown that only the correct solution can give a realistic behavior of the correlation function at large distances. The relevance of the saddle point methods for describing phase transitions is also discussed.

KEY WORDS: Correlation functions; functional formalism; Ising model; integral solutions; saddle point approximation.

1. INTRODUCTION

Functional methods providing an ultimate hope for going beyond conventional approximation methods are now widely used in manybody theory and statistical mechanics.[1,2] Their essential attraction lies in the fact that they formulate these formidable problems in an appealing and condensed (although formal) way. Their difficulties are mainly of a mathematical nature, and especially when dealing with functional integrals, their rigorous meaning may be questioned. Further, they have not been able to provide

[1] Department of Theoretical Physics, Royal Institute of Technology, Stockholm, Sweden.

much more than conventional approximation methods. In order to look for their potentialities for the provision of more general methods, it seems to be important to investigate them in detail for models such as the Ising model, where many exact results are known.

Recently, Schwabl[3] has studied the generating functional of the correlation functions for the Ising model, and obtained a functional differential equation of this. The general approach is similar to that of the present author.[4] In Ref. 4, the generating functional approach to the continuum gas was studied and functional integrals were obtained as formal solutions of the basic equations. These integrals were not unique, since different integrations paths could be admitted. This ambiguity occurs since we are dealing with an infinite system where no end can be assigned for the chain of equations of correlation functions. It was argued that the different solutions may correspond to different phases and that they are intimately connected with the complex limiting structure of the partition function. Further, molecular field equations occur very naturally from this approach as conditions for saddle points of the integrals.[5] It is then an interesting question whether each solution corresponds to a unique saddle point solution, and if therefore the number of molecular field solutions reflects the nonuniqueness of the basic problem. In the Ising model the different solutions should, according to the discussion in Ref. 4, correspond to different eigenvalues of the transfer matrix used in the solution of this problem.[6] The molecular field equations are widely studied for this problem, which therefore provides a suitable field for testing the basic ideas.

Another important task of this work is to study the meaning of the saddle points of the integral solutions for the correlation functions. The equations for these points, discussed in Ref. 5, yield generalizations to the molecular field equations, but are far more complicated since, besides being nonlinear, they lose the homogeneous character of the latter. In order to see what can be obtained from these equations and what is required to achieve a workable result, we find it useful to study these equations in a comparatively simple limit case.

We start in Section 2 by discussing the general arguments, and show, in a simple way, that Schwabl's equation has different solutions corresponding to different eigenvalues of the transfer matrix. In Section 3 we use an integral transform for solving the basic equation. This solution is much the same as the integral representation of Siegert.[7] It also has, however, the interesting feature of being nonunique. Its properties, together with the saddle point equations, are discussed in Section 4.

We finally remark that some of the solutions are immediately found to be nonphysical. In spite of this, we think that they are important in this context since we believe that the principle of getting nonequivalent solutions is

fruitful for the study of general phase transitions. In order to do so, more should be known about the solutions and how to find the correct one. Therefore, at this first stage it seems to be more appropriate to study the simplest possible situation rather than one that is physically more interesting but where no exact results are known.

2. CORRELATION FUNCTIONS IN THE ISING CASE

The Hamiltonian of the problem is given by

$$H(\{\sigma_i\})/\kappa T = -\tfrac{1}{2}\sum_{ij}\sigma_i\sigma_j K_{ij} - \sum_i h\sigma_i \tag{1}$$

where $\sigma_i = \pm 1$ and the indices i, j stand for the atoms of a lattice. We use essentially the same notations as in Ref. 3. Here K_{ij} and h are the dimensionless interaction and magnetic field parameters,

$$K_{ij} = v_{ij}/\kappa T \qquad \text{and} \qquad h = \mu B/\kappa T \tag{2}$$

We put $K_{ii} = 0$. Often we have only nearest-neighbor interactions

$$K_{ij} = \begin{cases} K & \text{if } i,j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

The partition function is

$$Z = \sum_{\sigma_i=\pm 1} \exp\left(\tfrac{1}{2}\sum_{ij}\sigma_i\sigma_j K_{ij} + h\sum_i \sigma_i\right) \tag{4}$$

Correlation functions are, as usual,

$$g^{(n)}_{i_1\cdots i_n} = (1/Z)\sum_{\sigma_i=\pm 1}(\sigma_{i_1}\sigma_{i_2}\cdots\sigma_{i_n})\, e^{-H(\{\sigma_i\})/\kappa T} \equiv \langle\sigma_{i_1}\sigma_{i_2}\cdots\sigma_{i_n}\rangle \tag{5}$$

We also introduce a generating functional:

$$\begin{aligned} F[x] &= \sum_n \sum_{\text{all } i} (1/n!)\, g^{(n)}_{i_1\cdots i_n} x_{i_1}\cdots x_{i_n} \\ &= (1/Z)\sum_{\{\sigma\}} \exp\left\{\sum x_i\sigma_i - [H(\{\sigma\})/\kappa T]\right\} \\ &\equiv (1/Z)\sum_{\{\sigma\}} \exp\left(-\tfrac{1}{2}\sum \sigma_i\sigma_j K_{ij} + \sum B_i\sigma_i\right) \end{aligned} \tag{6}$$

where, for convenience, we put $B_i = h + x_i$.

