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**THE CLUSTER MODEL
AND THE SADDLE POINT METHOD**

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In the paper of one of the authors [1] it was shown that at a certain choice of the exchanged integrals the Model Hamiltonian of the Ising interaction system with $2\mathcal{X}$ spins ($\mathcal{X} < \infty$) can take the form:

$$H(\mathcal{X}) = g_1 - hNS - N \sum_{n=1}^{\mathcal{X}} g_n S^{2n}, \quad S = \frac{1}{N} \sum_{j=1}^N S_j^2. \quad (I)$$

Thermodynamics and correlation effects in systems modelled by (I) were studied in [1] by means of majorizing method developed by N.N. Bogolubov (Jr.) [2]. They succeeded in getting the estimation for density difference of free energies calculated with the approximative hamiltonian

$$H_0(c, \mathcal{X}) = g_1 - (h + \sum_{n=1}^{\mathcal{X}} 2ng_n C^{2n-1})NS - N \sum_{n=1}^{\mathcal{X}} (g_n - 2ng_n) C^{2n} \quad (2)$$

and alongside (1). The estimation has the following form:

$$0 < f_0(h, \theta) - f_N(h, \theta) \leq \frac{\alpha(\theta)}{N^{3/5}}. \quad (3)$$

Thus the parameter C in $H_0(c, \mathcal{X})$ is obtained from equation

$$C = th \beta (h + \sum_{n=1}^{\mathcal{X}} 2ng_n C^{2n-1}), \quad (4)$$

which gives good possibilities of using the approximation method (2) in different physical problems, especially in magnetism.

In this connection we should mention the method of N.N. Bogolubov (Jr.) originally developed for studying BCS model then successfully used in magnet systems, and quite recently it was applied in studying the problems in which Bose-operators are of great significance (unlimited in norm). The cluster interaction of a general type (1) was also successfully investigated in paper [1] by the method mentioned in [2]. Sometimes in cases of great physical significance like $\mathcal{K}=1$, $\mathcal{K}=2$, the improvement of estimation (3) is possible if the saddle-point method is applied. In this paper we shall consider $g_n \geq 0$ only, - it will allow to use a simple Laplas formulation [3] for the saddle-point method taking into consideration the fact that it is possible to follow the asymptotic $f_N(h, \theta)$ at phase transition for $\mathcal{K}=1$.

1. Let us consider the model Hamiltonian as a part of (1) with $g_{2i} = g_i$ correspondingly:

$$H(p) = g_1 - hNS - N \sum_{i=1}^p g_i S^{2i}. \quad (5)$$

It is easy to show that

$$\text{Tr} e^{-\beta H(p)} = e^{-\tau^2 \frac{N}{2}} \int_{-\infty}^{\infty} d\lambda_1 \int_{-\infty}^{\infty} d\lambda_2 \dots \int_{-\infty}^{\infty} d\lambda_p e^{-N\mathcal{F}(\lambda_1, \dots, \lambda_p)}, \quad (6)$$

where

$$\mathcal{F}(\lambda_1, \dots, \lambda_p) = \sum_{i=1}^p \lambda_i^2 - \text{en}ch(\beta h + 2\lambda_i \tau_i), \quad (7)$$

$$\tau_i = (\beta g_i + 2\lambda_{i+1} \tau_{i+1})^{1/2}, \quad i = 1, 2, \dots, p-1,$$

$$\tau_p = (\beta g_p)^{1/2}, \quad \tau = (\beta g_1)^{1/2}.$$

The function $\mathcal{F}(\lambda_1, \dots, \lambda_p)$ is analytical in $\{\lambda_i\}$ and we suppose that the minimum of the function is simple. The corresponding quadratic form is positively determined and $\Delta = \text{Det} \left\| \frac{\partial^2 \mathcal{F}}{\partial \lambda_i \partial \lambda_j} \right\| > 0$. The minimum will be defined from the set of the equations

$$\bar{\lambda}_j = \frac{\partial(\bar{\lambda}_i \tau_i)}{\partial \lambda_j} \text{th}(\beta h + 2\bar{\lambda}_i \tau_i), \quad j = 1, \dots, p. \quad (8)$$

In this case as it is known [3,4] the asymptotic expansion is valid:

$$\text{Tr} e^{-\beta H(p)} = 2^N \left(\frac{N}{\pi}\right)^{p/2} e^{-N\mathcal{F}(\bar{\lambda})} \left\{ \alpha_0 N + \alpha_1 N + O(N^{-1/2}) \right\}, \quad (9)$$

where

$$d_0 = \pi^{1/2} \Delta^{-1/2}, \quad \mathcal{F}(\bar{\lambda}) = \mathcal{F}(\bar{\lambda}_1, \bar{\lambda}_2, \dots, \bar{\lambda}_p).$$

