ORDER PARAMETER AND THE GROUND STATE ENERGY FOR THE ISING MODEL WITH THE PERPENDICULAR FIELD

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The long-range parameters and the ground state energy for the Ising model with the perpendicular field component are calculated up to the fourth order in the perturbation expansion by applying the cumulant expansion method for spin operators and corresponding diagrammatic technique given by Arai, Goodman. A comparison is made with other approximate methods.

1. *Introduction*

We consider a system composed of N lattice points described by the simple Hamiltonian

$$H = \lambda^z \sum_{h=1}^{N} S_h^z + \lambda^x \sum_{h=1}^{N} S_h^x - 2J \sum_{\langle h,k\rangle} S_h^z S_k^z \tag{1.1}$$

where $S^\alpha(\alpha = x, y, z)$ are the spin operators for $S = 1/2$, $J > 0$ denotes the exchange constant and λ^α are the external field components in energy units. The summation $\langle h, k\rangle$ runs over all pairs of nearest-neighbour points.

Models of this kind have been treated in papers of many authors. Fisher [1] found the expansions for the static initial susceptibility at high and low-temperatures, Allan and Betts [2] obtained a general expression for the perpendicular response function and for the frequency-dependent initial perpendicular susceptibility. Recently, Essam and Garelick [3] have investigated the dynamical properties of such a model for a general spin.

On the other hand, models similar to that described by (1.1) have been frequently used in the theory of order-disorder ferroelectrics [4–9]. De Gennes [4] was the first to propose this model as an effective spin Hamiltonian describing the proton net-work in hydrogen bonded ferroelectrics. The eigenvalues of the spin operator S^z correspond, in this case, to the two possible equlibrium positions of the hydrogen ions, and the Ising term $-2J \sum_{\langle h,k\rangle} S_h^z S_k^z$ describes their interactions. The $\lambda^x \sum_h S_h^x$ term in (1.1) represents the tunneling motion of protons and λ^z corresponds to the external electric field.

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The aim of this paper is to obtain the perturbation expansion for the ground state energy and for the order parameters at $T = 0$ up to the fourth order term in perturbation parameter $q = \lambda^x/zJ$ (z — the coordination number) for the Hamiltonian (1.1), and to compare the results with the expressions and estimations given by other approximate theories, such as the molecular field approximation (MFA), the Green functions (GF) [8] and "statistical perturbation" (SP) [9] methods.

The method of calculation is based on the cumulant expansion and Wick's theorem for spin operators given by Arai, Goodman [10] which procedure is also applicable for a general spin. We shall also emphasize the influence of the two-fold degeneracy of the unperturbed ground state (arising when $\lambda^z = 0$) on the result. In practice, this degeneracy should be accounted only for small systems, when the number of spin is smaller or equal to the number of terms taken into account in the perturbation expansion.

2. *Method of calculations*

Let us divide the Hamiltonian (1.1) into the unperturbed part H_0 and the perturbation H_I:

$$H = H_0 + \lambda^x H_I, \tag{2.1}$$

$$H_0 = \lambda^z \sum_h S_h^z - 2J \sum_{\langle h,k \rangle} S_h^z S_k^z, \tag{2.2}$$

$$H_I = \sum_h S_h^x = \frac{1}{2} \sum_h (S_h^+ + S_h^-). \tag{2.3}$$

The unperturbed part contains here the interaction between the S^z and is not of a single-particle type. The use of such H_0 is the main advantage of the method given in [10], and ensures a good convergence.

The basic expression for our calculation is the well-known Gell-Mann-Low formula for the ground state energy E:

$$E = E_0 + \lim_{\beta \to 0+} i\beta\lambda^x \frac{\partial}{\partial \lambda^x} [\ln \langle 0| U_\beta(0, -\infty)|0\rangle] \tag{2.4}$$

where E_0 is the energy of the ground state $|0\rangle$ of H_0, and

$$U_\beta(t, -\infty) = \exp_T \left[\frac{\lambda^x}{i} \int_{-\infty}^{t} H_{I\beta}(t')dt' \right], \tag{2.5}$$

$$H_{I\beta}(t) = H_I(t) \exp \beta t. \tag{2.6}$$

$H_I(t)$ is here, as usual, the Hamiltonian (2.3) in the interaction representation and $\exp_T \ldots$ denotes the Dyson's chronological ordered exponential.