We assume that the interaction is of a finite range, i.e., $K_{ij} = 0$ for atoms i and j separated by more than a given distance. In that case the problem can

always be formulated by a transfer matrix[6] **A** relating the state of a group of atoms, which may consist of lines or sheets, with that of the other atoms inside their interactions range. If there are n such groups, the partition function is

$$Z = \operatorname{Tr} A^n = \sum_\alpha A_\alpha{}^n \tag{7}$$

where $\{A_\alpha\}$ are the eigenvalues. In fact, we can write

$$\mathbf{A} = \sum_\alpha A_\alpha \mathbf{e}_\alpha , \qquad \mathbf{e}_\alpha \cdot \mathbf{e}_\beta = \delta_{\alpha\beta}\mathbf{e}_\alpha \tag{8}$$

The components of A are denoted by the letter r, which in general is a vector, indicating the configuration of the corresponding group of atoms. We assume S to be an operator which involves a finite number of groups, and for the configurations $r_1 , r_2 ,...$ obtain values $S(r_1 , r_2 ...)$. Then, for the average of S, we obtain (the correlation functions are averages of this kind):

$$\begin{aligned}\langle S\rangle = (1/Z) \sum_{\text{all } r} & S(r_1 , r_2 ,..., r_m)\, A(r_1 , r_2) \\ & \times A(r_2 , r_3) \cdots A(r_m , r_{m+1})\, A^{n-m}(r_{m+1} , r_1)\end{aligned} \tag{9}$$

provided we have periodic boundary conditions.

If we use (8) and assume

$$| A_\alpha / A_\beta | < 1, \qquad \text{all} \quad \alpha \neq \beta \tag{10}$$

for sufficiently large n, we have

$$\langle S\rangle_\beta = (1/A_\beta{}^m) \sum_{\text{all } r} S(r_1 ,..., r_m)\, A(r_1 , r_2) \cdots A(r_m , r_{m+1})\, e_\beta(r_{m+1} , r_1) \tag{11}$$

Irrespectively of the assumption (10), Eq. (11) defines a welldefined average associated with the eigenvalue A_β. It was argued in Ref. 4, that, if we have a linear chain of equations for determining averages of this type, all $\langle S\rangle_\beta$ should be solutions of these equations. The reason for this is that when the relevant parameters are continued into a complex space, for any β, there are regions U_β where (10) is valid. In such a region (11) is a true solution, which in general is well-defined everywhere except, possibly, for singularities on some set of zero measure. Because of the linearity of the equations, (11) also should be a solution outside the region where (10) is valid and where it is the "true" solution.

The situation is simplest for the one-dimensional Ising model with nearest-neighbor interactions. Then, the matrix **A** has elements

$$A(\sigma, \sigma') = \exp[+ \tfrac{1}{2}K\sigma\sigma' + \tfrac{1}{2}h(\sigma + \sigma')] \tag{12}$$

with eigenvalues

$$A_{1,2} = e^{+K/2}(\cosh h) \pm (e^{+K} \sinh^2 h + e^{-K})^{1/2} \tag{13}$$

The e matrices can be written as

$$\mathbf{e}_1 = \begin{pmatrix} \cos^2\theta & \cos\theta \sin\theta \\ \cos\theta \sin\theta & \sin^2\theta \end{pmatrix}, \qquad \mathbf{e}_2 = \begin{pmatrix} \sin^2\theta & -\cos\theta \sin\theta \\ -\cos\theta \sin\theta & \cos^2\theta \end{pmatrix} \tag{14}$$

where

$$\tan\theta = (2^{+2K} \sinh^2 h + 1)^{1/2} - e^{+K} \sinh h \tag{15}$$

Then for a chain of n atoms

$$Z = \operatorname{Tr} \mathbf{A}^n = A_1{}^n + A_2{}^n \sim A_\alpha{}^n \qquad (|A_\alpha| \text{ is the largest}) \tag{16}$$

$$\langle \sigma_i \sigma_{i+\mu} \rangle = (1/Z) \sum_{\sigma_i, \sigma_{i+\mu}} \sigma_i \sigma_{i+\mu} A^\mu(\sigma_i, \sigma_{i+\mu}) A^{n-\mu}(\sigma_{i+\mu}, \sigma_i) \tag{17}$$

