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Некоторые неравенства для классических непрерывных и решетчатых систем

Целью работы является получение строгих соотношений между статистическими средними наблюдаемых величин и термодинамическими потенциалами в классической статистической механике. С единой точки зрения рассмотрены решетчатые и непрерывные системы, а также микроканонический, канонический и большой канонический ансамбли. Математически строго доказаны классические аналоги неравенства Иенсена и неравенства Боголюбова.

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Some Inequalities for Classical Continuous and Lattice Systems

The purpose of the paper is to obtain some rigorous relations between statistical averages and thermodynamic potentials in classical statistical mechanics. The lattice and continuous systems as well as the microcanonical, the canonical, and the great canonical ensembles are considered from the single point of view. The classical analogues of the Iensen and the Bogolubov inequolity are proved rigorously.

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

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The Bogolubov inequality and the Bogolubov variational principle are of great importance for various branches of quantum statistical physics. For this reason it seems promising to extend them to classical many-particle systems. In the present paper we consider the Bogolubov inequality and some connected problems in classical statistical mechanics.

In classical mechanics a state of a system is described[1] by a set of canonical conjugate variables - generalized coordinates q_i and generalized momenta p_i ,- where the index i runs over intergers from 1 to $\mathcal{H}$, $\mathcal{H}$ being the number of degrees of freedom. The behaviour of the system is specified by a Hamiltonian H depending on these $2\mathcal{H}$ variables

$$H = H(q_1, \dots, q_{\mathcal{H}}, p_1, \dots, p_{\mathcal{H}}). \tag{1}$$

For a continuous system the subsystems composing it are called particles which move in d -dimensional space. These particles may be of different kinds and may have internal degrees of freedom.

For simplicity we restrict ourselves to the case when they have no internal degrees of freedom. Then the state of every particle may be specified by the position $q_i \in R^d$ and the momentum $p_i \in R^d$ and $\mathcal{H} = dN$, where $N = N_1 + \dots + N_2$ is the total number of particles, N_j being that of the j -th kind, so that the collection of particles is characterized by a vector in Z^r $\underline{N}=\{N_1,\dots,N_r\}$, where r is the number of species. Thus the Hamiltonian H has the form

$$H=H(\underline{q}_1,\dots,\underline{q}_N,\underline{p}_1,\dots,\underline{p}_N). \tag{2}$$

If all the particles are of the same kind and the interaction between them does not depend on their velocity, H is written as

$$H=T(\underline{p}_1,\dots,\underline{p}_N)+U(\underline{q}_1,\dots,\underline{q}_N)=\sum_{1\le i\le N}{}^{'}\frac{p_i^2}{2m}+U(\underline{q}_1,\dots,\underline{q}_N), \tag{3}$$

but so far we do not need such a concretization.

The system (2) is assumed to be enclosed in a finite measurable (in the sence of Lebesgue) subset of $\mathbb{R}^d$ - $V\subset\mathbb{R}^d$.

Thus, in the <u>microcanonical</u> and the <u>canonical ensembles</u> where the numbers of particles N_j are fixed and play the role of thermodynamic parameters the state space of a system is the phase space

$$\Omega^{(m,c)}=\Omega_{V,\underline{N}}=(\mathbb{R}^d)^N\otimes(V)^N. \tag{4}$$

In the <u>grand canonical ensemble</u> the numbers of particles are replaced as thermodynamic parameters by the chemical potentials μ_j of the j-th species, the former becoming variables. So, the state space is the direct sum over all integers N_j of $\Omega_{V,\underline{N}}$

$$\Omega^{(g)}=\Omega_V=\bigoplus_{\underline{N}\in Z^r}\Omega_{V,\underline{N}}=\bigoplus_{\underline{N}\in Z^r}(\mathbb{R}^d)^N\otimes(V)^N. \tag{5}$$

