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DIAGRAM TECHNIQUE FOR SPIN-OPERATORS
AND ITS APPLICATIONS TO SOME PROBLEMS OF FERROMAGNETISM

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Résumé. — On propose une technique de diagramme pour le calcul des fonctions de corrélation d’un ferromagnétique décrit par le modèle d’Ising, et son approximation zéro correspond au champ self-consistant.

La dépendance principale d’un facteur numérique du diagramme d’après sa structure est la particularité importante de cette technique en comparaison avec la technique de diagramme habituelle pour les opérateurs de Fermi ou de Boson. Elle conduit au caractère particulier des séries analytiques correspondant à certaines séries de diagramme et aux méthodes particulières de leur sommation. On a obtenu les expressions formelles exactes pour la moyenne du moment spontané en termes de fonctions de corrélation irréductibles à plusieurs particules.

On a extrait certaines séries pour le moment spontané qui correspondent aux fluctuations de Gauss du champ self-consistant.

On a obtenu une relation entre la technique de diagramme proposée et le développement d’intégrales fonctionnelles pour les fonctions de corrélation du modèle d’Ising.

En conclusion, on a donné les références des publications où une technique de diagramme pour les modèles d’Heisenberg et s-d est développée.

Abstract. — A diagram technique for calculation of correlation functions of ferromagnet being described by the Ising model is proposed here and its zero approximation corresponds to the selfconsistent field.

The essential dependence of a numerical factor of a diagram upon its structure is the important peculiarity of this technique in comparison with the usual diagram technique for fermion or boson operators. It leads to the special character of analytical series corresponding to the certain diagram series and to the special ways of their summarizing. The exact formal expression for the average spontaneous moment in terms of irreducible many-particle correlation functions had been obtained.

A certain series of graphs for spontaneous moment which corresponds to the Gaussian fluctuations of the selfconsistent field being taken into account had been extracted.

A relation between the proposed diagram technique and the expansion of functional integrals for the correlation functions of the Ising model had been obtained as well.

In conclusion the references to authors papers where a diagram technique for Heisenberg and s-d models are developed are given there.

In the Ising model the ferromagnetic system of atomic magnetic moment of the crystal being placed in external magnetic field is characterized by Hamiltonian which for convenience sake may be written as $H = H_0 + H_{\text{int}}$ where $H_0 = -[\mu H + \sum_I I(1-1') < S_I^+ >] \sum_I S_I^+$, (1.1)

$H_{\text{int}} = -\frac{1}{2} \sum_{i \neq j} I(1-1') (S_i^+ - < S_i^+ >) \times (S_j^- - < S_j^- >)$. (1.2)

Here and thereafter indices 1, 2, ... run over the lattice sites occupied by magnetic atoms; $I(1-1')$ is the exchange interaction integral of two spins in 1 and 1' sites; symbol $< ... >$ denote a statistical average with Hamiltonian $H$:

$< ... > = \text{Sp} (e^{-\beta H_0})/\text{Sp} e^{-\beta H}, \quad (\beta = 1/kT)$. (1.3)

The main problem is to develop the perturbation theory for calculation of correlation function of any order:

$< S_1^+ S_2^+ ... S_n^+ > = < S_1^+ S_2^+ ... S_n^+ e^{-\beta H_{\text{int}}} >_0 \quad \text{where} \quad < ... >_0 \quad \text{is a statistical average with Hamiltonian } H_0.$

It’s easy to show that all those averages are expressed in terms of function $b(y) = S_B(y)$ $B(y) - \text{Brilloin's function}$ and its derivatives $b^{(k)}$ over $y$, where

$y = \beta \left\{ \mu H + \sum_I I(1-1') < S_I^+ > \right\}$. (1.5)

is the value of the selfconsistent field which acts on the spin in site 1. For example

$< S_1^+ >_0 = b$

$< S_1^+ S_2^+ >_0 = b^2 + b^{(1)} \delta_{12}$

$< S_1^+ S_2^+ S_3^+ >_0 = b^3 + b^{(1)} b \delta_{12} + b \delta_{13} + b \delta_{23} + ...$