The limit functions are

$$\begin{aligned} \langle \sigma_i \sigma_{i+\mu} \rangle_\alpha &= \sum_{\sigma,\sigma'} (1/A_\alpha{}^\mu)\, \sigma\sigma' A^\mu(\sigma, \sigma')\, e_\alpha(\sigma', \sigma) \\ &= \sum \sigma\sigma' [e_\alpha(\sigma, \sigma') + (A_\beta/A_\alpha)^\mu\, e_\beta(\sigma, \sigma')]\, e_\alpha(\sigma', \sigma) \\ &= \cos^2 2\theta + (A_\beta/A_\alpha)^\mu \sin^2 2\theta \end{aligned} \tag{18}$$

If $h = 0$, we get

$$\langle \sigma_i, \sigma_{i+\mu} \rangle_1 = \tanh^\mu K, \qquad \langle \sigma_i \sigma_{i+\mu} \rangle_2 = \tanh^{-\mu} K \tag{19}$$

Here, (14) and (15) have been used.

It is easy to see that the limit function $\langle \cdots \rangle_2$ increases with μ, and thus behaves nonphysically. This fact can immediately be generalized to the general case, given by (9). It is then found that the nonphysical solutions for the correlation function between atoms which are sufficiently far apart from each other always increase with the distance. This fact seems to be the most suitable one for selecting the correct solutions in methods of this kind. The increase depends on terms $(A_\beta/A_\alpha)^\mu$, which can always make the correlation function increase if A_α is not the largest eigenvalue. For large μ (this parameter describes the separation) such terms will dominate the correlation function. The free energy of the different solutions ("phases") can be defined to be NkT times the negative logarithm of the corresponding eigenvalue. The correct solution, evidently, is given by the largest eigenvalue and our condition above is therefore equivalent to choosing the solution with the smallest free energy.

We first show how the different solutions occur in the chain of equations for correlation functions in the case of the one-dimensional nearest-neighbor Ising model. Schwabl obtained the following equation for the second-order correlation function (put $\langle \sigma_i \sigma_{i+\mu} \rangle = g_\mu$, $g_0 = 1$):

$$g_\mu - \tfrac{1}{2}(g_{\mu-1} + g_{\mu+1}) \tanh 2K = \tfrac{1}{2}\delta_{\mu,0}(\operatorname{sech}^2 2K + 1 - g_2 \tanh^2 2K) \quad (20)$$

For the Fourier transform defined by $C(k) = \sum_{-\infty}^{\infty} g_\mu e^{i\mu k}$ this yields

$$C(k) = \gamma(1 - \tanh 2K \cos k)^{-1} \quad (21)$$

where γ is the expression on the righthand side of (20). Then, g_μ is obtained using

$$g_\mu - \frac{\gamma}{2\pi}\int_{-\pi}^{\pi} \frac{e^{i\mu k}}{1 - \tfrac{1}{2}(\tanh 2K)(e^{ik} + e^{-ik})}\, dk$$
$$= \frac{\gamma}{2\pi i}\int_C \frac{x^{|\mu|}}{x - \tfrac{1}{2}(\tanh 2K)(x^2 + 1)}\, dx = \gamma \times (\text{sum of residues}) \quad (22)$$

C is a closed curve. The integrand has poles at $x_1 = \tanh K$ and $x_2 = \coth K$. The residues yield

$$g_\mu^{(1)} = \gamma(\tanh K)^{|\mu|} \cosh 2K, \qquad g_\mu^{(2)} = -\gamma(\tanh K)^{-|\mu|} \operatorname{sech} 2K \quad (23)$$

The definition of γ then yields

$$g_\mu^{(1)} = (\tanh K)^{|\mu|}, \qquad g_\mu^{(2)} = (\tanh K)^{-|\mu|} \quad (24)$$

which are the ones previously obtained. We note that with this method Schwabl calculated $g_\mu^{(1)}$, which is, of course, the only physically acceptable solution. From our point of view, however, the other solution is of equal interest.

3. THE FUNCTIONAL EQUATION AND ITS SOLUTION

We shall start with the expression for the generating functional $F[x]$ in (6).

Schwabl obtained the following linear equation for F:

$$(\partial/\partial x_i) F[x] = \left[\tanh\left(x_i + h + \sum_j K_{ij}\, \partial/\partial x_j\right)\right] F[x] \quad (25)$$

There are several integral representations for the generating functional[7,8] based on the general definitions. Here we shall derive such a representation

from Eq. (25). This will not provide any new kind of integral but it will be important for getting more information about the equation.

