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THE BOGOLUBOV GENERATING FUNCTIONAL METHOD IN STATISTICAL PHYSICS AND "COLLECTIVE" VARIABLES TRANSFORM WITHIN THE GRAND CANONICAL ENSEMBLE

МЕТОД ПОРОДЖУЮЧИХ ФУНКЦІОНАЛІВ БОГОЛЮБОВА В СТАТИСТИЧНІЙ ФІЗИЦІ ТА ПЕРЕТВОРЕННЯ ДО „КОЛЕКТИВНИХ" ЗМІННИХ У ВЕЛИКОМУ КАНОНІЧНОМУ АНСАМБЛІ

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We show that the Bogolubov generating functional method is a very effective tool for studying distribution functions of both equilibrium and nonequilibrium states of classical many-particle dynamical systems. In some cases the Bogolubov generating functionals can be represented by means of infinite Ursell – Mayer diagram expansions, whose convergence holds under some additional constraints on the statistical system under consideration. The classical Bogolubov idea to use the Wigner density operator transformation for studying the nonequilibrium distribution functions is developed, a new analytic nonstationary solution to the classical Bogolubov evolution functional equation is constructed.

Доведено, що метод породжуючих функціоналів Боголюбова є досить ефективним для вивчення функцій розподілу рівноважних та нерівноважних станів класичних багаточастинкових динамічних систем. У деяких випадках породжуючі функціонали Боголюбова можна виразити через нескінченні розвинення діаграм Урселла – Мартіна, які збігаються при накладанні додаткових умов на розглядувані статистичні системи. Розвинуто класичну ідею Боголюбова про використання перетворення Вігнера оператора щільності для вивчення нерівноважних функцій розподілу та побудовано новий нестаціонарний розв'язок класичного рівняння еволюції функціонала Боголюбова.

1. Introduction. Bogolubov functional equation and distribution functional. Let a large system of $N \in \mathbb{Z}_+$ (one-atomic and spinless) bose-particles with a fixed density $\bar{\rho} := N/\Lambda$ in a volume $\Lambda \subset \mathbb{R}^3$ be specified by a quantum-mechanical Hamiltonian operator $\hat{H} : L_2^{(\mathrm{sym})}(\mathbb{R}^{3N}; \mathbb{C}) \to L_2^{(\mathrm{sym})}(\mathbb{R}^{3N}; \mathbb{C})$ of the form

$$\hat{H} := -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{j<k}^{N} V(x_j - x_k), \tag{1.1}$$

where $\nabla_j := \partial/\partial x_j$, $j = \overline{1,N}$, $\hbar$ is the Plank constant, $m \in \mathbb{R}_+$ a particle mass and $V(x-y) := V(|x-y|)$, $x, y \in \Lambda$, a two-particle potential energy allowing for a partition $V = V^{(l)} + V^{(s)}$ with $V^{(s)}$ being a short range potential of the Lennard – Johns type and $V^{(l)}$ a long range potential of the Coulomb type. Making use of the second quantization representation [1, 2], the Hamiltonian (1.1), as $\Lambda \to \mathbb{R}^3$ and $N \to \infty$, can be written as a sum $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$, where

$$\begin{gathered} \mathbf{H}_0 := -\frac{\hbar^2}{2m}\int\limits_{\mathbb{R}^3} d^3x\psi^+\nabla_x^2\psi, \\ \mathbf{V} := \frac{1}{2}\int\limits_{\mathbb{R}^3} d^3x\int\limits_{\mathbb{R}^3} d^3yV(x-y)\psi^+(x)\psi^+(y)\psi(y)\psi(x), \end{gathered} \tag{1.2}$$

and the operator $\mathbf{H} : \mathbf{\Phi} \to \mathbf{\Phi}$ acts on a suitable Fock space [1, 2] with the standard scalar product $(\cdot,\cdot)$, and $\psi^+(x), \psi(y)$: $\mathbf{\Phi} \to \mathbf{\Phi}$ are creation and annihilation operators defined, correspondingly, at points $x \in \mathbb{R}^3$ and $y \in \mathbb{R}^3$.