$+ b^{(2)} \delta_{12} \delta_{23}$. (1.6)

In general case

$< S_1^+ S_2^+ ... S_n^+ >_0 = b^n + b^{(1)} b^{(p-1)} \sum_{\text{perm}} \delta_{12} + ...$ + $b^{(2)} b^{p-3} \sum_{\text{perm}} \delta_{12} \delta_{23} + ...$ + $b^{(p-n)} \delta_{12} \delta_{23} ... \delta_{p-1,p}$. (1.7)

One can see from (1.7) that factor $b^{k-11}$ corresponds to every group of $\delta$-symbols which bind up, say, $k$ lattice sites and therefore the structure of $\delta$-symbols in every single term in (1.7) adequately determines the factor.

Due to the expansion (1.7) the contribution of $H_{\text{int}}, n$-power in (1.4) is divided into the sum of terms everyone of which contains a product of $n$ exchange...
integrals, a set of $\delta$-symbols and a corresponding set of factors $b$ and its derivatives. Everyone of these terms may be drawn as a graph. For this reason we shall draw all site indices in a number of $2 \, n + l$ ($l$ are the outer indices and $2 \, n$ are the inner ones), by points on a plane and call them vertices. The groups of coincident sites (due to $\delta$-symbols) will be drawn by oval and the corresponding part of diagram will be called block. An exchange interaction $I(l - 1')$ will be drawn by a wavy line connecting site 1 with site 1'. Thus a diagram with certain links will correspond to the certain term.

Thus we've got the following rules for diagram technique.

To draw the contribution of $n$-power in (1.4) it is necessary:

1. To draw up all the bound not equivalent graphs with 1 outer and $2 \, n$ inner vertices. Every graph is a set of blocks all the inner vertices of which are linked by $n$ interaction lines. The graphs which contain the elements without outer vertices and which are linked by only one interaction line to the rest part of the graph (the so-called one-taileds) should not be drawn for they have been already taken into account by renormalization of Hamiltonian.

2. The analytical expression

$$p_n = \beta_n ! \sum_{1 \neq 1'} I(1 - 1') ... \times (n - n') \delta(...\delta(...))$$

(1.8)

corresponds to a single graph.

$\beta$ is an index of blocks in the diagram ; $\beta_n$ is a number of vertices in $n$-th block ; $\delta(...\delta(...)$ means the coincidence of all $\beta_n$ vertices in a block.

$$p_n = \frac{1}{n_1 ! n_2 ! ...}$$

(1.9)

is a numerical factor, where $n_1, n_2, ...$ are the numbers of indistinguishable parts of a, b, ... types in the graph.

The dependence of a numerical factor upon the diagram structure is the essential distinction of our technique in comparison with the usual technique for fermion or boson operators. That gives rise to a very particular analytical structure of diagram series and to the special ways of their summarizing. Instead of having been usually gotten power series we had expansions of Taylor series type with intervals. But due to the multiplicative character of the numerical coefficient in which every factor corresponds to a certain part of the graph it had been possible to summarize the diagram series and to use the so-called << fattened >> elements.

Consider as an example a diagram series for $< S_1 >$ i. e. for spontaneous moment. Any graph for of this series may be considered as a mere reconstruction of a block containing the outer vertex 1 by attaching of any elements by interaction lines to it. We shall call these elements many-taileds.

The complete set of graphs with two, three, ... taileds will be drawn as on figure 1.

Consider a series of graphs (Fig. 2) containing in $< S_1 >$. Analytical series corresponds to the diagram series (Fig. 2). Here $x_2$ is an analytical expression corresponding to the two-tailed. Any graph for $< S_1 >$ contains $p_2$ two-taileds, $p_3$ three-taileds, ... $p_n$ $n$-taileds and according to the diagram rules its analytical expression is

$$b(p_2 + p_3 + ... + p_n) (y) \times x_1^{p_2} x_3^{p_3} ... x_n^{p_n}$$

(1.11)

Here factorials are in accordance with (1.9). It is obvious that

$$< S_1 > = \lim_{n \to \infty} \sum_{p_2=0}^{\infty} \sum_{p_3=0}^{\infty} b(p_2 + p_3 + ... + p_n) (y) \times x_1^{p_2} x_3^{p_3} ... x_n^{p_n}$$