We note that the expression

$$\Phi_i(B_i) = \exp\left(p_i B_i - \tfrac{1}{2}\sum A_{ij} B_i B_j\right) \tag{26}$$

with $B_i = x_i + h$ is an eigenstate of the complicated tanh operator in (25) provided that $A_{ij} = A_{ji}$ satisfies

$$\sum_j K_{ij} A_{jk} = \delta_{ik} \tag{27}$$

The eigenvalue is $\tanh(\sum_j K_{ij} p_j)$. Therefore, we look for a solution of the form:

$$F[x] = C \int_S \prod_i dp_i \left[\exp\left(\sum_i p_i B_i - \tfrac{1}{2}\sum_{ij} A_{ij} B_i B_j\right)\right] f[p] \tag{28}$$

where S is some integration path, and C a constant, chosen such that $F[0] = 1$. This is a solution if (i) f obeys the equation

$$\left[p_i - \tanh \sum_j K_{ij} p_j\right] f[p] = \sum_j A_{ij}\, \partial f[p]/\partial p_j \tag{29}$$

and (ii) S is such that

$$\int_S \prod_i dp_i \,(\partial/\partial p_j)\left\{f[p] \exp\left(\sum_i p_i B_i\right)\right\} = 0 \tag{30}$$

The solution of (29) is

$$f[p] = \left[\exp\left(-\tfrac{1}{2}\sum_{ij} K_{ij} p_i p_j\right)\right] \prod_i \cosh\left(\sum_j K_{ij} p_j\right) \tag{31}$$

Condition (30) means that $f[p]$ shall vanish at the boundaries of S. Therefore on S either (a) the p variables go from $-\infty$ to $+\infty$ passing regions where $\mathrm{Re}\sum K_{ij} p_i p_j$ is bounded below (in order to make the absolute value of the integrand bounded), or (b) the p variables vary along the imaginary hyperplane between points p_i^0, where the cosh factors vanish. The p_i^0 are defined as

$$\sum_j K_{ij} p_j^0 = (n + \tfrac{1}{2})\,\pi i \tag{32}$$

n being any (positive or negative) integer. It is also possible that a combination of the different ways of integration exists. Generally, symmetric paths with respect to the origin shall be chosen.

Formulas (28) and (31) with the choice (a) for S can directly be transformed to the Siegert integral[7] if one puts

$$p_i - \sum_k A_{ik} B_k = u_i \tag{33}$$

Then

$$F[x] = C \int_{-\infty}^{+\infty} \prod du_i \left[\exp\left(-\tfrac{1}{2} \sum_{ij} K_{ij} u_i u_j \right) \right] \prod_i \cosh\left(\sum_j K_{ij} u_j + x_i + h \right) \tag{34}$$

The integration path of type (a) is the only one which appears from a direct transformation of the sum of the last part of (6). As mentioned above, this sum has a strict meaning only for finite systems. In that case, no ambiguity should occur. In the infinite system, however, the limit can be nonunique. The form of Eq. (25) is not changed in the limit but a constraint on its solutions for correlation functions of very large order will disappear. This is what introduces the ambiguity. We therefore expect the anomalous type (b) solutions to be meaningful in some sense for the infinite system. This is in accord with the ideas of Ref. 4.

We here make a few remarks about the paths of integration. As the quadratic form $\sum K_{ij} u_i u_j$ is not necessarily positive-definite, we should instead transform it to a diagonal form (accomplished by a Fourier transformation) and integrate the variables in an appropriate way along the real and the imaginary axes. Since the basic equation (25) is linear, any linear combination of solutions is also a solution. The true solution shall be chosen as the one with lowest free energy which fulfills important physical restrictions. The free energy can be directly calculated from the knowledge of the second-order correlation function.

Clearly there are very many solutions. Most of the solutions, however, are far too irregular to be accepted. In addition, there are evidently solutions with a broken symmetry, i.e., for which $\langle \sigma_i \rangle = \partial F[x]/\partial x$ does not vanish for $x_i = h = 0$. This property is not shared with the representations from the partition function approach, where the first-order correlation functions always vanish. The "anomalous" property occurs for asymmetric paths, e.g., between $\sum K_{ij} p_j = i(2n - 1)\pi/2$ and $i(2n + 1)\pi/2$ or from $\sum K_{ij} p_j = i(2n + 1)\pi/2$ to infinity. We see that linear combinations of such paths can yield symmetric ones with the "normal" symmetry property $\langle \sigma_i \rangle = 0$. Further, from the symmetric structure of the integrals it follows that paths which are reflections of each other in the real hyperplane yield complex conjugate results, and therefore correspond to solutions (possibly combinations) of the same real eigenvalues. For this reason, anomalous, asymmetric solutions can only be accepted if they yield degenerate symmetric solutions

(of degenerate eigenvalues). This is a well-known condition for symmetry-breaking solutions in, e.g., matrix methods.

