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APPROXIMATION OF CLASSICAL CONTINUOUS AND LATTICE SYSTEMS

Курбатов А.М. **E5 - 12432**

Аппроксимация классических непрерывных и решетчатых систем

В работе рассматривается возможность аппроксимации модельных систем классической статистической механики. Анализ проводится сразу для решетчатых и непрерывных систем. Для модельных гамильтонианов с отрицательным взаимодействием доказан классический аналог основной теоремы об аппроксимации Боголюбова /мл./. Сформулированы условия, при которых является точной аппроксимация систем с сепарабельным отрицательным и положительным взаимодействием. Доказанные теоремы охватывают и случай бесконечного числа мод взаимодействия. Полученные результаты справедливы для всех ансамблей за исключением микроканонического.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Approximation of Classical Continuous and Lattice Systems

The possibility of the approximation of model systems in classical statistical mechanics is considered. The analysis is carried out for lattice and continuous systems altogether. For the model Hamiltonians with negative interaction the classical analogue of the main approximation theorem by Bogolubov Jr., is proved. The conditions are formulated under which the approximation of the systems with separable negative and positive interactions is exact. The theorems proved cover the case of in finite number of modes as well. The results obtained are valid for all the ensembles except for the microcanonical one.

The investigations has been performed at the Laboratory of Theoretical Physics, JINR.

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The method of exact approximation of many-particle systems has been developed in quantum statistical mechanics /1/. Here we shall make an attempt to extend it to classical systems.

In the present paper we consider the possibility of reducing model Hamiltonians to much more simple ones, that enables us to tackle the former ones exactly. We make use essentially of the results and notations of our paper /2/.

We coside simultaneously the continuous canonical and the grand canonical ensembles as well as the lattice systems, that is our consideration covers the cases $P=P^{(c,g,\ell)}$.

To begin we need to define the norm $\|\cdot\|_\infty$ in the spaces $\Omega=\Omega_{V,N},\Omega_V,\Omega_N$ in the usual way.

Def. 1 (norm $\|\cdot\|_\infty$):

The norm $\|\cdot\|_\infty$ in $\Omega=\Omega_{V,N},\Omega_V,\Omega_N$ of any function A defined on Ω is

$$\|A\|_\infty=\sup_{\Omega}|A|. \tag{1}$$

The statistical average may be appreciated by this norm. Namely, if $P_H\in L_1^1[\Omega]$, $A\in Av_{P_H}[\Omega]$ and $\|A\|_\infty<\infty$,

$$|\langle A\rangle_H| = \frac{|(P_H, A)_\Omega|}{|(P_H, \mathbb{1})_\Omega|} \leqslant \frac{|\,\|A\|_\infty (P_H, \mathbb{1})_\Omega|}{|(P_H, \mathbb{1})_\Omega|} = \|A\|_\infty . \tag{2}$$

We are interested in model systems with Hamiltonians of the form

$$H = \Lambda G - \Lambda \sum_{\alpha=1}^{S} A_\alpha^* A_\alpha , \tag{3}$$

where G , A_α are dynamic variables, i.e., the functions in the states space Ω . The real positive namber Λ is a parameter of the system, the integer S , generally speaking, may depend on Λ .

We note that in most cases of interest the parameter Λ for $\Omega = \Omega_{V,N}, \Omega_V$ represents the volume of a system V , and for $\Omega = \Omega_N$ - the number of sites N , but it need not be like that, it is an arbitrary characteristic of a system under consideration.

For further investigation it is convenient to add to the Hamiltonian H or to single out of G - it is just the same - the terms with sources

$$H = \Lambda G - \Lambda \sum_{\alpha=1}^{S} A_\alpha^* A_\alpha + \Lambda \sum_{\alpha=1}^{S} (\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha), \tag{4}$$

where ν_α^* are complex numbers.

The following theorem shows how the density of the thermodynamic potential

$$f_\Lambda [H] = \frac{1}{\Lambda} F[H] \tag{5}$$

for Hamiltonians of the form (1) or (4) may be calculated exactly in the limit as $\Lambda \to \infty$.

Theorem 1 (Bogolubov,Jr Theorem for classical systems [1]):

Let for $P = P^{(c,q,\ell)}$ the model Hamiltonian of a system be

$$H = \Lambda G - \Lambda \sum_{\alpha=1}^{S} A_\alpha^* A_\alpha + \Lambda \sum_{\alpha=1}^{S} (\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha), \tag{6}$$

the norm $\|\cdot\|_\infty$ of the functions A_α be finite,

$$(\forall \alpha) \quad \|A_\alpha\|_\infty = M_{\alpha\Lambda} < \infty , \tag{7}$$

and for any Λ

$$\sum_{\alpha=1}^{S} M_{\alpha\Lambda} = M_\Lambda < \infty , \tag{8}$$

where the constant M_Λ may depend on Λ .