For a <u>lattice system</u> the subsystems are called lattice sites and may be parameterised by d-tuples of integers $\underline{x}=\{x_1,\dots,x_d\}\in\mathbb{Z}^d$. All the sites hereinafter are assumed to be identical and may be situated in a finite number $r+1$ states labeled by integers $n_{\underline{x}}\in\{0,1,\dots,r\}=V\in Z^1$, $\|V\|=r<\infty$. The Hamiltonian depends on $n_{\underline{x}}$ only

$$H=H(n_{\underline{0}},\dots). \tag{6}$$

The system is supposed to consist of a finite number of the sites, i.e., $\underline{x}\in N\subset Z^d$, where N is bounded - $\|N\|=N<\infty$ - subset of Z^d, N - the number of the sites. Thus, the state space is

$$\Omega^{(l)}=\Omega_N=(V)^N. \tag{7}$$

We denote as $\mathbb{F}[\Omega]$ the space of all mesurable functions defined on Ω ($\Omega=\Omega_{V,\underline{N}},\Omega_V,\Omega_N$) and define the mapping $(\cdot,\cdot)_\Omega:\langle\mathbb{F}[\Omega],\mathbb{F}[\Omega]\rangle\to R^1$.

<u>Def. 1</u> ($(\cdot,\cdot)_\Omega$ for $\Omega_{V,\underline{N}}$):

For any two functions $A_{V,\underline{N}}, B_{V,\underline{N}}\in\mathbb{F}[\Omega_{V,\underline{N}}]$, for which there exists the finite integral

$$\int_{\Omega_{V,\underline{N}}} A_{V,\underline{N}}(\underline{q}_1,\dots,\underline{q}_N)B_{V,\underline{N}}(\underline{q}_1,\dots,\underline{p}_N)\,d\underline{q}_1\dots d\underline{p}_N,$$

$$(A_{V,\underline{N}},B_{V,\underline{N}})_{\Omega_{V,\underline{N}}}=\frac{1}{\underline{N}!}\int A_{V,\underline{N}}(\underline{q}_1,\dots,\underline{p}_N)B_{V,\underline{N}}(\underline{q}_1,\dots,\underline{p}_N)\times d\underline{q}_1\dots d\underline{p}_N.^{*)} \tag{8}$$

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*) Hereinafter we use the notation $\underline{N}!=\prod_{1\le j\le r}N_j!$.

Def. 2 ($(\cdot,\cdot)_\Omega$ for Ω_V):

For any two functions $A_V=\{A_{V,\underline{N}} | \underline{N}\in Z^2\}$, $B_V=\{B_{V,\underline{N}} | \underline{N}\in Z^2\}\in$ $\in F[\Omega_V]$ such that $(\forall \underline{N}\in Z^2)\ \exists (A_{V,\underline{N}})_{\Omega_{V,\underline{N}}}$:
$|(A_{V,\underline{N}}, B_{V,\underline{N}})|<\infty$; $|\sum_{\underline{N}\in Z^2}(A_{V,\underline{N}}, B_{V,\underline{N}})_{\Omega_{V,\underline{N}}}|<\infty$,

$$(A_V, B_V)_{\Omega_V}=\sum_{\underline{N}\in Z^2}(A_{V,\underline{N}}, B_{V,\underline{N}})_{\Omega_{V,\underline{N}}}=$$

$$=\sum_{\underline{N}\in Z^2}\frac{1}{\underline{N}!}\int_{\Omega_{V,\underline{N}}} A_{V,\underline{N}}(\underline{r}_1,\dots,\underline{p}_N)B_{V,\underline{N}}(\underline{r}_1,\dots,\underline{p}_N)d\underline{r}_1\dots d\underline{p}_N. \quad (9)$$

Def. 3 ($(\cdot,\cdot)_\Omega$ for Ω_N):

For any two functions $A_N, B_N\in F[\Omega_N]$

$$(A_N, B_N)_{\Omega_N}=\sum_{n_\ell\in V}{}'\dots\ A_N(n_\ell,\dots)B_N(n_\ell,\dots). \quad (10)$$

Note that the mappings (8)-(10) are bilinear.

Now we define the spaces $L^1[\Omega_{V,\underline{N}}]$, $L^1[\Omega_V]$, $L^1[\Omega_N]$ in usual way.