4. THE SADDLE POINT APPROXIMATION

The most-used approximation of infinite integrals of the type above is the saddle point approximation. We shall demonstrate this method here for the case of the second-order correlation function. For simplicity, h is put equal to zero. We write

$$\langle \sigma_k \sigma_l \rangle = F_1^{kl}/F_0 \tag{35}$$

where

$$F_0 = \int_S \prod dp_i \left[\exp\left(-\tfrac{1}{2}\sum_{ij} K_{ij} p_i p_j\right)\right] \prod_i \cosh\left(\sum_j K_{ij} p_i\right) \tag{36}$$

and

$$F_1^{kl} = \int_S \prod dp_i \left[\exp\left(-\tfrac{1}{2}\sum_{ij} K_{ij} p_i p_j\right)\right] \sinh\left(\sum_j K_{kj} p_j\right) \sinh\left(\sum_j K_{lj} p_j\right) \times \prod_{i \neq k,l} \cosh\left(\sum_j K_{ij} p_j\right) \tag{37}$$

Saddle points of the integrands are obtained when (presuming K_{ij} can be inverted)

$$\text{for } F_0: \qquad \bar{p}_i = \tanh\left(\sum_j K_{ij} \bar{p}_j\right) \tag{38}$$

$$\text{for } F_1^{kl}: \qquad \bar{p}_i(kl) = \delta_{ik} \coth\left(\sum_j K_{kj} \bar{p}_j\right) + \delta_{il} \coth\left(\sum_j K_{lj} \bar{p}_j\right) + (1 - \delta_{ik} - \delta_{il}) \tanh\left(\sum_j K_{ij} \bar{p}_j\right) \tag{39}$$

Equation (38) becomes the familiar molecular field equation:

$$\bar{p} = \tanh(2K\bar{p}) \tag{40}$$

if we assume $\bar{p}_i$ is independent of i, i.e., $\bar{p}_i = \bar{p}$, $\sum_j K_{ij} = K$. This is also the equation obtained in the appendix, where some of its properties are discussed.

When integrating along the (a) type of path [i.e., the Fourier sums of the p_i are integrated from $-\infty$ to $+\infty$ (or $-i\infty$ to $+i\infty$ according to the signs of the eigenvalues of K_{ij})], this equation yields a maximum when all $p_i = \bar{p} = 0$ when $2K < 1$, and two maxima at points $p_i = \pm\bar{p} = 0$ when $2K > 1$. In the latter case the origin is a minimum. The integration along the type (b)

path closest to the origin (namely $\sum K_{ij} p_j$: $-i\pi/2 \to i\pi/2$) has a converse structure: There are two maxima for $2K < 1$ and one maximum (at the origin) when $2K > 1$. In general, when there are several maxima the approximated integral should be the sum of their contributions.

Equation (39) is more complicated since it distinguishes two lattice points k and l (the indices should be looked upon as vectors). For points far away from these we should get the solution of (38):

$$\bar{p}_i(kl) \xrightarrow[|i-k|,|i-l|\to\infty]{} \bar{p}_i = \bar{p} \tag{41}$$

In fact, the solutions converge fairly rapidly toward this value (at least unless $2K \approx 1$).

There is a symmetry property in (39) for points around the point $m = (k + l)/2$. The solutions are either symmetric or antisymmetric with respect to that point:

$$\text{either} \quad \bar{p}^s_{m-\mu} = \bar{p}^s_{m+\mu} \quad \text{or} \quad \bar{p}^a_{m-\mu} = -\bar{p}^a_{m+\mu} \tag{42}$$

If the asymptotic point $\bar{p}$ of (41) is not zero, only the symmetic solution is possible. (Note that m and μ need not be points of the lattice.) The complete expression shall be the sum of the contributions of these solutions, which yield the two maxima of the integral.

As for the factors of the integrand of (37), the cosh factors are essentially the same for the symmetric and the antisymmetric solutions. The two sinh factors, however, get different signs. In order to get the sum of the contributions of the symmetric and the antisymmetric solutions, it is then necessary to know the difference of the sinh factors in these cases. Some consideration shows that this difference is essentially determined by the difference between the corresponding solutions for the $\bar{p}$ values in the middle of the interval between k and l.

In order to show the general features of Eq. (39), we consider the one-dimensional case, and also restrict ourselves to the limits of large and small K. (There is no difficulty in one dimension in obtaining a numerical solution for the general case. The qualitative features are, however, apparent already in the limiting cases.) The equations in one dimension are, with nearest-neighbor interactions,

$$\begin{aligned} \bar{p}_i(kl) &= \tanh\{K[\bar{p}_{i-1}(kl) + \bar{p}_{i+1}(kl)]\}, \qquad i \neq k, l \\ \bar{p}_k(kl) &= \coth\{K[\bar{p}_{k-1}(kl) + \bar{p}_{k+1}(kl)]\} \\ \bar{p}_l(kl) &= \coth\{K[\bar{p}_{l-1}(kl) + \bar{p}_{l+1}(kl)]\} \end{aligned} \tag{43}$$

When K is small ($\ll 1$), for the "normal" solution, $\bar{p}_k$ and $\bar{p}_l$ become large. $\bar{p}_{k-1}$, $\bar{p}_{k+1}$, $\bar{p}_{l-1}$, and $\bar{p}_{l+1}$ are not small, but the rest are of order K or less.