Let, also, the form of approximating Hamiltonian be

$$H_0(\underline{a}) = \Lambda G - \Lambda \sum_{\alpha=1}^{S} (a_\alpha A_\alpha^* + a_\alpha^* A_\alpha - a_\alpha a_\alpha) + \Lambda \sum_{\alpha=1}^{S} (\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha), \tag{9}$$

where a_α are complex numbers.

Then, if $P_H \in L^1[\Omega]$, $P_{H_0} \in L^1[\Omega]$, $G \in L^1[\Omega]$, $\sum_{\alpha=1}^{S} |A_\alpha - a_\alpha|^2 \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$, $e^{\pm\Lambda \sum_{\alpha=1} |A_\alpha - a_\alpha|^2} \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$.

a) There exists a minimum for the density of the thermodynamic potential function $f_\Lambda [H_0(\underline{a})]$ which is attained at some point $\overline{\underline{a}}^{(\Lambda)}$:

$$f_\Lambda [H_0(\overline{\underline{a}}^{(\Lambda)})] = \min_{\underline{a}} f_\Lambda [H_0(\underline{a})] \tag{10}$$

such that

$$(\forall\alpha)\quad |\bar{a}_\alpha^{(\Lambda)}| \leq M_{\alpha\Lambda} \leq M_\Lambda . \tag{11}$$

b) The difference of the densities of the thermodynamic potentials for the Hamiltonians H and $H_0(\underline{\bar{a}}^{(\Lambda)})$ is bounded by

$$0 \leq f_\Lambda[H_0(\underline{\bar{a}}^{(\Lambda)})] - f_\Lambda[H] \leq 2\left[\frac{1}{\beta}+4\right]\frac{M_\Lambda}{\sqrt{\Lambda}} . \tag{12}$$

c) If

$$\frac{M_\Lambda}{\sqrt{\Lambda}} \xrightarrow[\Lambda\to\infty]{} 0 , \tag{13}$$

the difference of the densities of the thermodynamic potentials for the Hamiltonians vanishes as $\Lambda \to \infty$:

$$f_\Lambda[H_0(\underline{\bar{a}}^{(\Lambda)})] - f_\Lambda[H] \xrightarrow[\Lambda\to\infty]{} 0 . \tag{14}$$

Proof:

a) The form of the approximating Hamiltonian $H_0(\underline{a})$ may be written as

$$H_0(\underline{a}) = \Lambda G - 2\Lambda\sum_{\alpha=1}^{s}\Big[A_\alpha^* A_\alpha - (A_\alpha - \tfrac{1}{2}a_\alpha)^*(A_\alpha - \tfrac{1}{2}a_\alpha) -$$

$$-\frac{1}{2}(\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha)\Big] + \frac{1}{2}\Lambda\sum_{\alpha=1}^{s}|a_\alpha|^2 . \tag{15}$$

Taking into account that $(A_\alpha - \frac{1}{2}a_\alpha)^*(A_\alpha - \frac{1}{2}a_\alpha) \geq 0$ and that according to (7),(8) $\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha \leq 2\max_\alpha|\nu_\alpha| M_{\alpha\Lambda}$, $\|A_\alpha^* A_\alpha\| \leq M_\Lambda M_{\alpha\Lambda}$, we find

$$H_0(\underline{a}) \geq -2\Lambda M_\Lambda \sum_{\alpha=1}^{s} M_{\alpha\Lambda} - \Lambda\max_\alpha|\nu_\alpha|\sum_{\alpha=1}^{s} M_{\alpha\Lambda} + \Lambda G + \frac{1}{2}\Lambda\sum_{\alpha=1}^{s}|a_\alpha|^2 . \tag{16}$$

Now it is clear that, since $G \in L^1[\Omega]$,

$$f_\Lambda[H_0(\underline{a})] \geq -2(M_\Lambda + \max_\alpha|\nu_\alpha|)M_\Lambda + f_\Lambda[\Lambda G] + \frac{1}{2}\sum_{\alpha=1}^{s}|a_\alpha|^2 . \tag{17}$$

Therefore the minimum of the function $f_\Lambda[H_0(\underline{a})]$ exists. The point at which it becomes a minimum satisfies the equations

$$\frac{\partial f_\Lambda[H_0(\underline{a})]}{\partial a_\alpha^*} = 0 . \tag{18}$$