(1.12)

Summing in (1.11) may be carried out if one use Caushy's formula for derivative:

$$b(q) = \frac{k!}{2 \pi i} \int_{\infty}^{b(z)} \frac{dz}{(z - y)^{k+1}}$$

(1.13)

Thus we've got the following formula

$$< S_1 > = \lim_{n \to \infty} \sum_{p_2=0}^{\infty} \sum_{p_3=0}^{\infty} b(p_2 + p_3 + ... + p_n) (y) \times x_1^{p_2} x_3^{p_3} ... x_n^{p_n}$$

(1.14)

which expresses the exact meaning of spontaneous moment in terms of the function of zero approximation $b(z)$ and of parameters $x_2, x_3, ...$ corresponding to the many-taileds which describe many-particle correlations of the system. Apparently taking the approximate values for parameters $x_k$ will give a possibility to find the asymptotic behaviour of spontaneous moment in the vicinity of phase transition. If we assume that all $x_k = 0$ then we will obtain $< S_1 > = b(y)$ that will correspond to zero approximation (or to the first graph on Fig. 2). If we keep only $x_2$ in (1.14) that will correspond to all graphs on figure 2 and to analytical series (1.10). The sum of the series is

$$A(x_2 | b) = \frac{1}{\sqrt{4 \pi x_2}} \int_{-\infty}^{+\infty} b(y + \xi) e^{-\xi^2/4x_2} d\xi$$

(1.15)
This expression has a simple physical meaning: it takes into account the Gaussian fluctuations of molecular field near its average value \( y \). The magnitude \( x_2 \) is the squareaverage fluctuation of the field. According to the formulated rules

\[
x_2 = \frac{1}{2N} \beta^2 \sum I(1 - 1') K_2(1, 2) I(2 - 1'), \quad (1.16)
\]

where \( K_2(1, 2) \) is the two-particle correlation function

\[
K_2(1, 2) = \langle S_1^x - \langle S_1^x \rangle \rangle \langle S_2^z - \langle S_2^z \rangle \rangle.
\]

(1.17)

The expansion of \( K_2(1, 2) \) is determined by all graphs with two outer vertices. If we denote the whole set of graphs which cannot be cut in one interaction line by \( \sum (1, 2) \) (the so-called proper (or irreducible) self-energy) then a following equation will take place:

\[
K_2(1, 2) = \sum (1, 2) + \sum (1, 3) \beta I(3, 4) K_2(4, 2). \quad (1.18)
\]

Passing to the Fourier’s expansions in (1.16) and (1.18) we will obtain

\[
x_2 = \frac{1}{2N} \sum q \frac{\beta \beta(q)}{1 - \beta \beta(q) \sum(q)}, \quad (1.19)
\]

where \( \beta(q) \) and \( \beta(q) \) are the Fourier’s transform of \( I(1 - 1') \) and \( \sum (1, 1') \) accordingly. If we confine ourselves by zero approximation for \( \sum(q) \) i.e. \( \sum(q) = K^{(1)}(y) \) then the expression under the sign of sum in (1.19) becomes the effective interaction of Ornstein-Zernike type. Thus the second graph for \( < S_1^x > \) on figure 2 corresponds to the Ornstein-Zernike approximation whereas the whole sum of graphs on figure 2 corresponds to the account of all field square fluctuations.

It may be shown [1] that the temperature dependence of magnetization (when \( T \to T_c \)) being obtained by approximate equation

\[
< S_1^x > = A(x_2 | b).
\]

(1.20)

is in agreement with scaling theory.

Let us consider now the partition function \( \zeta = \sum e^{-\beta E} \). The graphs for it are constructed by the above mentioned rules but they have not a single outer vertex. As in the usual technique it may be proved that

\[
\zeta = \exp \beta \beta_{\text{bound}}.
\]

(1.21)

which expresses \( \zeta \) only in terms of the bound diagrams. The diagram technique developed here is in a close connection with functional integral representation of partition function [2].

References