In fact, for $i < k - 1$ (assume $l > k$)

$$\bar{p}_i \approx K\bar{p}_{i+1} \qquad \text{and} \qquad \bar{p}_{k-1} \approx \tanh(K\bar{p}_k) \tag{44}$$

We get similar relations for $i > l + 1$. For i between k and l, the situation is also similar, the $\bar{p}_i$ decrease rapidly when i goes from k or l toward the central point m. The situation, however, depends on the distance $| l - k |$ and also upon the symmetric character of the solutions. In fact, the symmetric and antisymmetric solutions in (42) yield the same contribution in first order, and higher-order terms must be considered to get the correct expression.

For $l = k + 1$, one gets

$$\bar{p}_k = \coth[K(\bar{p}_l + \bar{p}_{k-1})] \approx \coth(K\bar{p}_k) \approx 1/\sqrt{K} \tag{45}$$

provided $\bar{p}_l = \bar{p}_k \gg \bar{p}_{k-1}$. There is no antisymmetric solution in this case.

For $l = k + 2$ the symmetric solution yields

$$\begin{aligned} \bar{p}_k &= \coth[K(\bar{p}_{k-1} + \bar{p}_{k+1})] \approx 1/K(p_{k-1} + p_{k+1}) \\ \bar{p}_{k-1} &\approx \tanh(K\bar{p}_k) \approx \tanh[1/(p_{k-1} + p_{k+1})] \\ \bar{p}_{k+1} &= \tanh(2K\bar{p}_k) \approx \tanh[2/(p_{k-1} + p_{k+1})] \end{aligned} \tag{46}$$

or if x is the solution of $x = \tanh(1/x) + \tanh(2/x)$,

$$\bar{p}_{k-1} = \tanh(1/x), \qquad \bar{p}_{k+1} = \tanh(2/x) \tag{47}$$

The antisymmetric solution is given by

$$\bar{p}_{k+1} = 0, \quad \bar{p}_k \approx 1/K\bar{p}_{k-1}, \quad \bar{p}_{k-1} \text{ is the solution of } x = \tanh(1/x) \tag{48}$$

When $l > k + 1$ the points between k and l are important. We get the following:

1. $l = k + 2\nu$; $m = k + \nu$ belongs to the lattice:

$$\bar{p}_m{}^s \approx K^{(\nu-1)}\bar{p}_{k+1}, \qquad \bar{p}_m{}^a = 0 \tag{49}$$

2. $l = k + 2\nu + 1$; m does not belong to the lattice:

$$\begin{aligned} \bar{p}^s_{k+\nu+1} = \bar{p}^s_{k+\nu} &\approx K^{(\nu-1)}\bar{p}_{k+1} = \tanh[K(\bar{p}_{k+\nu-1} + \bar{p}_{k+1})] \\ -\bar{p}^a_{k+\nu+1} = +\bar{p}^a_{k+\nu} &\approx K^{\nu-1}\bar{p}_{k+1} = \tanh[K(\bar{p}_{k+\nu-1} - \bar{p}_{k+1})] \end{aligned} \tag{50}$$

from which we obtain

$$\bar{p}^s_{k+\nu} \approx (K^{\nu-1} + K^{\nu})\,\bar{p}_{k+1}, \qquad \bar{p}^a_{k+\nu} \approx (K^{\nu-1} - K^{\nu})\,\bar{p}_{k+1} \tag{51}$$

We then use these points in the integrals (36) and (37). The integrands are transformed to the form

$$f[\bar{p}]\exp\{-\kappa_{ij}[\bar{p}]\,\delta_i\delta_j\} \tag{52}$$

where $\delta_i = p_i - \bar{p}_i$ and higher-order terms are neglected. Equation (35) is then obtained in the form

$$\langle\sigma_k\sigma_l\rangle = \frac{f_1[\bar{p}(kl)]}{f_0[\bar{p}]}\left(\frac{\mathrm{Det}\{\kappa_{ij}[\bar{p}]\}}{\mathrm{Det}\{\kappa_{ij}[\bar{p}(kl)]\}}\right)^{1/2} \tag{53}$$