Assume now that our particle system is under the thermodynamic equilibrium at an "inverse" temperature $\mathbb{R}_+ \ni \beta \to \infty$. Then the corresponding Bogolubov n-particles distribution functions can be written [1, 3] as

$$F_n(x_1, x_2, \ldots, x_n) := (\Omega, : \rho(x_1)\rho(x_1)\ldots\rho(x_n) : \Omega), \tag{1.3}$$

where $n \in \mathbb{Z}_+$, $\rho(x) := \psi^+(x)\psi(x)$ is the density operator at $x \in \mathbb{R}^3$, $: :$ the usual [1, 2] Wick normal ordering over the creation and annihilation operators, and $\Omega \in \mathbf{\Phi}$ is the ground state of the Hamiltonian (1.2) at the temperature $\beta \to \infty$, normalized by the condition $(\Omega, \Omega) = 1$. If we introduce the Bogolubov generating functional

$$\mathcal{L}(f) := (\Omega, \exp[i\rho(f)]\Omega) \tag{1.4}$$

for any "test" Schwartz function $f \in \mathcal{S}(\mathbb{R}^3; \mathbb{R})$, where $\rho(f) := \int_{\mathbb{R}^3} d^3xf(x)\rho(x)$, then for n-particle distribution functions we can get the expression

$$F_n(x_1, x_2, \ldots, x_n) =: \frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}\ldots\frac{1}{i}\frac{\delta}{\delta f(x_n)} : \mathcal{L}(f)|_{f=0}. \tag{1.5}$$

Here $x_j \in \mathbb{R}^3$, $j = \overline{1,n}$, $n \in \mathbb{Z}_+$, and the symbol $: \frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}\ldots\frac{1}{i}\frac{\delta}{\delta f(x_n)} :$ imitates the application of the symbol $: :$ to the operator expressions $\rho(x_1)\rho(x_1)\ldots\rho(x_n)$, that is,

$$\begin{gathered} : \frac{1}{i}\frac{\delta}{\delta f(x_1)} : = \frac{1}{i}\frac{\delta}{\delta f(x_1)}, \\ : \frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)} : = \frac{1}{i}\frac{\delta}{\delta f(x_1)}\left[\frac{1}{i}\frac{\delta}{\delta f(x_2)} - \delta(x_1 - x_2)\right], \end{gathered} \tag{1.6}$$

and so on. Consider now the expression (1.4) at some $\beta \in \mathbb{R}_+$, making use of the statistical operator $\mathcal{P}$: $\mathbf{\Phi} \to \mathbf{\Phi}$ and the "shifted" Hamiltonian $\mathbf{H}^{(\mu)} := \mathbf{H} - \mu \int_{\mathbb{R}^3} d^3x\rho(x)$ with $\mu \in \mathbb{R}$, which give a suitable "chemical" potential,

$$\mathcal{L}(f) := \operatorname{tr}(\mathcal{P}\exp[i\rho(f)]), \quad \mathcal{P} := \frac{\exp(-\beta\mathbf{H}^{(\mu)})}{\operatorname{tr}\exp(-\beta\mathbf{H}^{(\mu)})}, \tag{1.7}$$

where "tr" means the operator trace-operation in the Fock space $\mathbf{\Phi}$. Posing within this work the problem of studying distribution functions (1.3) in the classical statistical mechanics case, we need to calculate the trace in (1.7) as $\hbar \to 0$. The latter gives rise to the following expressions:

$$\begin{gathered}\mathcal{L}(f) = \frac{Z(f)}{Z(0)}, \quad Z(f) := \exp[-\beta V(\delta)]\mathcal{L}_0(f),\\ \mathcal{L}_0(f) = \exp\left(z\int_{\mathbb{R}^3} d^3x\{\exp[if(x)]-1\}\right),\end{gathered} \tag{1.8}$$

where $z := \exp(\beta\mu)(2\pi\hbar^2\beta m - 1)^{-3/2}$ is the system "activity" [1], and

$$V(\delta) := \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : . \tag{1.9}$$

Based now on expressions (1.8) and (1.9) we can formulate the following proposition.