Def. 4 ($L^1[\Omega]$):

$$L^1[\Omega_{V,\underline{N}}]=\{A_{V,\underline{N}}\in F[\Omega_{V,\underline{N}}] | \exists(A_{V,\underline{N}},\mathbb{1})_{\Omega_{V,\underline{N}}} : |(A_{V,\underline{N}},\mathbb{1})_{\Omega_{V,\underline{N}}}|<\infty\},$$

$$L^1[\Omega_V]=\{A_V\in F[\Omega_V] | \exists(A_V,\mathbb{1})_{\Omega_V} : |(A_V,\mathbb{1})_{\Omega_V}|<\infty\}, \quad (11)$$

$$L^1[\Omega_N]=F[\Omega_N].$$

Let us introduce also the spaces $Av_\ell[\Omega_{V,\underline{N}}]$, $Av_\ell[\Omega_V]$, $Av_\ell[\Omega_N]$.

Def. 5 ($Av_\ell[\Omega]$):

$$Av_\ell[\Omega_V]=\{A\in F[\Omega] | \exists(\ell,A)_\Omega : |(\ell,A)_\Omega|<\infty\}, \quad (12)$$

$$\Omega=\Omega_{V,\underline{N}}, \Omega_V, \Omega_N.$$

Obviously, $Av_\ell[\Omega_N]=F[\Omega_N]$.

We define likewise the scalar product, mapping $\underline{a}=\{a_1,\dots,a_z\}$ and $\underline{b}=\{b_1,\dots,b_z\}$ into the number $(\underline{a}\circ\underline{b})=a_1b_1+\dots+a_zb_z$, and for Ω_V the mapping $\varphi(\cdot)=\{\varphi_{\underline{N}}(\cdot):\underline{N}\in Z^2\}$, transforming $A_V=\{A_{V,\underline{N}}:\underline{N}\in Z^d\}$ into $\varphi(A_V)=\{\varphi_{\underline{N}}(A_{V,\underline{N}}):\underline{N}\in Z^2\}$.

Now we are able to express the partition function, the thermodynamic potential, and the statistical average for all the ensembles in terms of the definitions given.

As is known, the probability measures for the statistical ensembles have the following form.

1. Continuous systems.

a) Microcanonical ensemble:

$$\frac{1}{\underline{N}!}P_H^{(m)}(\Omega_{V,\underline{N}})d\Omega_{V,\underline{N}}=\frac{1}{\underline{N}!}\delta^\Delta(H(\underline{r}_1,\dots\underline{p}_N)-\mathcal{E})d\underline{r}_1\dots d\underline{p}_N, \quad (13)$$

where $\delta^\Delta(i)$ is the characteristic function of the interval $(-\Delta,0)$, $\mathcal{E}$ is the total energy of the system.

b) Canonical ensemble:

$$\frac{1}{\underline{N}!}P_H^{(c)}(\Omega_V)d\Omega_V=\frac{1}{\underline{N}!}e^{-\beta H(\underline{r}_1,\dots\underline{p}_N)}d\underline{r}_1\dots d\underline{p}_N. \quad (14)$$

c) Grand canonical ensemble:

$$\frac{1}{N!} P_H^{(g)}(\underline{N}, \Omega_{V,\underline{N}}) d\Omega_{V,\underline{N}} = \frac{1}{\underline{N}!} e^{\beta(\underline{\mu} \circ \underline{N}) - \beta H(\underline{r}_1, \ldots, \underline{p}_N)} \times d\underline{r}_1 \ldots d\underline{p}_N, \tag{15}$$

where $\underline{\mu} = \{\mu_1, \ldots, \mu_z\} \in R^z$.

2. Lattice systems.

$$P_H^{(\ell)}(\Omega_N) = e^{\beta \sum_{\underline{x} \in N} \mu(n_{\underline{x}}) - \beta H(n_2, \ldots)} . \tag{16}$$

In the alloy interpretation /1/ $\mu(n_{\underline{x}})$ is the chemical potential for the species $n_{\underline{x}}$, in the lattice gas interpretation $\mu(n_{\underline{x}}) = \mu n_{\underline{x}}$, being the chemical potential of the gas, in the spin-system interpretation $\mu(n_{\underline{x}}) = S_{\underline{x}} h$, where h is external magnetic field, $S_{\underline{x}} = n_{\underline{x}} - \frac{1}{2} z$ is the spin component.