After introducing the cumulants $\langle 0| \ldots |0\rangle_c$ defined by the relation

$$\langle 0|T\{X_n(t_1)\ldots X_1(t_1)\}|0\rangle_c = \sum_{l=1}^{n} \sum_{\substack{\text{all possible}\\ \text{partitions}}} (-1)^{l-1} \langle 0|T\{X_{i_1}(t_{i_1})\ldots\}|0\rangle \times$$

$$\times \langle 0|T\{X_{i_2}(t_{i_2})\ldots\}|0\rangle \ldots \langle 0|T\{X_{i_l}(t_{i_l})\ldots\}|0\rangle \qquad (2.7)$$

(2.4) may be rewritten in the form

$$E = E_0 + \lim_{\beta\to 0+} i\beta\lambda^x \frac{\partial}{\partial\lambda^x} [\langle 0|U_\beta(0, -\infty) - 1|0\rangle_c]. \qquad (2.8)$$

Starting from (2.8) Arai and Goodman [10] proved an analogue of Wick's theorem for the time-ordered products of $S^{\pm}(t)$ operators, and applied it to the ground state energy calculation of an antiferromagnet. The calculation in this case may be formalised by using the diagrammatic technique introduced in [10]. The same, slightly modified, technique may be used also for our H given by (1.1).

As the ground state of H_0 we can take $|0\rangle \equiv |-\frac{1}{2}, \ldots, -\frac{1}{2}\rangle$ (if we assume that $\lambda^z > 0$). Our task is now to calculate the averages of the type (2.7) where $X_i(t)$ is equal to $S_i^{\mp}(t)$. According to Kubo's theorem on the cumulants [11] such averages vanish when the operators

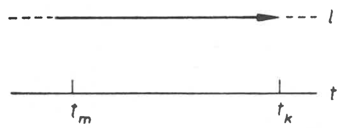

Fig. 1. The graphical representation of the $S_l^-(t_m)$, $S_l^+(t_k)$ pair (when $t_m = t_2$, $t_k = t_1$ Fig. 1 represents the unique second order diagram)

$X_{j_n}(t_n), \ldots, X_{j_1}(t_1)$ are divided into two or more groups which are independent of each other in calculating the average $\langle 0|X_{j_n}(t_n)\ldots X_{j_1}(t_1)|0\rangle$. On the other hand, using Wick's theorem [10] we obtain that the non-zero contributions give only such time-ordered products of $S^{\pm}(t)$ operators which may be decomposed into pairs $S_1^-(t_m)$, $S_1^+(t_k)$ with $t_m > t_k$ and hence, evidently only even n's contribute. Such pairs can be represented graphically as in Fig. 1. The pairs with different lattice indices can be drawn at different levels and, whenever possible, neighbouring lattice points will be shown on neighbouring lines. Thus we can connect with each term of the order $n = 2k$, admitting such decompositions, a set of corresponding diagrams. Each diagram consists of k "arrows" lying on the suitable levels in definite time sequence. The diagram is called interacted if it cannot be divided into two spatially separated, with respect to the nearest-neighbour interaction, parts. Evidently, only interacted diagrams contribute.

Without going into details, we shall formulate the prescriptions for the calculation of the n-th order term of our expansion.

(i). Draw all interacting configurations consisting of $n/2$ "arrows" in a definite time sequence. This introduces the factor $(\lambda^x/2)^n$.

(ii). For the numerical value of a diagram of the n-th order before the cumulant correction calculate for each time interval (t_k, t_{k+1}) the quantity

$$\varepsilon = 2gJ - p(zJ + \lambda) \qquad (2.9)$$

where p is the number of arrows belonging to this interval and g is the number of interactions between them. Further, multiply the product of the inverse of all these quantities by factors η defined for each site level as follows

$$\eta = 1-2r \tag{2.10}$$

where r is the number of arrows lying entirely on the other arrows.

(*iii*). For the cumulant correction to a diagram form all distinct partitions of the diagram into subdiagrams composed of one or more arrows. The subdiagrams are treated as spatially separated. Apply the procedure (*ii*) to each, in some manner decomposed, diagram and multiply the result by the factor$(-1)^{l-1}(l-1)!$ where l is the number of subdiagrams. Sum over all partitions.

(*iv*). Add (*iii*) to (*ii*) and multiply by the number of times the diagram appears.