Proposition 1.1. *The functional (1.4) satisfies [1, 3, 4] the following functional Bogolubov type equation:*

$$[\nabla_x - i\nabla_x f(x)]\frac{1}{i}\frac{\delta\mathcal{L}(f)}{\delta f(x)} = -\beta\int_{\mathbb{R}^3} d^3y\nabla_x V(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : \mathcal{L}(f), \tag{1.10}$$

with the expression (1.8) being its exact functional-analytic solution.

Below we proceed to construct effective analytic tools allowing to find exact functional-analytic solutions to the Bogolubov functional equation (1.10), describing equilibrium many-particle dynamical systems, as well as, we will generalize the obtained results to the case of nonequilibrium dynamical many particle systems.

2. The Bogolubov – Zubarev "collective" variables transform. Taking into account two-particle potential energy partition $V = V^{(s)} + V^{(l)}$, owing to representation (1.8), one can easily write the following expression for the generating functional $Z(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$:

$$Z(f) = \exp[-\beta V^{(s)}(\delta)]\mathcal{L}^{(l)}(f), \quad \mathcal{L}^{(l)}(f) := \exp[-\beta V^{(l)}(\delta)]\mathcal{L}_0(f), \tag{2.1}$$

where we put

$$V^{(l)}(\delta) := \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V^{(l)}(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : ,$$
$$V^{(s)}(\delta) := \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V^{(s)}(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : . \tag{2.2}$$

To calculate the functional $\mathcal{L}^{(l)}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, corresponding to the long range part $V^{(l)}$ of the full potential energy $V : \mathbf{\Phi} \to \mathbf{\Phi}$, we will apply the analog of Bogolubov – Zubarev [5] "collective" variables transform within the grand canonical ensemble, suggested before in [4, 6, 7]. Namely, denote by $\mathcal{L}^{(l)}_{(n)}(f)$, $n \in \mathbb{Z}_+$, a partial solution to the functional equation (1.10), possessing exactly $n \in \mathbb{Z}_+$ particles. Then, owing to the results of [3], for $\mathcal{L}^{(l)}(f)$, $n \in \mathbb{Z}_+$, the following exact expression holds:

$$\mathcal{L}^{(l)}_{(n)}(f) = \int_{\mathbb{R}^3} d^3x_1 \int_{\mathbb{R}^3} d^3x_2 \ldots \int_{\mathbb{R}^3} d^3x_n \prod_{j=1}^{n} \exp[if(x_j)] \exp(-\beta V^{(l)}_n), \tag{2.3}$$

where $V^{(l)}_n$ is the long term part potential energy of an n-particle group of the system. Then we get that

$$\mathcal{L}^{(l)}(f) := \sum_{n\in\mathbb{Z}_+} \frac{z^n}{n!}\mathcal{L}^{(l)}_{(n)}(f) Q_{0,}^{-1} \quad Q_0 := \left(\sum_{n\in\mathbb{Z}_+} \frac{z^n}{n!}\mathcal{L}^{(l)}_{(n)}(0)\right)^{-1}. \tag{2.4}$$

The sum in (2.3) can be calculated exactly, giving rise to the expression

$$\mathcal{L}^{(l)}_{(n)}(f) = \int \mathcal{D}(\omega) \left\{ z \int_{\mathbb{R}^3} d^3x \exp[if(x)] g(x;\omega) \right\}^n J(\omega), \tag{2.5}$$

where $\mathcal{D}(\omega) := \prod_{k\in\mathbb{R}^3} \frac{i}{2}(d\omega_k \wedge d\omega_k)$, $\omega^*_k := \omega_{-k} \in \mathbb{C}$, $k \in \mathbb{R}^3$,