From above, we see that for small K, $f_0 \approx 1$. The important f_1 terms are primarily the sinh factors and the difference between the symmetric and antisymmetric expressions. These terms yield the K dependence. The two sinh factors are each proportional to $\sqrt{K}$ if $l = k + 1$ and to K otherwise. From the formulas (46)–(51) one finds that the difference between the symmetric and antisymmetric solutions is proportional to $K^{(l-k-2)}$ if $l \geqslant k + 2$. Therefore f_1/f_0 is proportional to $K^{(l-k)}$. The determinants of the κ matrices both turn out both to be proportional to $K^{N/2}$, where N is the number of lattice points. Thus, we get

$$\langle\sigma_k\sigma_l\rangle \sim K^{|l-k|} \tag{54}$$

which is the right behavior. It is not as easy (but not impossible) to get the numerical factor. Primarily because the integral gets important contributions from regions where higher-order terms of the hyperbolic functions are appreciable, this factor does not come out correctly in this approximation except for the case $l = k + 1$, when it becomes equal to one, as it should.

The situation for large K is simpler. Then, from (43), one finds that all $\bar{p}_i$ are approximately equal to one (or minus one). (There is no antisymmetric solution in this case.) Then, for all finite distances $|\, l - k \,|$ the correlation functions become one, as they should.

Finally, we briefly discuss the behavior of the "anomalous" solution where the p_i are integrated along the imaginary axis, and

$$-\pi/2 \leqslant \mathrm{Im}\sum K_{ij}\,p_j^0 \leqslant \pi/2$$

The saddle points of (38) are given by

$$\bar{x} = \tan 2K\bar{x} \tag{55}$$

where $p = ix$. The positive solution for small K is

$$\bar{x} = x_0 = (\pi/4K) - (4/\pi) + O(K) \tag{56}$$

(i.e., $2K\bar{x} \approx \pi/2$, $\cos 2K\bar{x} \approx K$). In this case, the main behavior close to the saddle point is determined by the (now) trigonometric factors, which vary

more rapidly than the Gaussian. In the F_1 integral of (39), we do not get any maximum for the sine factors, which together with the Gaussian, increase in the entire interval. Its arguments $\sum K_{ij} p_j$, $i = k$ or l, should therefore be at the boundary. With this constraint, the maximum point can be obtained as before. The convergence toward the value in (56) is slower than it was earlier. As before we expand around the maximum points and get an expression $\exp(-\kappa_{ij}\, \delta x_i\, \delta x_j)$. In this case the matrix κ_{ij} is in lowest order independent of K, in contrast to the previous case, where it was proportional to K. Each of the cosh factors (now cos factors!) of (36) and of (37), for at least $i \ll k$ and $i \gg l$ ($l > k$ assumed), is proportional to K and the corresponding quotients of these factors in the approximate expression are of order one. For the factors in (36), this fact is obtained from (56). In (37) for $i < k$ and $i > l$, the $-4/\pi$ term of (56) is replaced by a constant which becomes equal to that value as $| i - k |$ and $| i - l |$ go to infinity. Close to k and l, this constant is dependent on K and is small. Because of this, all the quotients of the cos factors for $i < k$ and $i > l$ in the approximate integrals yield a factor proportional to K.

For points i between k and l, the sums $\sum K_{ij}\bar{x}_j$ are no longer close to $\pi/2$ and, correspondingly, the cosh factors are of order one instead of K. This means that in the quotient F_1/F_0 we get a factor

$$1/K \text{ from } \sinh\left[\sum K_{kj}\bar{x}_0(kl)\right]\Big/\cosh\left[\sum K_{kj}\bar{x}_j\right]$$

$$\text{or from } \cosh\left[\sum K_{ij}\bar{x}_j(kl)\right]\Big/\cosh\left[\sum K_{ij}\bar{x}_j\right]$$

for every i such that $k \leqslant i \leqslant l$. The result is therefore

$$\langle \sigma_k \sigma_l \rangle \sim K^{-|k-l|} \tag{57}$$

as it shall be for the anomalous solution. Because the ranges of the approximating Gaussians are not small, the numerical coefficient can not be expected to come out correctly.

5. DISCUSSION

Before going deeper into the results of the previous sections, there are a few important questions that remain to be cleared up. The first concerns a subsidary condition, which is a direct consequence of (6):

$$\partial^2 F[x]/\partial x_i^2 = F[x] \tag{58}$$

This relation was used by Schwabl. It can be shown that the functional equation with this condition must have a unique solution for a finite system.

It is also easily seen that among the integral representations derived above, only the one with the integral path of type (a) fulfills (58) strictly. However, it is also quite clear that the importance of the functionals lies very much in the fact that they provide the correlation functions. It is therefore only necessary that (58) have a local meaning. It follows from the integral representations that, for an infinite system,

$$\frac{\partial^2}{\partial x_i^2} \frac{\partial^m}{\partial x_{j_1} \cdots \partial x_{j_m}} F[x] = \frac{\partial^m}{\partial x_{j_1} \cdots \partial x_{j_m}} F[x] \tag{59}$$

when all x_i are zero for all finite m for any of the possible solutions. Therefore all solutions are acceptable if (58) is considered in its local sense (59).