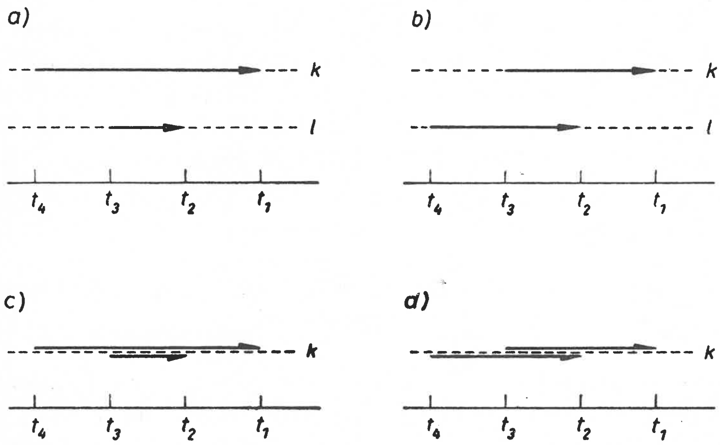

Fig. 2. Fourth order diagrams giving the non-zero contribution (k and l are two neighbouring lattice points)

Thus we obtain finally the numerical contribution of the given diagram to the expansion. Fig. 2 shows all diagrams involved in our calculation for the fourth order terms. For example, the contribution of the diagram (2*a*) is

$$Nz\left(\frac{\lambda^x}{2}\right)^4\left[\frac{1}{-(zJ+\lambda^z)\,(2J-2\,(Jz+\lambda^z))\,(-(zJ+\lambda^z))}-\right.$$
$$\left.-\frac{1}{-(zJ+\lambda^z)(-2(zJ+\lambda^z))\,(-(zJ+\lambda^z))}\right]. \tag{2.11}$$

3. Results and comparison with other methods

By using the prescriptions given above we can easily calculate the ground state energy up to the fourth order term for the Hamiltonian (1.1) with $\lambda^z > 0$. The result is

$$E = E_0+E_2+E_4+\ldots \tag{3.1}$$

where

$$E_0 = -\frac{N\lambda^z}{2} - \frac{NzJ}{4}, \tag{3.2}$$

$$E_2 = -N\frac{1}{4(zJ+\lambda^z)} \cdot (\lambda^x)^2 \tag{3.3}$$

and

$$E_4 = -N\frac{1}{16(zJ+\lambda^z)^3}\frac{J-\lambda^z}{zJ+\lambda^z-J} \cdot (\lambda^x)^4. \tag{3.4}$$

At this stage arises the problem of obtaining the expansion for the ground state energy at $\lambda^z = 0$. The expansion (3.1) was evaluated under assumption that the unperturbed ground state is undegenerate ($\lambda^z > 0$). For $\lambda^z = 0$ the usual two-fold degeneracy occurs. Thus we cannot, in general, put simply $\lambda^z = 0$ in (3.1). Indeed, the first obvious difficulty is connected with ε quantities which in this case are

$$\varepsilon = 2gJ - pzJ. \tag{3.5}$$

Because of the inequality $g \leqslant pz/2$ we obtain that $\varepsilon \leqslant 0$. ε becomes equal to zero (for such ε's (3.1) has no sense) in time intervals containing "interacted group of arrows". In the interacted group of arrows any pair of arrows is interacted and any arrow of the group appears with all its neighbours. The interacted groups occur when $N = 2$ ($z = 1$), $N = 3$ ($z = 2$) and $N = 4$ ($z = 3$) only. For $N > 4$ we have $\varepsilon < 0$.

Let us examine, for illustration, the case $N = 2$ ($z = 1$). For two interacted spins the eigenvalues of the operator H may be obtained from the equation

$$\left(\lambda^z - \frac{J}{2} - E\right)\left(\frac{J}{2} - E\right)\left(-\lambda^z - \frac{J}{2} - E\right) + (\lambda^x)^2\left(\frac{J}{2} + E\right) = 0. \tag{3.6}$$

It is easily shown, that the root of Eq. (3.6) which corresponds to the lowest eigenvalue of H for $\lambda^z > 0$ has an expansion identical with (3.1) (for $N = 2$, $z = 1$) and that the exact ground state energy for $\lambda^z = 0$ is

$$E(0) = -\frac{J}{2}[1+(2q)^2]^{1/2} = -\frac{J}{2}[1+2q^2-2q^4+\dots]; \left(q = \frac{\lambda^x}{zJ}\right). \tag{3.7}$$

On the other hand, if we put in (3.1) $\lambda^z = 0$ we obtain for $N = 2$, $z = 1$ the senseless result $E(0) = -J/2\,[1+q^2+\text{infinite term}]$.