$$g(x;\omega) := \exp\left[-2\pi i \int_{\mathbb{R}^3} d^3k \omega_k \exp(ikx) + \frac{\beta}{2}\int_{\mathbb{R}^3} d^3k \nu(k)\right],$$
$$J(\omega) := \exp\left[-\int_{\mathbb{R}^3} d^3k \frac{2\pi^2}{\beta\nu(k)}\omega_k\omega_{-k} + \int_{\mathbb{R}^3} d^3k \ln\frac{\pi}{\beta\nu(k)}\right], \tag{2.6}$$

and $\nu(k) := (2\pi)^{-3} \int\limits_{\mathbb{R}^3} d^3x V^{(l)} \exp(-ikx)$, $k \in \mathbb{R}^3$. Now from (2.4), (2.5) and (2.6) one easily finds that

$$\mathcal{L}^{(l)}(f) = \int \mathcal{D}(\omega) \exp\left(\bar{z} \int\limits_{\mathbb{R}^3} d^3x \{\exp[if(x) - 1]\} g(x;\omega)\right) J^{(l)}(\omega) Q^{-1}, \tag{2.7}$$

where $\bar{z} := z \exp\left(\frac{\beta}{2} \int\limits_{\mathbb{R}^3} d^3k \nu(k)\right) = z \exp\left[\frac{\beta}{2} V^{(l)}(0)\right]$ and the function $J^{(l)}(\omega), \omega \in \mathbb{R}^3$, allows for the following series expansion:

$$J^{(l)}(\omega) := J(\omega) \exp\left[\int\limits_{\mathbb{R}^3} d^3x g(x;\omega)\right] = J(\omega) \exp\left[-\frac{(2\pi)^2}{2!}(2\pi)^3 \int\limits_{\mathbb{R}^3} d^3k \omega_k \omega_{-k} + \right.$$

$$\left. + \sum_{n \neq 2} \frac{(-2\pi i)^n}{n!} (2\pi)^3 \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \ldots \int\limits_{\mathbb{R}^3} d^3k_n \prod_{j=1}^{n} \omega_{k_j} \delta\left(\sum_{J=1}^{N} k_j\right)\right]. \tag{2.8}$$

The expression (2.7) can be represented now [6] in the following cluster Ursell form:

$$\mathcal{L}^{(l)}(f) = \exp\left(\sum_{n=1}^{\infty} \frac{\bar{z}^n}{n!} \int\limits_{\mathbb{R}^3} d^3x_1 \int\limits_{\mathbb{R}^3} d^3x_2 \ldots \int\limits_{\mathbb{R}^3} d^3x_n \prod_{j=1}^{n} \{\exp[if(x) - 1]\} g_n(x_1, x_2, \ldots, x_n)\right). \tag{2.9}$$

Here, for any $n \in \mathbb{Z}_+$,

$$g_n(x_1, x_2, \ldots, x_n) := \sum_{\sigma[n]} (-1)^{m+1} (m-1)! \prod_{j=1}^{m} R_{\sigma[j]}(x_k \in \sigma[j]),$$
$$R_n(x_1, x_2, \ldots, x_n) := \sum_{\sigma[n]} \prod_{j=1}^{m} g_{\sigma[j]}(x_k \in \sigma[j]), \tag{2.10}$$

where $g_n(x_1, x_2, \ldots, x_n), n \in \mathbb{Z}_+$, are called the n-particle Ursell cluster functions, $R_n(x_1, x_2, \ldots \ldots, x_n)$, $n \in \mathbb{Z}_+$, are suitable "correlation" functions [1, 4, 6] and $\sigma[n]$ denotes a partition of the set $\{1, 2, \ldots, n\}$ into nonintersecting subsets $\{\sigma[j] : j = \overline{1, m}\}$, that is, $\sigma[j] \cap \sigma[k] = \varnothing$ for $j \neq k = \overline{1, m}$, and $\sigma[n] = \cup_{j=1}^{m} \sigma[j]$. Having separated from the function $J^{(l)}(\omega)$, $\omega \in \mathbb{C}^3$, the natural "Gaussian" part $J_0^{(l)}(\omega)$, $\omega \in \mathbb{R}^3$, one can write down that

