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SOME THEOREMS FOR FREE ENERGY OF MODEL SYSTEMS OF STATISTICAL PHYSICS

Asymptotically exact methods of studying of many-particle systems were developed in Bogolubov's papers [1,2] in the course of creating microscopical theory of superconductivity. Mathematically rigorous background of the offered methods was essentially pointed in paper [3]. The problems which admit exact solution in limiting thermodynamical sense ($V \to \infty$, $N \to \infty$, $\frac{N}{V} = const$, where V - volume of the system, N - the number of particles) occupy particular place among the model problems of modern statistical physics. Later on rigorous from the mathematical point of view methods of proving asymptotical exactness of the results obtained for such model systems have been suggested by N.N.Bogolubov (Jr.), and there has been also constructed a general method of studying asymptotical behaviour of such values as free energy (and its derivatives), one-time and many-time correlation functions, and Green's functions [4,5].

These methods, originally developed for studying Bardin-Bogolubov model systems [1-5] with Hamiltonian[1]:

$$H = \sum_f T_f a_f^+ a_f - \frac{1}{V} \sum_{f,f'} I(f,f') a_f^+ a_{-f}^+ a_{-f'} a_{f'} \qquad (1)$$

[1] Here and further we use the following notations: $f=(\vec{p},s)$; $-f=(-\vec{p},s)$ p -momentum, s -spin, $T_f = \frac{p^2}{2} - \mu$; μ being the chemical potential; a_f^+, a_f are the Fermi operators. Positive value T_c means the constant of interaction; $\sigma_p, \sigma_p^+, \sigma_t^z$ are Pauli operators; Ω - pairstates number; N is the number of particles, and $\mathcal{H}$ - external magnetic field.

got successful application in the studies on quasi-spin models [6-7] with Hamiltonian of the Thirring type:

$$H=\sum_{p=1}^{\Omega}\mathcal{E}(1-\sigma_p^z)-\frac{2T_c}{\Omega}\sum_{p=1}^{\Omega}\sigma_p^-\sum\sigma_p^+ \qquad (2)$$

and on the Ising model [8,9]

$$H=-{}^{I}/_{N}\sum_{i,j}\sigma_i^z\sigma_j^z-\mu_0\mathcal{H}\sum_{i=1}^{N}\sigma_i^z \qquad (3)$$

Later on we shall show that for model problems with Hamiltonian of more general type such as in case of the superconductivity type system, inhomogeneous in spin variables

$$H=\sum_{\vec{p},s,s'}T(p)a^+_{\vec{p},s}a_{\vec{p},s'}-\frac{1}{2V}\sum_{\vec{p},\vec{p}'}\sum_{s,s'}I(\vec{p},\vec{p}';s,s')a^+_{\vec{p},s}a^+_{-\vec{p},-s}a_{-\vec{p}',-s'}a_{\vec{p}',s'} \qquad (4)$$

our method [1-5] gives a possibility to find asymptotically exact expressions for correlation functions, one-time and many-time ones, and Green's functions as well.

Further development of mathematical methods for studying model problems is undoubtedly very interesting.

Here we shall consider the expression with Hamiltonian of a general type:

$$H=T-2V\sum_{\alpha=1}^{\ell}g_\alpha\mathcal{J}_\alpha\mathcal{J}_\alpha^+ \quad , \qquad (5)$$

where dynamical operators $T,\mathcal{J}_\alpha,\mathcal{J}_\alpha^+$ are not concretized but the fulfillment of the following conditions is demanded

$$T=T^+ \quad \|\mathcal{J}_\alpha\|\leq A_1 \quad \|T\mathcal{J}_\alpha-\mathcal{J}_\alpha T\|\leq A_2$$
$$\|\mathcal{J}_\alpha\mathcal{J}_\beta-\mathcal{J}_\beta\mathcal{J}_\alpha\|\leq\frac{A_3}{V} \quad \|\mathcal{J}_\alpha^+\mathcal{J}_\beta-\mathcal{J}_\beta\mathcal{J}_\alpha^+\|\leq\frac{A_4}{V}\ , \qquad (6)$$

where V is a finite volume of the system, A_i are some positive constants under $V\to\infty$ $(\frac{N}{V}=const)$. Coefficients g_α in (5) are taken positive in connection with the fact that only the systems with negative interaction are discussed in this work.