Similarly, for $N = 3$, $z = 2$ after solving directly the eigenvalue problem for $\lambda^z = 0$ we find

$$E(0) = -\frac{3J}{2}\left[\frac{1}{3} + \frac{2}{3}|q| + \frac{2}{3}(1-2|q|+4q^2)^{1/2}\right]$$
$$= -\frac{3J}{2}\left(1+q^2+|q|^3+\frac{1}{4}q^4+\dots\right). \tag{3.8}$$

We see that the "strange" term $|q|^3$ occurs in (3.8), whenever (3.1) gives $E(0) = -3J/2\times$ $\times(1+q^2+1/4q^4+\dots)$.

The general situation becomes clear if we perform the appropriate calculations by the conventional perturbation method for two-fold degenerate level. The following statement can be then proved. The decoupling of the E_0-level appears when n (order of the perturbation correction) becomes equal to N (number of spins in system). When $n < N$, the calculations are the same as for the undegenerate case, and hence the formula

$$E(0) = E_0(0)\left(1+q^2+\frac{1}{4(z-1)}q^4+\ldots\right) \tag{3.9}$$

which may be obtained from (3.1) for $\lambda^z = 0$ holds for $N > 4$.

The perturbation theory for a degenerate level gives, of course, the appropriate expansions (3.7) and (3.8) for $N = 2, 3$ as well as the expansion (3.9) for $N > 4$. However, the calculations are rather long in this case, and it is difficult to formalise them. In practice, we calculate such quantities as E/N and long-range parameters only in the $N \to \infty$ limit. Then the condition $n < N$ plays no role, and the presented above simple diagrammatic technique may be employed.

The value of $E(0)$ for any N must belong to the following interval

$$E_0(0)(1+(2q)^2)^{1/2} \leqslant E(0) \leqslant E_0(0)(1+q^2)\,. \tag{3.10}$$

The upper bound for $E(0)$ may be obtained easily when $|q| \leqslant 1$ by variational principle. The lower bound was given by Kijewski and Perkus [12–13] by using the density-matrix method. $E(0)$ is equal to its lower bound only for $N = 2$.

Equations (3.9) and (3.10) seem to indicate that for $z \to \infty$, $q = \text{const}$ $E(0) \to E_0(1+q^2)$ which is an MFA result, similarly as for the usual Ising model for which MFA is exact in the limit case of N spins all interacting with the same intensity Jz/N $(N \to \infty)$ [14].

The corresponding theorem for our case oan be proved after writing our Hamiltonian with the interaction $-\dfrac{Jz}{N}\sum\limits_{h,k}^{N} S_h^z S_k^z$ the summation goes here over all pairs of spins in the form

$$H = -\frac{JzN}{4}\left(1+\frac{1}{N}+q^2\right)+\frac{Jz}{N}\left(\left[S^x+q\,\frac{N}{2}\right)^2+(S^y)^2\right] \tag{3.11}$$

where $S^x = \sum\limits_h S_h^x$, $S^y = \sum\limits_h S_h^y$.

From (3.11) and variational principle we can easily obtain the following inequality

$$E_0(0)\left(1+\frac{1}{N}+q^2\right) \leqslant E(0) \leqslant E_0(0)\,(1+q^2) \quad (|q| < 1). \tag{3.12}$$

Hence

$$\lim_{\substack{N\to\infty \\ q=\text{const}}} \frac{E(0)}{N} = -\frac{Jz}{4}\,(1+q^2) \tag{3.13}$$

as should be expected.

Now, let us calculate the long-range parameters. Corresponding expansions following from other theories are then easily comparable.