Note that $\dfrac{\partial H_0(\underline{a})}{\partial a_\alpha^*} = -\Lambda(A_\alpha - a_\alpha) \in A_{V_{P_{H_0}}}[\Omega]$, hence

$$\frac{\partial f_\Lambda[H_0(\underline{a})]}{\partial a_\alpha^*} = \frac{\partial}{\partial a_\alpha^*}\left[-\frac{1}{\Lambda\beta}\ln\left(P_{H_0(\underline{a})}, \mathbb{1}\right)_\Omega\right] =$$

$$= \frac{\partial}{\partial a_\alpha^*}\left[-\frac{1}{\Lambda\beta}\left(e^{\beta C - \beta H_0(\underline{a})}, \mathbb{1}\right)_\Omega\right] = -\frac{1}{\Lambda}\left(\frac{\partial H_0(\underline{a})}{\partial a_\alpha^*}e^{\beta C - \beta H_0(\underline{a})}, \mathbb{1}\right)_\Omega \Big/$$

$$\Big/\left(e^{\beta C - \beta H_0(\underline{a})}, \mathbb{1}\right)_\Omega = \frac{\left(P_{H_0}(\underline{a}), A_\alpha - a_\alpha\right)_\Omega}{\left(P_{H_0}(\underline{a}), \mathbb{1}\right)_\Omega} = \langle A_\alpha - a_\alpha\rangle_{H_0(\underline{a})} , \tag{19}$$

that is $\underline{\bar{a}}^{(\Lambda)}$ satisfies the set of equations

$$a_\alpha = \langle A_\alpha \rangle_{H_0(\underline{a})} . \tag{20}$$

According to (2)

$$\langle A_\alpha \rangle_{H_0(\underline{a})} \le M_{\alpha\Lambda} , \tag{21}$$

therefore

$$(\forall \alpha) \quad |\bar{a}_\alpha^{(\Lambda)}| \le \| A_\alpha \|_\infty \le M_{\alpha\Lambda} \le M_\Lambda . \tag{22}$$

Thus the first statement of the Theorem 1 is proved.

b) We represent now H in the form

$$H = H_0(\underline{a}) + H_1(\underline{a}), \tag{23}$$

where

$$H_1(a) = -\Lambda \sum_{\alpha=1}^{S} |A_\alpha - a_\alpha|^2 . \tag{24}$$

Since $P_H \in L_1^1[\Omega]$, $P_{H_0} \in L_1^1[\Omega]$ and $\sum_{\alpha=1}^{S} |A_\alpha - a_\alpha|^2 \in$ $\in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$, $e^{\pm\Lambda \sum_{\alpha=1}^{S} |A_\alpha - a_\alpha|^2} \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$, we are able to make use of the Bogolubov inequality for classical systems /2/ which yields

$$\sum_{\alpha=1}^{S} \langle |A_\alpha - a_\alpha|^2 \rangle_{H_0(\underline{a})} \le f_\Lambda[H_0(\underline{a})] - f_\Lambda[H] \le \sum_{\alpha=1}^{S} \langle |A_\alpha - a_\alpha|^2 \rangle_H , \tag{25}$$

Since $|A_\alpha - a_\alpha|^2 \ge 0$,

$$0 \le f_\Lambda[H_0(\underline{a})] - f_\Lambda[H] \le \sum_{\alpha=1}^{S} \langle |A_\alpha - a_\alpha|^2 \rangle_H . \tag{26}$$

So, we have to estimate the difference

$$\Delta(\underline{\nu}, \underline{\nu}^*) = f_\Lambda[H_0(\bar{\underline{a}}^{(\Lambda)})] - f_\Lambda[H] . \tag{27}$$

Taking into account that

$$\frac{\partial^2 f_\Lambda[H]}{\partial \nu_\alpha^* \partial \nu_\alpha} = -\beta\Lambda \langle |A_\alpha - \langle A_\alpha \rangle|^2 \rangle_H , \tag{28}$$

we find

$$0 \le \Delta(\underline{\nu}, \underline{\nu}^*) \le -\frac{1}{\beta\Lambda} \sum_{\alpha=1}^{S} \frac{\partial^2 f_\Lambda[H]}{\partial \nu_\alpha^* \partial \nu_\alpha} . \tag{29}$$

Denoting $\nu_\alpha = u_\alpha + i v_\alpha$ and integrating we obtain

$$0 \le \frac{1}{\ell^{2S}} \int_{u_1}^{u_1+\ell}\int_{v_1}^{v_1+\ell} \ldots \int_{u_S}^{u_S+\ell}\int_{v_S}^{v_S+\ell} \Delta(\underline{u}', \underline{v}')\, du_1' dv_1' \ldots du_S' dv_S' \le -\frac{1}{\beta\Lambda} \cdot \frac{1}{\ell^{2S}} \int_{u_1}^{u_1+\ell} \ldots \int_{v_S}^{v_S+\ell} \sum_{\alpha=1}^{S}$$