As "approximative" system for the model with Hamiltonian (5) we suggest the system, described by Hamiltonian

$$H_a(C)=T-2V\sum_\alpha g_\alpha(C_\alpha\mathcal{J}_\alpha^+ + C_\alpha^*\mathcal{J}_\alpha)+\mathcal{K}(C), \qquad (7)$$

which depends upon the parameter C, representing the vector $C=(C_1,C_2,\dots,C_\ell$ in ℓ-dimensional complex space E_ℓ ; $\mathcal{K}(C)$ constant and, if it is necessary, can serve as parameter of normalization.

We must note that for Hamiltonian (7) free energy per unit volume[2)] is a function of the parameter C, determined on space E_ℓ of all points C. Later on the expression $\min_{(C)} f(C)$ will denote absolute minimum of the function $f_V(H_a)$ in E_ℓ.

Note, that the procedure of minimization of free energy per unit volume for Hamiltonian(7),as function of the parameter C,allows one to get conditions determining the set of points $\bar{C}=(\bar{C}_1,\bar{C}_2,\dots,\bar{C}_\ell)$ in which absolute minimum of $f_V(H_a)$ is reached, i.e., the equality

$$f_V\{H_a(\bar{C})\}=\min_{(C)} f_V\{H_a(C)\} \qquad (8)$$

is correct.

2) Under free energy per unit volume for system with arbitrary Hamiltonian H we mean the expression $f_V=-\frac{\theta}{V}\ln Sp\,e^{-\frac{H}{\theta}}$, where parameter θ is temperature (in energetic units).

In this paper we shall show that the expression for free energy per unit volume for Hamiltonian (5) is asymptotically close to the corresponding expression for free energy of "approximative system" with Hamiltonian (7) under the assumption of fulfillment of conditions (6).

For our investigation it is more convenient to treat the so-called Hamiltonian with sources:

$$h = T - 2V\sum_\alpha g_\alpha J_\alpha J_\alpha^+ - V\sum_\alpha (\nu_\alpha J_\alpha^+ + \nu_\alpha J_\alpha) \qquad (9)$$

in which including source parameters are proportional, accordingly, to $\bar C_\alpha$, $\bar C_\alpha^*$ with positive coefficients of proportionality:

$$\nu_\alpha = \tau_\alpha \bar C_\alpha \quad \nu_\alpha^* = \tau_\alpha \bar C_\alpha^* \quad \tau_\alpha = \tau_\alpha^* > 0,\ \alpha = 1,2,\dots,\ell. \qquad (10)$$

As it is shown in [5], the choice of these parameters in form (10) allows one to avoid difficulties under true definition of quasi-averages for considered model systems.

In order to have a possibility of true selection of quasi-average for "systems with sources" (9) it is necessary to choose a corresponding approximative Hamiltonian [5]:

$$h_a = T - 2V\sum_\alpha g_\alpha (\bar C_\alpha J_\alpha^+ + C_\alpha^* J_\alpha) - V\sum_\alpha \tau_\alpha (\bar C_\alpha^* J_\alpha^+ + \bar C_\alpha^* J_\alpha) + \mathcal{K}(C), \qquad (11)$$

which evidently corresponds to approximative Hamiltonian (7) for model Hamiltonian (5) under alteration of parameters g_α in the latter according to the rule

$$g_\alpha \to g_\alpha + \frac{\tau_\alpha}{2}, \quad \alpha = 1,2,\dots,\ell \qquad (12)$$

Therefore only "renormalization"3) of g_α constants in expression (9) for h with necessity results in that Hamiltonian (11) becomes approximative for primary Hamiltonian (5). We emphasize that term K was not necessary for it, obviously, does not contain itself neither in motion equation nor in finite expression for average $\langle\dots\rangle_h$. Hence, we have the right to add arbitrary but constant part to a model Hamiltonian which will be

$$h = T - 2V\sum_\alpha \left(g_\alpha - \frac{\tau_\alpha}{2}\right) J_\alpha J_\alpha - V\sum_\alpha \tau_\alpha (\bar C_\alpha J^+ + \bar C_\alpha^* J_\alpha). \qquad (13)$$