Then with the help of (9) it is easy to write the asymptotic expansion for the free energy density at fixed $N \gg 1$:

$$f_N = -\frac{\theta}{N} \ln \text{Tr} e^{-\beta H(p)} = -\theta \ln 2 + \theta \mathcal{F}(\bar{\lambda}) + \frac{2g_1 - \theta \ln \Delta}{2N} + O(N^{-1}). \quad (10)$$

Taking into account (8) and by definition of the specific magnetization $\sigma = -\left. \frac{\partial f}{\partial h} \right|_{\theta}$ we get the equation for σ :

$$\sigma = th \beta \left(h + \sum_{i=1}^p g_i 2^i \sigma^{-2^i - 1} \right), \quad (11)$$

which is a detailed transformation of (4) in our case. The expansion (10) can and may be modified at $\Delta = 0$ which first of all may occur when $h=0$ and $\beta = \beta_c$; $\{\bar{\lambda}_j(\beta_c)\} = 0$.

In this case the expansion $\mathcal{F}(\lambda_1, \lambda_2, \dots, \lambda_p)$ in the neighbourhood of $\bar{\lambda}_j(\beta_c)$ may start with the terms of a higher degree $(\lambda_j - \bar{\lambda}_j)^n$; $(n > 2)$, as the first terms of the expansion tend to zero. Therefore we may have $\ln N$ in expansion (10). Let us consider in detail for $p=1$.

Here the asymptotic expansion (9) under the assumption that $\frac{\partial^2 \mathcal{F}}{\partial \lambda_i^2} > 0$ can be written in the following way:

$$\text{Tr} e^{-\beta H(1)} = 2^N \left(\frac{N}{\pi} \right)^{1/2} e^{-N \mathcal{F}(\bar{\lambda})} \left\{ \gamma_0 N^{-1/2} + \gamma_1 N^{-3/2} + O(N^{-5/2}) \right\}, \quad (12)$$

$$\gamma_0 = \left\{ \frac{\pi}{2\bar{\lambda}^2 - 2\tau^2 + 1} \right\}^{1/2},$$

$$\gamma_1 = \frac{\Gamma(\frac{5}{2})}{2\bar{\lambda}^2 - 2\tau^2 + 1} \left\{ \frac{5}{4} + \frac{8}{3} \frac{\bar{\lambda}(\tau^2 - \bar{\lambda}^2)}{2\bar{\lambda}^2 - 2\tau^2 + 1} \right\},$$

where the stationary point is determined by the equation

$$\bar{\lambda} = \tau th (\beta h + 2\bar{\lambda} \tau). \quad (13)$$

We should note that the following terms of asymptotic in (12) contributing $O(N^{-5/2})$ are easily calculated and give credit for $O(N^{-1/2})$ [3]. However, we shall not put down $h=0$, $\beta = \beta_c$, at $\theta < \theta_c$ and $\theta > \theta_c$, because we shall consider this case later.

The solutions of the equation of selfconsistency (13) are well known. Here we want to point out the case when $h=0$ resulting in nontrivial solution $\bar{\lambda}_0(\tau)$ when $2\tau^2 > 1$. And thus we observe the phenomenon of spontaneous magnetization. Let us note that the limited value of spontaneous magnetization is usually calculated:

$$\sigma = th \beta (h + 2g_1 \sigma)$$

and obtained by means of:

$$G_0(\beta) = th \, 2\bar{\lambda}_0(\tau)\tau = \frac{\bar{\lambda}_0(\tau)}{\tau}. \quad (14)$$

At first a trivial case is investigated ($2\tau^2 < 1$) for which only $\bar{\lambda}_0 = 0$ is known. The function $\mathcal{F}(\lambda)$ has a simple absolute minimum at this point: $\mathcal{F}''(0) = 2(1-2\tau^2) > 0$.

The asymptotic expansion (12) is valid, where γ_0, γ_1 are obtained from (12), when $\bar{\lambda} = 0$ correspondingly. The free energy is expressed by

$$f_N(h=0, 2\tau^2 < 1) = -\theta \ln 2 + \frac{\theta}{N} \left\{ \tau^2 + \frac{\ln(1-2\tau^2)}{2} \right\} + O(N^{-1}). \quad (15)$$

The asymptotic expansion (12) is also valid below the phase transition point ($2\tau^2 > 1$), where the choice of the two simple absolute maxima depends on the sign of h . Let us assume that $h > 0$ fixes the "right" maximum with a further transition $h \Rightarrow +0$: average values are understood as Bogolubov's quasi-averages. Then we receive

$$f_N(h=0, 2\tau^2 > 1) = -\theta \ln 2 + \frac{\theta}{N} \left\{ \tau_0^2 + \frac{\ln(1-\sigma_0^2)}{2} \right\} + \frac{\theta}{N} \left\{ \tau^2 + \frac{\ln[1-2\tau^2(1-\sigma_0^2)]}{2} \right\} + O(N^{-1}), \quad (16)$$

using (12) and (14).