$$\frac{1}{4}\left[\frac{\partial^2}{\partial u_\alpha'^2} + \frac{\partial^2}{\partial v_\alpha'^2}\right] f_\Lambda[H]\, du_1' \ldots dv_S' \le \frac{1}{\beta\Lambda} \frac{1}{\ell^{2S}} \sum_{\alpha=1}^{S} \left\{ \int_{u_1}^{u_1+\ell} \ldots \int_{v_S}^{v_S+\ell} \frac{1}{4}\left[\left|\frac{\partial f_\Lambda[H]}{\partial u_\alpha'}\right|\right]_{u_\alpha}^{u_\alpha+\ell} \times \right.$$

$$\left. \times \frac{du_1' \ldots dv_S'}{du_\alpha'} + \int_{u_1}^{u_1+\ell} \ldots \int_{v_S}^{v_S+\ell} \frac{1}{4}\left[\left|\frac{\partial f_\Lambda[H]}{\partial v_\alpha'}\right|\right]_{v_\alpha}^{v_\alpha+\ell} \frac{du_1' \ldots dv_S'}{dv_\alpha'} \right\} , \tag{30}$$

where ℓ is an arbitrary positive parameter that may depend on Λ . Note that

$$\frac{\partial}{\partial u_\alpha} f_\Lambda[H] = \langle A_\alpha^* + A_\alpha \rangle_H \, , \; \frac{\partial}{\partial v_\alpha} f_\Lambda[H] = i \langle A_\alpha^* - A_\alpha \rangle_H \, , \tag{31}$$

therefore according to (2)

$$\left| \frac{\partial}{\partial u_\alpha} f_\Lambda[H] \right| \le 2 \| A_\alpha \|_\infty \, , \; \left| \frac{\partial}{\partial v_\alpha} f_\Lambda[H] \right| \le 2 \| A_\alpha \|_\infty \, , \tag{32}$$

and we arrive at

$$\frac{1}{\ell^{2s}} \int_{u_1}^{u_1+\ell} \cdots \int_{v_s}^{v_s+\ell} \Delta(\underline{u}, \underline{v}) \, du_1 \ldots dv_s \le 2 \frac{1}{\beta \Lambda} \frac{1}{\ell} \sum_{\alpha=1}^{s} \| A_\alpha \|_\infty = 2 \frac{1}{\beta} \frac{1}{\Lambda} \frac{1}{\ell} M_\Lambda . \tag{33}$$

The mean value theorem yields

$$\Delta(\underline{u}'', \underline{v}'') \le 2 \cdot \frac{M_\Lambda}{\beta \Lambda \ell} \, , \tag{34}$$

where

$$u_\alpha'' \in [u_\alpha, u_\alpha + \ell] \, , \; v_\alpha'' \in [v_\alpha, v_\alpha + \ell] . \tag{35}$$

From the other hand

$$\Delta(\underline{u}, \underline{v}) - \Delta(\underline{u}'', \underline{v}'') \le \sum_{\alpha=1}^{s} \left[\ell \max_{\nu} \left| \frac{\partial \Delta(\underline{u}, \underline{v})}{\partial u_\alpha} \right| + \ell \max_{\nu} \left| \frac{\partial \Delta(\underline{u}, \underline{v})}{\partial v_\alpha} \right| \right] , \tag{36}$$

and, since

$$\frac{\partial \Delta(\underline{u}, \underline{v})}{\partial u_\alpha} = \langle A_\alpha^* + A_\alpha \rangle_H - \langle A_\alpha^* + A_\alpha \rangle_{H_0(\underline{\bar{a}}(\Lambda))} \, ,$$

$$\frac{\partial \Delta(\underline{u}, \underline{v})}{\partial v_\alpha} = i \langle A_\alpha^* - A_\alpha \rangle_H - i \langle A_\alpha^* - A_\alpha \rangle_{H_0(\underline{\bar{a}}(\Lambda))} \, , \tag{37}$$

the right-hand side of (36) is bounded by

$$\Delta(\underline{u}, \underline{v}) - \Delta(\underline{u}'', \underline{v}'') \le 8 \ell \sum_{\alpha=1}^{s} \| A_\alpha \|_\infty = 8 \ell M_\Lambda . \tag{38}$$

Thus, summing up (34) and (38) we obtain

$$\Delta(\underline{\nu}, \underline{\nu}^*) \le \left[\frac{2}{\beta \Lambda} \frac{1}{\ell} + 8 \ell \right] M_\Lambda . \tag{39}$$

Setting $\ell = \Lambda^{-1/2}$ and taking into account that $\Delta(\underline{\nu}, \underline{\nu}^*) \ge 0$ (29) we find finally

$$0 \le f_\Lambda[H_0(\underline{\bar{a}}(\Lambda))] - f_\Lambda[H] \le 2 \left[\frac{1}{\beta} + 4 \right] \frac{M_\Lambda}{\sqrt{\Lambda}} . \tag{40}$$

c) The statement (c) is now trivial. ■

Now we consider the Hamiltonians of the form

$$H = \Lambda G - \Lambda \sum_{\alpha=1}^{S_A} A_\alpha^* A_\alpha + \Lambda \sum_{\alpha=1}^{S_B} B_\alpha^* B_\alpha \, , \tag{41}$$

where G, A_α, B_α are dynamic variables, the integers S_A and S_B, generally speaking, depend on real positive parameter Λ, S_A and/or S_B may be infinite at finite Λ. We will prove that the following theorem holds.