$$g_1(x_1) = \frac{G(\xi_k^{(1)})}{G(0)}, \quad g_2(x_1, x_2) = \frac{G(\xi_k^{(2)})}{G(0)} - g_1(x_1) g_1(x_2), \ldots, \tag{2.11}$$

where $\xi_k^{(n)} := -2\pi i \sum_{s=1}^{n} \exp(ikx_s),\ k \in \mathbb{R}^3, n \in \mathbb{Z}_+,$

$$G(\xi_k^{(n)}) := \exp[\mathcal{M}(\xi_k^{(n)})] \int D(\omega) g^{(l)}(\xi_k^{(n)};\omega) J_0(\omega),$$

$$\mathcal{M}(\xi_k^{(n)}) := \sum_{m\neq 2} \frac{(-2\pi i)^m}{m!}(2\pi)^3 \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \ldots \int\limits_{\mathbb{R}^3} d^3k_m \delta\left(\sum_{s=1}^{m} k_s\right) \prod_{s=1}^{m} \frac{\delta}{\delta\xi_{k_s}^{(n)}}, \tag{2.12}$$

$$g^{(l)}(\xi_k^{(n)};\omega) := \prod_{j=1}^{n} g(x_j;\omega).$$

Since the integrals $\int \mathcal{D}(\omega) g^{(l)}(\xi_k^{(n)};\omega) J^{(l)}(\omega),\ n \in \mathbb{Z}_+$, are calculated exactly, the formulae (2.9) and (2.10) are sources of the so-called "virial" variables for the Ursell – Mayer "cluster" correlation functions $g_n(x_1, x_2, \ldots x_n),\ n \in \mathbb{Z}_+$, which have important applications. In particular, from the function $J^{(l)}(\omega),\ \omega \in \mathbb{C}^3$, one gets right away that the cluster expansion for the functions $g_n(x_1, x_2, \ldots x_n),\ n \in \mathbb{Z}_+$, are fulfilled by means of the "screened" potential function $\bar{V}^{(l)}(x - -y),\ x, y \in \mathbb{R}^3$, where

$$\bar{V}^{(l)}(x-y) := \int\limits_{\mathbb{R}^3} d^3k \frac{\nu(k)\exp[ik(x-y)]}{1+\nu(k)\beta\bar{z}(2\pi)^3}. \tag{2.13}$$

In particular, from (1.5) and (2.9) one easily finds that

$$\begin{aligned} F_1(x_1) &= z \int \mathcal{D}(\omega) g(x;\omega) J^{(l)}(\omega) \left[\int \mathcal{D}(\omega) J^{(l)}(\omega)\right]^{-1} = \\ &= \bar{\rho} \simeq \bar{z} \exp\left[\frac{\beta}{2} \int d^3k \frac{\beta\nu^2(k)(2\pi)^3\bar{z}}{1+\nu(k)\beta\bar{z}(2\pi)^3}\right], \end{aligned} \tag{2.14}$$

$$\begin{aligned} F_2(x_1,x_2) &= z^2 \int \mathcal{D}(\omega) g(x_1;\omega) g(x_2;\omega) J^{(l)}(\omega) \left[\int \mathcal{D}(\omega) J^{(l)}(\omega)\right]^{-1} \simeq \\ &\simeq \bar{\rho}^2 \exp[-\beta\bar{V}^{(l)}(x_2-x_1)] \Bigg\{ 1 + \bar{\rho} \int\limits_{\mathbb{R}^3} d^3x_3 \Big[\exp\left(-\beta\bar{V}^{(l)}(x_1-x_3)\right) - 1 + \\ &+ \beta\bar{V}^{(l)}(x_1-x_3)\Big] \Big[\exp\left(-\beta\bar{V}^{(l)}(x_2-x_3)\right) - 1 + \beta\bar{V}^{(l)}(x_2-x_3)\Big] + \\ &+ \bar{\rho} \int\limits_{\mathbb{R}^3} d^3x_3 [-\beta\bar{V}^{(l)}(x_1-x_3)][\exp(-\beta\bar{V}^{(l)}(x_2-x_3)) - 1 + \beta\bar{V}^{(l)}(x_2-x_3)] + \\ &+ \bar{\rho} \int\limits_{\mathbb{R}^3} d^3x_3 [-\beta\bar{V}^{(l)}(x_2-x_3)][\exp(-\beta\bar{V}^{(l)}(x_1-x_3)) - 1 + \beta V^{(l)}(x_1-x_3)] + \ldots \Bigg\} \ldots, \end{aligned}$$