The choice of corresponding constant term in the form $V\sum_\alpha \tau_\alpha \bar C_\alpha \bar C_\alpha^*$ gives us an opportunity to rewrite (13) as

$$h = T - 2V\sum_\alpha \left(g_\alpha - \frac{\tau_\alpha}{2}\right) J_\alpha J_\alpha^+ - V\sum_\alpha \tau_\alpha (\bar C_\alpha J_\alpha^+ + \bar C_\alpha^* J_\alpha) + \qquad (14)$$
$$+ V\sum_\alpha \tau_\alpha \bar C_\alpha \bar C_\alpha^* = H + V\sum_\alpha \tau_\alpha (J_\alpha - \bar C_\alpha)(J_\alpha^+ - \bar C_\alpha^*),$$

where H is the primary Hamiltonian (5). Positive coefficients $\mathcal{T}_\alpha$ and dispersion σ_α according to the rules:

$$\tau_\alpha = 2\mathcal{T}_\alpha g_\alpha, \quad \mathcal{T}_\alpha > 0 \qquad (15)$$
$$\sigma_\alpha = (J_\alpha - \bar C_\alpha)(J_\alpha^+ - \bar C_\alpha^*), \quad \alpha = 1,2,\dots,\ell$$

give us a possibility to rewrite (14) in the form convenient for us:

$$h = H - 2V\sum_\alpha \mathcal{T}_\alpha g_\alpha \sigma_\alpha \qquad (16)$$

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3) i.e., transformation according to the rule:

$$g_\alpha \to g_{\alpha'} = g_\alpha - \frac{\tau_\alpha}{2} \qquad (12')$$

Let us start obtaining asymptotical behaviour of free energy for Hamiltonian (16). First of all, we state Theorem 1, which confirms the possibility for asymptotically exact describing the model system (5) with the help of Hamiltonian (7).

Theorem 1.

If the operators $T, \mathcal{J}$ in Hamiltonian (5) satisfy condition (6) and free energy for Hamiltonian T is limited

$$|f_V(T)| \leq A_0 = const,$$

then we have the inequality

$$0 \leq \min_{(C)} f_V\{H_a(C)\} - f_V(H) \leq \mathcal{E}\left(\tfrac{1}{V}\right). \qquad (17)$$

in which positive constant $\mathcal{E}(\frac{1}{V}) \to 0$ in thermodynamical limit $V \to \infty$ uniformly with respect to θ in the interval $0 \leq \theta \leq \theta_0$, where θ_0 is an arbitrary fixed temperature.

The proof of Theorem 1 is given in [4]. We mention here that Theorem 1 does not answer the question whether the limited expression

$$f_\infty(H) = \lim_{V \to \infty} f_V(H)$$

exists.

The answer is in

Theorem 2.

If in Hamiltonian (5) the operators T and $\mathcal{J}$ are defined for all points of ρ-space and the set of discontinuities of the functions is a set of measure zero, then under the fulfillment of condition (6) the asymptotic free energy

for Hamiltonian (7) exists and for all C_α from set $\{C : |C_\alpha| \leq \bar{A} = 2A_1\}$, inequality

$$|f_V\{H_a(C)\} - f_\infty\{H_a(C)\}| \leq \delta_V \qquad (18)$$

is correct. Here $\delta_V \to 0$ uniformly with respect to θ in the interval $0 \leq \theta \leq \theta_0$ and $f_\infty\{H_a(C)\}$ possesses continuous partial derivatives of all orders with respect to variables

$$C_1, C_2, \ldots, C_\ell, \quad C_1^*, C_2^*, \ldots, C_\ell^*$$

for all complex values of these variables. This function reaches in space E_ℓ absolute minimum realized on a set $\{\bar{C}\}$, i.e.,

$$\min_{(C)} f_\infty\{H_a(C)\} \equiv f_\infty\{H_a(\bar{C})\}$$

and here will be fulfilled the inequality

$$|f_V(H) - f_\infty\{H_a(C)\}| \leq \bar{\bar{\delta}}_V \equiv \mathcal{E}\left(\tfrac{1}{V}\right) + \delta_V, \qquad (19)$$

where $\bar{\bar{\delta}}_V \to 0$ uniformly with respect to θ in the interval $0 \leq \theta \leq \theta_0$.