Theorem 2 (Bogolubov,Jr Theorem for separable interaction): Let for $P = p^{(c,g,e)}$ a model Hamiltonian has the form

$$H = \Lambda G - \Lambda \sum_{\alpha=1}^{S_A} A_\alpha^* A_\alpha + \Lambda \sum_{\alpha=1}^{S_B} B_\alpha^* B_\alpha + \Lambda \sum_{\alpha=1}^{S_A} \left(\nu_\alpha A_\alpha^* + \nu_\alpha^* A_\alpha \right), \tag{42}$$

where G, A_α, B_α are dynamical variables of additive type

$$G = \frac{1}{\Lambda} \sum_{i=1}^{\Lambda} \mathcal{G}(\underline{r}_i, \underline{p}_i), \quad A_\alpha = \frac{1}{\Lambda} \sum_{i=1}^{\Lambda} \mathcal{A}_\alpha(\underline{r}_i, \underline{p}_i), \quad B_\alpha = \frac{1}{\Lambda} \sum_{i=1}^{\Lambda} \mathcal{B}_\alpha(\underline{r}_i, \underline{p}_i), \tag{43}$$

$\mathcal{G}(\underline{r}_i, \underline{p}_i)$ · $\mathcal{A}_\alpha(\underline{r}_i, \underline{p}_i)$ · $\mathcal{B}_\alpha(\underline{r}_i, \underline{p}_i)$, depend on the state of the i-th particle only, the norms $\|\cdot\|_\infty$ of the functions $\mathcal{A}(\underline{r}_i, \underline{p}_i)$, $\mathcal{B}_\alpha(\underline{r}_i, \underline{p}_i)$ are finite

$$(\forall i)(\forall \alpha) \quad \|\mathcal{A}_\alpha(\underline{r}_i, \underline{p}_i)\|_\infty \le M_{\alpha\Lambda}, \quad \|\mathcal{B}_\alpha(\underline{r}_i, \underline{p}_i)\|_\infty \le M_{\alpha\Lambda}, \tag{44}$$

and for any Λ

$$\sum_{\alpha=1}^{\max\{S_A, S_B\}} M_{\alpha\Lambda} = M_\Lambda < \infty, \tag{45}$$

where the constant M_Λ may depend on Λ.

Then, if $P_H \in L^1[\Omega]$, $P_{H_0} \in L^1[\Omega]$, $\sum_{\alpha=1}^{S_A} |A_\alpha - a_\alpha|^2 \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$,

$\sum_{\alpha=1}^{S_B} |B_\alpha - b_\alpha|^2 \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$, $\exp\left[\pm\Lambda \left(\sum_{\alpha=1}^{S_A} |A_\alpha - a_\alpha|^2 - \sum_{\alpha=1}^{S_B} |B_\alpha - b_\alpha|^2 \right)\right] \in A_{V_{P_H}}[\Omega] \cap A_{V_{P_{H_0}}}[\Omega]$,

a) There exists the solution $\langle \bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)} \rangle$ of the minimax problem for the density of the thermodynamic potential function $f_\Lambda[H_0(\underline{a}, \underline{b})]$:

$$\begin{aligned} & f_\Lambda\left[H_0(\underline{a}, \tilde{\underline{b}}^{(\Lambda)}(\underline{a}))\right] = \max_{\underline{b}} f_\Lambda\left[H_0(\underline{a}, \underline{b})\right], \\ & f_\Lambda\left[H_0(\bar{\underline{a}}^{(\Lambda)}, \tilde{\underline{b}}^{(\Lambda)}(\bar{\underline{a}}^{(\Lambda)}))\right] = \min_{\underline{a}} f_\Lambda\left[H_0(\underline{a}, \tilde{\underline{b}}^{(\Lambda)}(\underline{a}))\right], \\ & \bar{\underline{b}}^{(\Lambda)} = \tilde{\underline{b}}^{(\Lambda)}(\bar{\underline{a}}^{(\Lambda)}), \end{aligned} \tag{46}$$