The long-range parameters are defined here by

$$\sigma^{\alpha} = \frac{-2\langle \sum_h S_h^{\alpha} \rangle}{N} \qquad (\alpha = x, z) \tag{3.14}$$

where $\langle \ldots \rangle$ denotes an average with respect to the exact ground state. The value of σ^x and σ^z can be obtained from the formulae

$$\sigma^{\alpha} = -\frac{2}{N}\frac{\partial E}{\partial \lambda^{\alpha}} \qquad (\alpha = x, z). \tag{3.15}$$

After differentiating the corresponding energy expression we obtain

$$\sigma^x = \frac{\lambda^x}{zJ+\lambda^z} + \frac{1}{2}\frac{J-\lambda^z}{(zJ+\lambda^z)^3(zJ+\lambda^z-J)}\cdot(\lambda^x)^3 + \ldots \tag{3.16}$$

$$\sigma^z = 1 - \frac{1}{2}\left(\frac{\lambda^x}{Jz+\lambda^z}\right)^2 - \frac{1}{8}\frac{[3(J-\lambda^z)(Jz+\lambda^z-J)+Jz(Jz+\lambda^z)]}{(zJ+\lambda^z)^4(zJ+\lambda^z-J)^2} - \ldots \tag{3.17}$$

Hence, for $\lambda^z = 0$ (and for $N > 4$ only!)

$$\sigma^x(0) = q + \frac{1}{2}\cdot\frac{1}{z-1}q^3 + \ldots \tag{3.18}$$

$$\sigma^z(0) = 1 - \frac{1}{2}q^2 - \frac{1}{8}\frac{z^2+3z-3}{(z-1)^2}q^4 - \ldots \tag{3.19}$$

It should be noted that $\sigma^z(0)$ may be obtained from (3.1) by making use of the formula

$$\sigma^z(0) = \frac{1}{2} - \frac{2}{N}\frac{\partial E(0)}{\partial(zI)}. \tag{3.20}$$

However, formal employment of (3.20) to (3.9) may lead to a wrong result if one forgets certain manipulations already made in the derivation of (3.9), as, *e.g.*, $\frac{J}{zJ-J} = \frac{1}{z-1}$.

From (3.18) and (3.19) we may also obtain corresponding static susceptibilities

$$\chi_{\perp}(\lambda^x) = \frac{\partial\sigma^x(0)}{\partial\lambda^x} = \frac{1}{zJ}\left(1 + \frac{3}{2}\cdot\frac{1}{z-1}q^2 + \ldots\right) \tag{3.21}$$

and

$$\chi_{\parallel}(\lambda^x) = \frac{\partial\sigma^z}{\partial\lambda^z|_{\lambda^z=0}} = \frac{1}{zJ}q^2\left[1 + q^2\frac{8z^3+9z^2-27z+12}{8(z-1)^3}\right]. \tag{3.22}$$

From (3.21) we obtain $\chi_{\perp}(0) = \frac{1}{zJ}$, which in this rather trivial case, agrees with Fisher's result for $T = 0$.

Now, we compare our expansion for $\sigma^z(0)$ (3.19) with other theories. MFA in this case gives

$$\sigma^z_{\text{MFA}}(0) = (1-q^2)^{1/2} = 1 - \frac{1}{2}q^2 - \frac{1}{8}q^4 - \ldots \tag{3.23}$$

From comparison of (3.23) and (3.19) it can be seen that σ^z should tend to σ^z_{MFA} in the same limit procedure ($z \to \infty$, $q = \text{const}$).

The "statistical perturbation" method and Green function theory adopted respectively in [9] and [8] give, after expanding the corresponding formulae derived at $\lambda^z = 0$ in the low temperature limit,

$$\sigma^z_{SP}(0) = 1 - \frac{1}{2}q^2 - \frac{1}{8}\frac{z+1}{z}q^4 - \dots \tag{3.24}$$

$$\sigma^z_{GF}(0) = 1 - \frac{1}{2}q^2 - \frac{1}{8}\frac{z-1}{z}q^4 - \dots \tag{3.25}$$

It is seen from (3.23), (3.24) and (3.25) that all theories give the exact result for the term of the second order. The numerical values of coefficients in the fourth order terms are tabulated in Table I.

TABLE I

The numerical value of the coefficient in the fourth order term

Method	$z=2$	$z=4$	$z=6$	$z=12$
GF	0.0625	0.0938	0.1042	0.1146
MFA	0.1250	0.1250	0.1250	0.1250
SP	0.1875	0.1562	0.1458	0.1354
exact	0.8750	0.3472	0.2550	0.2305

From inspection of the Table I it is seen that the largest discrepancies among approximate and exact results occur for small coordination numbers. The difference between σ^z_{GF} and σ^z_{SP}, emphasized in [15], calls here again in favour of σ^z_{SP}, although both are rather far from the exact result for $z \leqslant 12$.

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