It is worthy noting that for all the ensembles except the microcanonical one the probability measure may be written as

$$P_H^{(c,g,\ell)}(\Omega^{(c,g,\ell)}) = e^{\beta C^{(c,g,\ell)} - \beta H}, \tag{17}$$

namely,

$$C^{(c)} = 0, \quad C^{(g)} = (\underline{\mu} \circ \underline{N}), \quad C^{(\ell)} = \sum_{\underline{x} \in N} \mu(n_{\underline{x}}). \tag{18}$$

Moreover, for $P_H(\Omega) = P_H^{(c,g,\ell)}(\Omega^{(c,g,\ell)})$ the identity holds

$$P_{H_1+H_2}^{(c,g,\ell)}(\Omega^{(c,g,\ell)}) = e^{-\beta C^{(c,g,\ell)}} P_{H_1}^{(c,g,\ell)}(\Omega^{(c,g,\ell)}) P_{H_2}^{(c,g,\ell)}(\Omega^{(c,g,\ell)}) = e^{-\beta H_1} P_{H_2}^{(c,g,\ell)}(\Omega^{(c,g,\ell)}). \tag{19}$$

Hereinafter in writing $(A, B)_\Omega$ we will imply one of the mappings $(A_{V,\underline{N}}, B_{V,\underline{N}})_{\Omega_{V,\underline{N}}}$, $(A_V, B_V)_{\Omega_V}$, $(A_N, B_N)_{\Omega_N}$ depending on the ensemble we deal with. In the same sense the notation $L^1[\Omega]$ and $P[\Omega]$ should be understood. Thus, in conformity with (13)-(16) we may give the definitions for the partition function, the thermodynamic potential and the statistical average for $\Omega = \Omega^{(m,c,g,\ell)}$.

Def. 6 (partition function):

For any Hamiltonian H such that $P_H \in L^1[\Omega]$, the partition function $Q[H]$ is given by

$$Q[H] = (P_H, \mathbb{1})_\Omega . \tag{20}$$

Def. 7 (thermodynamic potential):

For any Hamiltonian H such that $P_H \in L^1[\Omega]$, the thermodynamic potential $F[H]$ is given by

$$F[H] = -\frac{1}{\beta} \ln Q[H] = -\frac{1}{\beta} \ln (P_H, \mathbb{1})_\Omega . \tag{21}$$

Def. 8 (statistical average):

For any Hamiltonian H such that $P_H \in L^1[\Omega]$, and any dynamical variable $A \in A_{V_{P_H}}[\Omega]$ the statistical average $\langle A \rangle_H$ is given by

$$\langle A \rangle_H = \frac{(P_H, A)_\Omega}{(P_H, \mathbb{1})_\Omega} . \tag{22}$$

Now we are able to prove a general theorem which is valid for all the ensembles both continuous and lattice.

Theorem 1 (Iensen inequality):

If $\rho_H \in L^1[\Omega], A \in Av_{\rho_H}[\Omega]$,

then for an arbitrary function $\varphi \in C^2(\mathbb{R}^1)$, such that

$$\varphi'' \geq 0, \tag{23}$$

$$\varphi(A) \in Av_{\rho_H}[\Omega], \tag{24}$$

the inequality holds

$$\varphi(\langle A\rangle_H) \leq \langle \varphi(A)\rangle_H . \tag{25}$$

Proof:

For $\rho_H \in L^1[\Omega], A \in Av_{\rho_H}[\Omega]$ the quantity $\langle A\rangle_H$ is defined and finite, hence

$$\varphi(A) = \varphi(\langle A_H\rangle) + (A - \langle A\rangle_H)\varphi'(\langle A_H\rangle) + \frac{1}{2}(A - \langle A\rangle_H)^2\varphi''(\xi), \tag{26}$$

where ξ lies between A and $\langle A\rangle_H$. By virtue of (23)

$$\varphi(A) \geq \varphi(\langle A\rangle_H) + (A - \langle A\rangle_H)\,\varphi'(\langle A\rangle_H). \tag{27}$$