Proof:

Let us estimate the difference

$$\delta f = f_V\{H_a(C)\} - f_{V+v}\{H_a(C)\},$$

i.e., the difference of free energies, corresponding to one and the same approximative Hamiltonian (7), but chosen for the systems with different values V and $V+v$, where V is the value, finite in the framework of this proof, and v is some arbitrary value. After some simple transformation and having made the limit transition $V \to \infty$ (in general statistical sense) we get the inequality (18) which together with the inequality (17) results in (19)

$$\left| f_V(H) - f_\infty\{H_a(\bar{C})\} \right| = \left| f_V(H) - \min_{(C)} f_\infty\{H_a(C)\} \right| =$$

$$= \left| f_V(H) - \min_{(C)} f_V\{H_a(C)\} + \min_{(C)} f_V\{H_a(C)\} - \min_{(C)} f_\infty\{H_a(C)\} \right| \le$$

$$\le \left| f_V(H) - \min_{(C)} f_V\{H_a(C)\} \right| + \left| \min_{(C)} f_V\{H_a(C)\} - \min_{(C)} f_\infty\{H_a(C)\} \right| \le \mathcal{E}\left(\tfrac{1}{V}\right) + \delta_V .$$

Thus, we proved limit theorems for free energy functions and got corresponding estimates for a model problem with the Hamiltonian of a general type without concretizing the dynamical operators $T, \mathcal{J}$.

We must mention that in the case of concrete systems exact expressions for limit values of free energy can be obtained. For example, in [10] it was shown that the expression for free energy per unit volume V ,answering Hamiltonian (1) preliminarily diagonalized with the help of Bogolubov-Tiablikov canonical transformation, could be found in the form:

$$f_V\{H_a(C)\} = 2\sum_\alpha g_\alpha C_\alpha C_\alpha^* - \frac{1}{2V}\sum_f (E_f - T_f) + \frac{\theta}{V}\sum_f \ln(1+e^{-E_f/\theta}) \quad (20)$$

and under $V \to \infty$ will be approximated by the following asymptotic expression

$$f_\infty\{H_a(C)\} = 2\sum_\alpha g_\alpha C_\alpha C_\alpha^* - \frac{1}{2(2\pi)^3}\int \left\{E_f - T_f - 2\theta \ln(1+e^{-E_f/\theta})\right\} df , \quad (21)$$

where

$$E_f = \sqrt{T_f^2 + \Delta_f^2} \qquad \Delta_f = 2\sum_\alpha g_\alpha C_\alpha \lambda_\alpha(f) \quad (22)$$

are standard notions and $\lambda_\alpha(f)$ are "constant of interaction" and satisfy conditions

$$\lambda_\alpha(-f) = -\lambda_\alpha(f), \quad \alpha = 1, 2, \ldots, \ell .$$

Further we discuss the problem of asymptotical proximity of free energies, obtained on the basis of Hamiltonian h and H , correspondingly:

$$f_V(h) = -\frac{\theta}{V} \ln Sp\, e^{-\frac{h}{\theta}}$$
$$f_V(H) = -\frac{\theta}{V} \ln Sp\, e^{-\frac{H}{\theta}} . \quad (23)$$

Evidently, under $\tau = 1$, i.e., under $\tau_1 = \tau_2 = \ldots = \tau_\ell = 1$ we obtain

$$h|_{\tau=1} = T - 2V\sum_\alpha g_\alpha(\bar{C}_\alpha \mathcal{J}_\alpha^+ + \bar{C}_\alpha^* \mathcal{J}_\alpha) + 2V\sum_\alpha g_\alpha \bar{C}_\alpha \bar{C}_\alpha^* \equiv H(\bar{C}) \quad (24)$$

and therefore

$$h \le H(\bar{C}) \quad (25)$$

so far as $\sigma_\alpha \ge 0$ always.

On the other hand, $h \ge H$ under $0 < \tau_\alpha < 1, \ \alpha = 1, 2, \ldots, \ell$ and we can affirm that the inequalities

$$f_V\{H(\bar{C})\} \ge f_V(h) \ge f_V(H) \quad (26)$$

are valid if: $0 < \tau_\alpha < 1 \qquad \alpha = 1, 2, \ldots, \ell$.

Then

$$0 \le f_V\{H_a(\bar{C})\} - f_V(H) \le |f_\infty\{H(\bar{C})\} - f_V(H)| + $$
$$+ |f_\infty\{H(\bar{C})\} - f_V\{H(\bar{C})\}|$$

or taking into account theorem 1:

$$0 \le f_V\{H(\bar{C})\} - f_V(H) \le \bar{\bar{\delta}}_V + \delta_V , \tag{27}$$

and, correspondingly,

$$0 \le f_V(h) - f_V(H) \le \bar{\bar{\delta}}_V + \delta_V \equiv \eta$$
$$0 \le f_V\{H(\bar{C})\} - f_V(h) \le \bar{\bar{\delta}}_V + \delta_V \equiv \eta \quad . \tag{28}$$

The application of these inequalities for obtaining of corresponding estimations for correlation averages is based on Bogolubov's (Jr.) majorizing inequalities [5] .