such that

$$(\forall \alpha) \quad |\bar{a}_\alpha^{\Lambda}| \le M_{\alpha\Lambda}, \quad |\bar{b}_\alpha^{(\Lambda)}| \le M_{\alpha\Lambda}. \tag{47}$$

b) The difference of the thermodynamical potentials of the Hamiltonians H and $H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})$ is bounded by

$$-2\left(\frac{M_\Lambda}{\sqrt{\Lambda}}\right)^2 \le f_\Lambda\left[H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})\right] - f_\Lambda[H] \le 2\left[\frac{1}{\beta} + 4\right] \frac{M_\Lambda}{\sqrt{\Lambda}}. \tag{48}$$

c) If

$$\frac{M_\Lambda}{\sqrt{\Lambda}} \xrightarrow[\Lambda \to \infty]{} 0, \tag{49}$$

the difference of the thermodynamic potentials of the Hamiltonians H and $H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})$ vanishes as $\Lambda \to \infty$:

$$f_\Lambda\left[H_0\left(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)}\right)\right] - f_\Lambda[H] \xrightarrow[\Lambda\to\infty]{} 0 . \tag{50}$$

Proof:

First, note that according to the inequalities (46) and (47)

$$(\forall\alpha) \quad \|A_\alpha\|_\infty \le M_{\alpha\Lambda}, \quad \|B_\alpha\|_\infty \le M_{\alpha\Lambda}, \tag{51}$$

$$\sum_{\alpha=1}^{S_A} \|A_\alpha\|_\infty \le \sum_{\alpha=1}^{S_A} M_{\alpha\Lambda} \le M_\Lambda, \quad \sum_{\alpha=1}^{S_B} \|B_\alpha\|_\infty \le \sum_{\alpha=1}^{S_B} M_{\alpha\Lambda} \le M_\Lambda . \tag{52}$$

a) Similarly to the proof of the statement (a) of the Theorem 1, the inequality

$$f_\Lambda\left[H_0(\underline{a},\underline{b})\right] \le 2\left(M_\Lambda + \max_\alpha|\nu_\alpha| + \max_\alpha|a_\alpha|\right)M_\Lambda + f_\Lambda[\Lambda G] + \sum_{\alpha=1}^{S_A}|a_\alpha|^2 - \frac{1}{2}\sum_{\alpha=1}^{S_B}|b_\alpha|^2 , \tag{53}$$

leads to the existence of the maximum $f_\Lambda\left[H_0(\underline{a}, \tilde{\underline{b}}^{(\Lambda)}(\underline{a}))\right] = \max_{\underline{b}} f_\Lambda\left[H_0(\underline{a},\underline{b})\right]$ and the equations for the extremum yield

$$\left|\tilde{b}_\alpha^{(\Lambda)}(\underline{a})\right| \le M_{\alpha\Lambda}. \tag{54}$$

In view of (54)

$$f_\Lambda\left[H_0(\underline{a}, \tilde{\underline{b}}^{(\Lambda)}(\underline{a}))\right] \ge -\left(5M_\Lambda + 2\max_\alpha|\nu_\alpha|\right)M_\Lambda + f_\Lambda[\Lambda G] + \frac{1}{2}\sum_{\alpha=1}^{S_A}|a_\alpha|^2 , \tag{55}$$

It is easy to see now that the minimum $f_\Lambda\left[H_0(\bar{\underline{a}}^{(\Lambda)}, \tilde{\underline{b}}^{(\Lambda)}(\bar{\underline{a}}^{(\Lambda)}))\right] = \min_{\underline{a}} f_\Lambda\left[H_0(\underline{a}, \tilde{\underline{b}}^{(\Lambda)}(\underline{a}))\right]$ exists and, therefore,

$$\left|\bar{a}_\alpha^{(\Lambda)}\right| \le M_{\alpha\Lambda} , \tag{56}$$

$$\left|\bar{b}_\alpha^{(\Lambda)}\right| \le M_{\alpha\Lambda} . \tag{57}$$

b) Since $P_H \in L^1[\Omega]$, $P_{H_0} \in L^1[\Omega]$, $\sum_{\alpha=1}^{S_A}|A_\alpha - a_\alpha|^2 \in A_{VP_H}[\Omega] \cap A_{VP_{H_0}}[\Omega]$, $\sum_{\alpha=1}^{S_B}|B_\alpha - b_\alpha|^2 \in A_{VP_H}[\Omega] \cap A_{VP_{H_0}}[\Omega]$, $\exp\left[\pm\Lambda\left(\sum_{\alpha=1}^{S_A}|A_\alpha - a_\alpha|^2 - \sum_{\alpha=1}^{S_B}|B_\alpha - b_\alpha|^2\right)\right] \in A_{VP_H}[\Omega] \cap A_{VP_{H_0}}[\Omega]$, the Bogolubov inequality for classical systems/2/ gives

$$-\sum_{\alpha=1}^{S_B}\left\langle\left|B_\alpha - \langle B_\alpha\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})}\right|^2\right\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})} \le f_\Lambda\left[H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})\right] - f_\Lambda[H] \le \sum_{\alpha=1}^{S_A}\left\langle\left|A_\alpha - \langle A_\alpha\rangle_H\right|^2\right\rangle_H . \tag{58}$$