and so on. The result, presented above, can be obtained by means of a little formal calculations, based on generalized functions and operator theories [4, 8]. Indeed, as $\hbar \to 0$, one has that

$$
\begin{aligned}
\mathcal{L}^{(l)}(f) &= \exp[-\beta V^{(l)}]\mathcal{L}_0(f)Q^{-1} = \\
&= \operatorname{tr}\left\{\exp(-\beta \mathbf{H}_0^{(\mu)})\exp\left[-\frac{\beta}{2}\int_{\mathbb{R}^3} d^3k\nu(k) : \rho_k\rho_{-k} :\right]\exp[i(\rho(f)]\right\} = \\
&= \operatorname{tr}\left\{\exp(-\beta \mathbf{H}_0^{(\mu)})\exp\left[\frac{\beta}{2}\int_{\mathbb{R}^3} d^3k\nu(k)\int_{\mathbb{R}^3} d^3x\rho(x)\right]\times\right. \\
&\times \left.\int \mathcal{D}(\omega)\exp\left[-\int_{\mathbb{R}^3} d^3k\frac{2\pi^2}{\beta\nu(k)}\omega_k\omega_{-k} - \int_{\mathbb{R}^3} d^3k 2\pi i\omega_k\rho_k\right]\exp[i(\rho, f)]\right\}Q^{-1} = \\
&= \int \mathcal{D}(\omega)J(\omega)\operatorname{tr}\left\{\exp(-\beta \mathbf{H}_0^{(\mu)})\exp\left[i\left(\rho, f - 2\pi\int_{\mathbb{R}^3} d^3k\omega_k\exp(ikx) - \right.\right.\right. \\
&\left.\left.\left. - \frac{i\beta}{2}\int_{\mathbb{R}^3} d^3k\nu(k)\right)\right]\right\}Q^{-1} = \\
&= \int \mathcal{D}(\omega)J(\omega)\mathcal{L}_0(f - 2\pi\int_{\mathbb{R}^3} d^3k\omega_k\exp(ikx) - \frac{i\beta}{2}\int_{\mathbb{R}^3} d^3k\nu(k))Q^{-1} = \\
&= \int \mathcal{D}(\omega)J^{(l)}(\omega)\exp\left(\int_{\mathbb{R}^3} d^3k\{\exp[if(x)] - 1\}g(x;\omega)\right),
\end{aligned}
\tag{2.15}
$$

where $\mathbf{H}_0^{(\mu)} := \mathbf{H}_0 - \mu\int_{\mathbb{R}^3} d^3x\rho(x)$, $\rho_k := \int_{\mathbb{R}^3} d^3x\rho(x)\exp(ikx)$, $k \in \mathbb{R}^3$. The expression (2.15) coincides exactly with that of (2.9), thereby proving the validity of our expressions (1.8) and (2.1) for the N. N. Bogolubov type generating functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, satisfying the functional equation (1.10) in Proposition 1.1.