Taking into account that $\rho_H > 0$ and $\varphi(A) \in Av_{\rho_H}[\Omega]$ we find

$$(\rho_H, \varphi(A))_\Omega \geq \varphi(\langle A\rangle_H)(\rho_H, \mathbb{1})_\Omega + \varphi'(\langle A\rangle_H)[(\rho_H, A)_\Omega -$$

$$- \langle A\rangle_H (\rho_H, \mathbb{1})_\Omega] = \varphi(\langle A\rangle_H)(\rho_H, \mathbb{1})_\Omega , \tag{28}$$

therefore

$$\varphi(\langle A\rangle_H) \leq \frac{(\rho_H, \varphi(A))_\Omega}{(\rho_H, \mathbb{1})_\Omega} . \qquad \blacksquare \tag{29}$$

In particular, setting $\varphi(t) = e^{-\beta t}$, we obtain

Corollary:

If $\rho_H \in L^1[\Omega], A \in Av_{\rho_H}[\Omega], e^{-\beta A} \in Av_{\rho_H}[\Omega]$,

$$e^{-\beta\langle A\rangle_H} \leq \langle e^{-\beta A}\rangle_H . \tag{30}$$

For $\rho = \rho^{(c,g,e)}$ the following theorem takes place.

Theorem 2 (Bogolubov inequality):

For $\rho = \rho^{(c,g,e)}$, if $\rho_A \in L^1[\Omega]$, $\rho_B \in L^1[\Omega]$, $A - B \in Av_{\rho_B}[\Omega]$, $e^{-\beta(H-B)} \in Av_{\rho_B}[\Omega]$.

then the inequality holds

$$F[A] - F[B] \leq \langle A - B\rangle_B , \tag{31}$$

if, besides, $A - B \in Av_{\rho_A}[\Omega]$, $e^{-\beta(B-A)} \in Av_{\rho_A}[\Omega]$,

$$\langle A - B\rangle_A \leq F[A] - F[B] \leq \langle A - B\rangle_B . \tag{32}$$

Proof:

The definition (21) of the thermodynamic potential and the property (19) yield

$$F[A] - F[B] = -\frac{1}{\beta}\ln\left[\frac{(\rho_A, \mathbb{1})_\Omega}{(\rho_B, \mathbb{1})_\Omega}\right] = -\frac{1}{\beta}\ln\left[\frac{(\rho_{(A-B)+B}, \mathbb{1})_\Omega}{(\rho_B, \mathbb{1})_\Omega}\right] =$$

$$= -\frac{1}{\beta}\ln\left[\frac{(e^{-\beta(A-B)}\rho_B, \mathbb{1})_\Omega}{(\rho_B, \mathbb{1})_\Omega}\right] = -\frac{1}{\beta}\ln\left[-\frac{(\rho_B, e^{-\beta(A-B)})_{L^2(\Omega)}}{(\rho_B, \mathbb{1})_\Omega}\right] =$$

$$= -\frac{1}{\beta}\ln\langle e^{-\beta(A-B)}\rangle_B . \tag{33}$$

Since $\rho_B \in L^1[\Omega]$, $A-B \in A_{v\rho_B}[\Omega]$, $e^{-\beta(A-B)} \in A_{v\rho_B}[\Omega]$,

by virtue of Corollary of Theorem 1 we find

$$\left\langle e^{-\beta(A-B)} \right\rangle_B \geq e^{-\beta\langle A-B \rangle_B}, \tag{34}$$

hence

$$F[A] - F[B] \leq \langle A-B \rangle_B . \tag{35}$$

If besides $A-B \in A_{v\rho_B}[\Omega]$, $e^{-\beta(B-A)} \in A_{v\rho_B}[\Omega]$, likewise $A-B \in A_{v\rho_A}[\Omega]$, $e^{-\beta(B-A)} \in A_{v\rho_A}[\Omega]$ we are able to make the change $A \longleftrightarrow B$

$$F[B] - F[A] \leq \langle B-A \rangle_A . \tag{36}$$

Multiplication by -1 together with (35) yield

$$\langle A-B \rangle_A \leq F[A] - F[B] \leq \langle A-B \rangle_B . \quad \blacksquare \tag{37}$$

Finally, it should be emphasized that the statistical ensemble we deal with has not been concretized in our consideration. So, Theorem 1 is valid for all the ensembles both continuous and lattice, Theorem 2 holds also for all the ensembles except the microcanonical one.

R e f e r e n c e s

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