Estimations similar to those used in the proof the Theorem 1 yield

$$\sum_{\alpha=1}^{S_A}\left\langle\left|A_\alpha - \langle A_\alpha\rangle_H\right|^2\right\rangle_H \le 2\left[\frac{1}{\beta} + 4\right]\frac{M_\Lambda}{\sqrt{\Lambda}} . \tag{59}$$

The left-hand side of (58) may be written as

$$\sum_{\alpha=1}^{S_B}\left\langle\left|B_\alpha - \langle B_\alpha\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})}\right|^2\right\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})} =$$

$$= \sum_{\alpha=1}^{S_B}\left[\langle B_\alpha^* B_\alpha\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})} - \langle B_\alpha^*\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})}\langle B_\alpha\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)}, \bar{\underline{b}}^{(\Lambda)})}\right] =$$

$$=\sum_{\alpha=1}^{S_B}\Big[\frac{1}{\Lambda^2}\sum_{i'=1}^{\Lambda}\sum_{i''=1}^{\Lambda}\big\langle \mathcal{B}_\alpha^*(\underline{z}_{i'},\underline{p}_{i'})\,\mathcal{B}_\alpha(\underline{z}_{i''},\underline{p}_{i''})\big\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)},\,\bar{\underline{b}}^{(\Lambda)})} -$$

$$-\big\langle \mathcal{B}_\alpha^*(\underline{z}_{i'},\underline{p}_{i'})\big\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)},\,\bar{\underline{b}}^{(\Lambda)})}\big\langle \mathcal{B}_\alpha(\underline{z}_{i''},\underline{p}_{i''})\big\rangle_{H_0(\bar{\underline{a}}^{(\Lambda)},\,\bar{\underline{b}}^{(\Lambda)})}\Big]. \qquad (60)$$

Note that for $P=P^{(c,g,e)}$

$$P_H = e^{\beta\left[\sum_{i=1}^{\Lambda}\mu(i)-\mathcal{H}\right]}\,, \qquad (61)$$

where

$$\mu^{(c)}(i)=0, \qquad (62)$$

$$\mu^{(g)}(i)=\mu_j, \qquad (63)$$

j is the number of the species, the i-th particle belongs to, and

$$\mu^{(e)}(i)=\mu(n\underline{x}), \qquad (64)$$

$\underline{x}$ is the site labeled by the integer i /2/. From the other hand

$$H_0(\underline{a},\underline{b})=\sum_{i=1}^{\Lambda}\mathcal{H}_0(\underline{a},\underline{b};\underline{z}_i,\underline{p}_i), \qquad (65)$$

where

$$\mathcal{H}_0(\underline{a},\underline{b};\underline{z}_i,\underline{p}_i)=\mathcal{T}(\underline{z}_i,\underline{p}_i)-\sum_{\alpha=1}^{S_A}\left[a_\alpha \mathcal{A}_\alpha^*(\underline{z}_i,\underline{p}_i)+a_\alpha^*\mathcal{A}_\alpha(\underline{z}_i,\underline{p}_i)-a_\alpha^* a_\alpha\right]+$$

$$+\sum_{\alpha=1}^{S_B}\left[b_\alpha \mathcal{B}_\alpha^*(\underline{z}_i,\underline{p}_i)+b_\alpha^*\mathcal{B}_\alpha(\underline{z}_i,\underline{p}_i)-b_\alpha^* b_\alpha\right]+$$

$$+\sum_{\alpha=1}^{S_A}\left[\nu_\alpha \mathcal{A}_\alpha^*(\underline{z}_i,\underline{p}_i)+\nu_\alpha^*\mathcal{A}_\alpha(\underline{z}_i,\underline{p}_i)\right], \qquad (66)$$

and

$$P_{H_0(\underline{a},\underline{b})}=e^{\beta\sum_{i=1}^{\Lambda}\left[\mu(i)-\mathcal{H}_0(\underline{a},\underline{b};\underline{z}_i,\underline{p}_i)\right]}\,. \qquad (67)$$