Another question is related to the problem of "too many solutions" already mentioned. The actual number of solutions is certainly smaller than the number provided by possible integration paths. The way out of this seems to be the fact that the solutions are linearly dependent and that different paths can give rise to the same correlation function. At the moment, however, it seems difficult to prove this statement in general (as most things are difficult to do directly with functional integrals).

We have found in this work that the functional equations for the Ising model have numerous solutions. From the discussions of the limiting cases of the one-dimensional model it is seen that the functional integral solutions really correspond to the true structure of the partition function. This is probably a general situation and the study of the "anomalous" solutions should therefore be a meaningful task since they can enter as "condensed" states of the system.

An interesting remark, which also was made by Schwabl, is that the functional approach is not a good one for the Ising model, where other methods give much more precise results in an easier way. However, the Ising model is not studied here for its own sake but for the aid it offers us in understanding other systems better. In fact, the continuum system is in many respects simpler than the lattice system in the functional presentation.

Among the important conclusions of the work is the statement, discussed in Section 2, that the "false" correlation functions behave in an unrealistic way. As was said there, this is an important criterion for choosing the correct solution. There are also always symmetry-broken solutions, yielded by asymmetric integration paths; such solutions are often found in molecular field theories, which here correspond to saddle points. The treatment shows that such solutions can only be accepted physically if it can be shown that there are degenerate solutions. In the molecular field approach the integrals along the "anomalous" paths are in fact negligible compared with the normal integral and, therefore, apparently proportional (the proportionality factor being zero). This is the reason why solutions of broken

symmetry turn up. Strictly speaking, the contributions of all saddle points should be added. The mere occurrence of anomalous solutions in molecular field equations is therefore in a strict sense never an indication of a phase transition. What must be shown is in some way the proportionality of the integrals. It may be possible to show this by saddle point methods, and, as discussed above, it suffices to show that the anomalous correlation functions (here given by the bounded imaginary integration paths) behave physically. If this can be shown in a limiting case of e.g., low temperatures, where the saddle point method is most likely to yield reasonable results, it is a clear indication that a phase transition has taken place.

APPENDIX

We briefly discuss the one-variable equation

$$\frac{df(x)}{dx} + \tanh\left(x + a\frac{d}{dx}\right) f(x) = 0 \tag{A.1}$$

The equation is closely related to the multidimensional one discussed here. Its features are important for us to study in order to get a better understanding of the functional treatment. By the method of this paper, we can obtain the general solution in terms of integral transforms:

$$\begin{aligned} f(x) &= C\int_S dp\, \exp[-(x^2/2a) - xp - \tfrac{1}{2}ap^2]\cosh ap \\ &= C'\int_{S'} du\, [\exp(-\tfrac{1}{2}au^2)]\cosh(au + x) \end{aligned} \tag{A.2}$$

The integration paths can be:

Type (a). S, S': $-\infty \to +\infty$

Type (b). Symmetric parallel to the imaginary axis:

b_1 : S: $-\frac{1}{2}i\pi \to \frac{1}{2}i\pi$; S': $x - \frac{1}{2}i\pi \to x + \frac{1}{2}i\pi$

b_2 : S: $-i(n + \frac{1}{2})\pi \to -i(n - \frac{1}{2})\pi$, $i(n - \frac{1}{2})\pi \to i(n + \frac{1}{2})\pi$;
S': the same $+x$

By these integration paths, we are sure to get $df(x)/dx = 0$ when $x = 0$. For other, asymmetric paths, we can get $df(x)/dx \neq 0$ for $x = 0$ (corresponding to nonzero magnetization).

We look for the saddle point approximation for the integrals representating $f(0)$. The saddle point occur for

$$u = \tanh au \tag{A.3}$$

It is easily seen that the saddle points are either along the real or (most of them) the imaginary axis. For the (b_2) paths, there is always one saddle point on each of the two symmetric components. For the (a) and the (b_1) paths, the situation is slightly different. When $a < 1$ there is no saddle point on the real axis but only at $u = 0$, which yields a maximum. On the (b_1) path there are two maxima for $u \neq 0$ and a minimum at $u = 0$. When $a > 1$ the situation on these paths is reversed. The only real value of a for which saddle points coincide is $a = 1$ at $u = 0$.

ACKNOWLEDGMENTS

I warmly thank Professor L. Hulthén for his kind interest and constant encouragement, and also P. Richter from the University of Marburg for a valuable discussion and for showing the relevance of the work of Schwabl.

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