For a system described by the Hamiltonian linear in parameter τ :

$$H_\tau = H_0 + \tau H_1 \tag{29}$$

we can determine the expression

$$f_V(H_\tau) = -\frac{\theta}{V} \ln Sp\, e^{-\frac{H_\tau}{\theta}} \tag{30}$$

as a function of free energy per unit volume for a given model system.

It is easily seen that

$$\frac{d}{d\tau} f_V(H_\tau) = \frac{1}{V} < H_1 >_{H_\tau} , \tag{31}$$

and, correspondingly,

$$\frac{d^2}{d\tau^2} f_V(H_\tau) = -\frac{1}{\theta V} \int_0^1 < \tilde{H}_1 e^{-\frac{H_\tau \xi}{\theta}} \tilde{H}_1 e^{\frac{H_\tau}{\theta}(1-\xi)} >_{H_\tau} d\xi \tag{32}$$

is permissible, where $\tilde{H}_1 = H_1 - < H_1 >_{H_\tau}$.

But it is known that

$$\frac{d^2}{d\tau^2} f_V(H_\tau) \le 0$$

and, correspondingly,

$$\left\{\frac{d}{d\tau} f_V(H_\tau)\right\}_{\tau=1} \le \frac{d}{d\tau} f_V(H_\tau) \le \left\{\frac{d}{d\tau} f_V(H_\tau)\right\}_{\tau=0} \tag{33}$$

and free energy difference may be taken in the form

$$f_V(H_0 + H_1) - f_V(H_0) = \int_0^1 \frac{d}{d\tau} f_V(H_\tau)\, d\tau , \tag{34}$$

where $0 \le \tau \le 1$.

Thus we obtain the inequality

$$\left\{\frac{d}{d\tau} f_V(H_\tau)\right\}_{\tau=1} \le f_V(H_0 + H_1) - f_V(H_0) \le \left\{\frac{d}{d\tau} f_V(H_\tau)\right\}_{\tau=0} \tag{35}$$

with the help of which we simply obtain:

$$\frac{1}{V} < H_1 >_{H_0 + H_1} \le f_V(H_0 + H_1) - f_V(H_0) \le \frac{1}{V} < H_1 >_{H_0} . \tag{36}$$

Definite choice of parameters in the inequality (36)

$$H_0 \equiv H \qquad H_1 \equiv h - H = 2V\sum_\alpha \tau_\alpha g_\alpha \sigma_\alpha \tag{37}$$

with the account of the first of inequalitites (28) permits one to obtain the following estimate for binary correlation function $\langle \sigma_\alpha \rangle_h$:

$$2\sum_\alpha \tau_\alpha g_\alpha \langle \sigma_\alpha \rangle_h \leq \bar{\bar{\delta}}_V + \delta_V \ . \tag{38}$$

Thus, is proved

Theorem 3.

Under the fulfillment of condition of theorem 2 for Hamiltonian h in form (14) the following inequalities hold:

$$0 \leq f_V(h) - f_V(H) \leq \eta \tag{39}$$

$$\sum_\alpha g_\alpha \langle (J_\alpha - \bar{C}_\alpha)(J_\alpha^+ - \bar{C}_\alpha^*) \rangle_h \leq \frac{\eta}{\tau_0} \ ,$$

here $\eta = \bar{\bar{\delta}}_V + \delta_V$ and it tends to zero as $V \to \infty$ and is the minimal of the quantities $\tau_1, \tau_2, \ldots \tau_\ell$ which satisfy the conditions $0 < \tau_\alpha < 1$, $\alpha = 1, 2, \ldots, \ell$.

The inequalities (39) confirm the possibility for asymptotically exact describing model system with Hamiltonian (5) with the help of Hamiltonian (14), because from Theorem 3 it follows

$$\lim_{V\to\infty} f_V(h) = \lim_{V\to\infty} f_V(H) .$$

In the next papers we shall develop methodics of calculation of a correlation function and quasi-averages for model system of such a general form, and an application to concrete system of statistical physics will be made.

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