Proceeding from the Definitions 1-5 of ref.2 for $P=P^{(c,g,e)}$ we obtain that, if $\sum_{i=1}^{\Lambda}\mathcal{H}(\underline{z}_i,\underline{p}_i)\in L^1[\Omega]$, $\mathcal{U}(\underline{z}_{i'},\underline{p}_{i'})\,\mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''})\in$ $\in Av_{\sum_{i=1}^{\Lambda}\mathcal{H}(\underline{z}_i,\underline{p}_i)}[\Omega]$, for $i'\neq i''$ we have

$$\big\langle \mathcal{U}(\underline{z}_{i'},\underline{p}_{i'})\,\mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''})\big\rangle_{\sum_{i=1}^{\Lambda}\mathcal{H}(\underline{z}_i,\underline{p}_i)}=$$

$$=\frac{\left(\mathcal{U}(\underline{z}_{i'},\underline{p}_{i'})\,\mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''}),\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}{\left(1,\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}=$$

$$=\frac{\left(\mathcal{U}(\underline{z}_{i'},\underline{p}_{i'}),\ e^{\beta[\mu(i')-\mathcal{H}(\underline{z}_{i'},\underline{p}_{i'})]}\right)_{\Omega_{i'}}}{\left(1,\ e^{\beta[\mu(i')-\mathcal{H}(\underline{z}_{i'},\underline{p}_{i'})]}\right)_{\Omega_{i'}}}\ \frac{\left(\mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''}),\ e^{\beta[\mu(i'')-\mathcal{H}(\underline{z}_{i''},\underline{p}_{i''})]}\right)_{\Omega_{i''}}}{\left(1,\ e^{\beta[\mu(i'')-\mathcal{H}(\underline{z}_{i''},\underline{p}_{i''})]}\right)_{\Omega_{i''}}}=$$

$$=\frac{\left(\mathcal{U}(\underline{z}_{i'},\underline{p}_{i'}),\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}{\left(1,\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}\ \frac{\left(\mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''}),\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}{\left(1,\ e^{\beta\sum_{i=1}^{\Lambda}[\mu(i)-\mathcal{H}(\underline{z}_i,\underline{p}_i)]}\right)_\Omega}=$$

$$=\big\langle \mathcal{U}(\underline{z}_{i'},\underline{p}_{i'})\big\rangle_{\sum_{i=1}^{\Lambda}\mathcal{H}(\underline{z}_i,\underline{p}_i)}\big\langle \mathfrak{B}(\underline{z}_{i''},\underline{p}_{i''})\big\rangle_{\sum_{i=1}^{\Lambda}\mathcal{H}(\underline{z}_i,\underline{p}_i)}\,, \qquad (68)$$

$$\Omega_i^{(c)}=R^d\otimes V,\quad \Omega_i^{(g)}=\bigoplus_{\underline{N}\in Z^2}R^d\otimes V,\quad \Omega_i^{(e)}=V,$$

in particular, for $i' \neq i''$

$$\langle \mathcal{B}_\alpha^*(i')\mathcal{B}_\alpha(i'')\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} = \langle \mathcal{B}_\alpha^*(i')\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} \langle \mathcal{B}_\alpha(i'')\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} . \qquad (69)$$

Thus, by virtue of (60),(44), and (45)

$$\sum_{\alpha=1}^{S_B} \left\langle \left| B_\alpha - \langle B_\alpha \rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} \right|^2 \right\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} =$$

$$= \sum_{\alpha=1}^{S_B} \Big[\frac{1}{\Lambda^2} \langle \mathcal{B}_\alpha^*(\underline{r}_i,p_i)\mathcal{B}_\alpha(\underline{r}_i,p_i)\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} - \langle \mathcal{B}_\alpha^*(\underline{r}_i,p_i)\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} \cdot$$

$$\cdot \langle \mathcal{B}_\alpha(\underline{r}_i,p_i)\rangle_{H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})} \leq 2\frac{1}{\Lambda}\sum_{\alpha=1}^{S_B} \| B_\alpha^*(\underline{r}_i,p_i)\|_\infty^2 \leq$$

$$\leq 2\frac{1}{\Lambda}\sum_{\alpha=1}^{S_B} M_{\alpha\Lambda}^2 = 2\frac{M_\Lambda^2}{\Lambda} = 2\left(\frac{M_\Lambda}{\sqrt{\Lambda}}\right)^2 . \qquad (70)$$

Taking into account (58),(59), and (70) we have finally

$$-2\left(\frac{M_\Lambda}{\sqrt{\Lambda}}\right)^2 \leq f_\Lambda[H_0(\underline{\bar{a}}^{(\Lambda)},\underline{\bar{b}}^{(\Lambda)})] - f_\Lambda[H] \leq 2\left[\frac{1}{\beta}+4\right]\frac{M_\Lambda}{\sqrt{\Lambda}} . \qquad (71)$$

c) The statement (c) is now trivial. ∎

Finally, it should be stressed that the results obtained are valid for all the ensembles both continuous and lattice, except for the microcanonical one.

R e f e r e n c e s

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