The asymptotic at the phase transition point $2\tau^2 = 1$, $\bar{\lambda}_0(2\tau^2=1) = 0$, requires a particular consideration as γ_0 calculated by a routine method with a partial summing up of the series over $\frac{1}{\mathcal{F}''(0)}$ (See [5] and [3]) and due to $\mathcal{F}''(0) = 2(1-2\tau^2) = 0$, and have a branch at a given point (See (12)). $\mathcal{F}(\lambda)$ at the point of $\lambda_0 = 0$ has one degenerated minimum. Thus for $2\tau^2 = 1$ we have:

$$\mathcal{F}'(0) = \mathcal{F}''(0) = \mathcal{F}'''(0) = 0; \quad \mathcal{F}^{(IV)}(0) = 8; \quad \mathcal{F}^{(V)}(0) = 0,$$

$$\mathcal{F}^{(VI)}(0) = -128;$$

whence

$$\mathcal{F}(\lambda, 2\tau^2=1) = \frac{1}{3}\lambda^4 - \frac{8}{45}\lambda^6. \quad (17)$$

It allows us to get the asymptotic expansion at the point of phase transition

$$\text{Tr} e^{-\beta H(1)} = 2^N \left(\frac{N}{\pi}\right)^{1/2} \left\{ \gamma_1 N^{-1/4} + \gamma_2 N^{-3/4} + O(N^{-5/4}) \right\} \quad (18)$$

with the valid coefficients

$$\gamma_1 = \frac{1}{2} 3^{1/4} \Gamma(\frac{1}{4}), \quad \gamma_2 = \frac{4}{3} 3^{3/4} \Gamma(\frac{2}{4}). \quad (19)$$

The expansion (18) results in the following asymptotic for free energy at $2\tau^2 = 1$:

$$f_N = -g \ln 2 - \frac{g}{4} \frac{\ln N}{N} + \frac{g\tau^2 - g \ln[2\pi^{-1/2} 3^{1/4} \Gamma(\frac{1}{4})]}{N} + O(N^{-1}). \quad (20)$$

Coming back to the discussion when $\rho = 1$, it should be mentioned that the saddle-point method, if made correctly, gives the possibility to obtain and to compare the asymptotics (over N^{-1}) in the phase transition. The fact of logarithmical asymptotic at the very point of the phase transition $2\tau^2 = 1$ is of significance. Taking into account that the asymptotic amendments for $f_N(h=0, 2\tau^2 \neq 1)$ are the values of the order $\frac{g\tau^4}{N}$ and $\frac{g\tau^2(\tau^2 - \sigma_0^2)}{N}$ for $2\tau^2 < 1$ and $2\tau^2 > 1$ respectively, we see that at the phase transition point $2\tau^2 = 1$ the asymptotic changes sharply and takes the form: $\frac{g}{4} \frac{\ln N}{N} = \frac{g}{2} \frac{\ln N}{N}$ (according to (20)). The case $g < 0$ when $\mathcal{K} = 1$ is not difficult and results in the asymptotic of N^{-1} type for any τ .

Now in a general approach (5)-(11) it is quite possible to consider a "more realistic" cluster hamiltonian:

$$H(2) = g_1 - hNS - N(g_1 s^2 + g_2 s^4), \quad g_i \geq 0, \quad (21)$$

which introduces a certain approximation for the systems with weak spin-phonon interaction. The case when g_i are of different signs is of interest and it requires another investigation of the "full form" of the saddle-point method [5]. The "Heuristic" use of the equations (4), (11) allows us to consider the systems with phase transition both the first and the second kind and to follow the realization of all possibilities at various relations between g_i (See [1], [6]).

2. Let us consider shortly another possibility of investigation of the cluster interaction, to some extent, which coordinates the approach mentioned above and powerful method of the approximative Hamiltonians by N.N. Bogolubov (Jr.). The idea is to select the Hamiltonian $H(\rho)$ of (5) type as the approximative Hamiltonian for the cluster Hamiltonian $H(\mathcal{K})$ of a general type given in [1]. Let us illustrate it for the system with the model Hamiltonian at $\mathcal{K} = 3$

$$H(3) = g_1 - hNS - N(g_1 s^2 + g_2 s^4 + g_3 s^6), \quad (22)$$

which cannot be considered only by means of the saddle-point method given in the first section. It can naturally

be studied in the general method [1]. Nevertheless, we shall choose the following form for the approximative Hamiltonian:

$$H(2) = g_1 + G - N(a_1 s^2 + a_2 s^4), \quad (23)$$

$$a_1 = g_1 + g_3 c^4, \quad a_2 = g_2 + g_3 c^2, \quad G = N g_3 c^6.$$

The inequality developed by Bogolubov for the free energies density can be written as follows:

$$0 \leq \min_{(c)} f[H(2)] - f[H(3)] \leq g_3 \langle (s^2 - \langle s^2 \rangle)(s^4 - \langle s^4 \rangle) \rangle, \quad (24)$$

where the averaging process in the right-hand side of the inequality is carried out with respect to $H(3)$. The estimation of $\mathcal{E}(N)$ will be received by method [2], as usual. Then we shall introduce the sources in $H(2)$ and $H(3)$:

$$\mathcal{H}_i = H(i) + N(\nu s^2 + \mu s^4), \quad (i=2,3). \quad (25)$$

Naturally, (24) is correct for \mathcal{H}_2 and \mathcal{H}_3 correspondingly.

Thus

$$\mathcal{E}(N) = -g_3 \frac{\theta}{N} \frac{\partial^2 f[\mathcal{H}_3]}{\partial \nu \partial \mu}. \quad (26)$$

Since $\left| \frac{\partial f[\mathcal{H}_3]}{\partial \mu} \right| \leq 1$, then $\int_{\nu_0}^{\nu_1} \mathcal{E}(N) d\nu \Big|_{\mu} \leq g_3 \frac{2\theta}{N}$.

Let $\delta f_N = \min_{(c)} f[\mathcal{H}_2] - f[\mathcal{H}_3]$, then it is evident,

that $0 \leq \delta f_N(\nu) \leq 2(\nu_1 - \nu_0) + \frac{1}{\nu_1 - \nu_0} \int_{\nu_0}^{\nu_1} \mathcal{E}(N) d\nu$. Assuming, at last,

that $\nu = \mu = 0$, $\nu_0 = 0$, we receive:

$$0 \leq \min_{(c)} f[H(2)] - f[H(3)] \leq 2\nu_1 + \frac{2g_3\theta}{\nu_1 N}.$$

Now we take ν_1 from the minimum of the right-hand part of the above-mentioned inequality. We receive $\mathcal{E}(N) = \frac{4\sqrt{g_3\theta}}{N^{3/2}}$.

For $f_N[H(2)]$ we have as shown above:

$$f_N[H(2)] = f[H(2)] + \frac{g_1 - c_1}{N} + O(N^{-1}),$$

$$f[H(2)] = -\theta \ln 2 + g_3 c^6 + \theta \mathcal{F}(\bar{\lambda}_1, \bar{\lambda}_2),$$

$$\mathcal{F}(\bar{\lambda}_1, \bar{\lambda}_2) = \bar{\lambda}_1^2 + \bar{\lambda}_2^2 - \text{en ch}(\beta h + 2\bar{\lambda}_1 \tau_1); \quad (27)$$

$$\tau_1 = \{\beta a_1 + 2\bar{\lambda}_2 (a_2 \beta)^{1/2}\}^{1/2}, \quad c_1 = \frac{\theta}{2} \text{en Det} \left\| \frac{\partial^2 \mathcal{F}}{\partial \bar{\lambda}_1 \partial \bar{\lambda}_2} \right\|.$$

The parameter C and stationary points $\bar{\lambda}_1, \bar{\lambda}_2$ are obtained from minimum condition $f[H(2)]$ (See (8)):

$$\bar{\lambda}_1 = \tau_1 \text{th}(\beta h + 2\bar{\lambda}_1 \tau_1),$$

$$\bar{\lambda}_2 = \bar{\lambda}_1 \frac{\partial \tau_1}{\partial \bar{\lambda}_2} \text{th}(\beta h + 2\bar{\lambda}_1 \tau_1), \quad \frac{\partial \mathcal{F}(\bar{\lambda}_1, \bar{\lambda}_2)}{\partial C} = -6g_3 c_1^5 \beta. \quad (28)$$

Hence we finally get the equation for magnetization (compare (4) and (11)).

$$G = \text{th} \beta (h + 2g_1 G + 4g_2 G^3 + 6g_3 G^5). \quad (29)$$

Evidently, we described only general features of such an approach. However, in cases where "more physical" approximation than that discussed in [I] is necessary, this approach is more useful.

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