3. The Ursell – Mayer type diagram expansion. Having considered expressions (2.1) and (2.7) as starting ones, with known functions $g_n(x_1, x_2, \ldots x_n)$, $n \in \mathbb{Z}_+$, for the functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, one can obtain the following result:

$$\mathcal{L}(f) = \frac{Z(f)}{Z(0)}, \ \ Z(f) = \exp[-\beta V^{(s)}(\delta)]\mathcal{L}^{(l)}(f) =$$

$$= \exp[-\beta V^{(s)}(\delta)] \exp\left[\sum_{n=1}^{\infty} \frac{z^n}{n!} \int\limits_{\mathbb{R}^3} d^3x_1 \int\limits_{\mathbb{R}^3} d^3x_2 \ldots \int\limits_{\mathbb{R}^3} d^3x_n \times\right.$$

$$\left. \times \prod_{j=1}^{n} \{\exp[if(x_j)] - 1\} g_n(x_1, x_2, \ldots, x_n)\right] =$$

$$= \exp\left[\sum_{N=1}^{\infty} \frac{1}{N!} W(G_N^{(c)})\right], \tag{3.1}$$

where the functionals $W(G_N^{(c)})$, $N = \overline{1,\infty}$, are calculated via the following rule. Denote by $G_N^{(c)}$, $N = \overline{1,\infty}$, a connected graph and that consists of exactly N generalized vertices of $[\gamma(n_j)]$ type, $j = \overline{1,N}$, and $\sum_{j=1}^{N} n_j$ ordinary vertices of $[\alpha]$ type. Let it each vertex $[y(n)]$ is necessarily connected with n vertices of type $[\alpha]$ by means of dashed lines, but between themselves $[\alpha]$ vertices can be connected arbitrarily by means of solid lines. If now we assign the factor $g_n(x_1, x_2, \ldots, x_n)$ to each generalized $[\gamma(n)]$-vertex the factor $z \int\limits_{\mathbb{R}^3} d^3x \exp[if(x)]$ to each simple $[\alpha]$-vertex, and the factor $\{\exp[-\beta V^{(s)}(x_{l_1} - x_{l_2})] - 1\}$ to the line connecting them, then the obtained resulting expression will be exactly equal to the functional $W(G_N^{(c)})$. The final summing up over all such connected graphs gives the expression (2.15), where the factor $1/N!$ counts for the symmetry order of the graph $G_N^{(c)}$ under permutations of the generalized vertices.

It is evident that, by representing the factor $\exp[if(x)]$ that enters the vertex $[\alpha]$ as $\{\exp[i \times \times f(x)] - 1\} + 1$, the expression (2.15) can be easily resumed into Ursell – Mayer type expressions but already with suitably another functions g_n, replacing the former ones and giving rise to expansions similar to (2.14), based already on the “screened” potential (2.13), which we will not discuss here in more details.

Thereby, taking into account the results of [4, 6] we can formulate the next proposition, characterizing the Bogolubov type generating functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, satisfying the functional equation (1.10).

Proposition 3.1. *Let the Bogolubov type generating functional* $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, *represented analytically as a series (3.1) of graph-generated functionals, satisfy the following conditions:*

i) continuity with respect to the natural topology on $\mathcal{S}(\mathbb{R}^3;\mathbb{R})$, $|\mathcal{L}(f)| \leq 1$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$;

ii) positivity, $\sum_{j,k=1}^{n} c_j c_k^* \mathcal{L}(f_j - f_k) \geq 0$ *for any* $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$ *and all* $c_j \in \mathbb{C}$, $j = \overline{1,n}$, $n \in \mathbb{Z}_+$;

iii) symmetry and normalization conditions, $\mathcal{L}^*(f) = \mathcal{L}(-f)$ *for all* $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$ *and* $\mathcal{L}(0) = 1$;

iv) translational-invariance, $\mathcal{L}(f) = \mathcal{L}(f_a)$, *where* $f_a(x) := f(x-a)$, $x, a \in \mathbb{R}^3$, *for any* $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$;

v) cluster condition or, equivalently, the Bogolubov correlation decay, $\lim_{\lambda\to\infty}[\mathcal{L}(f+g_{\lambda a}) - -\mathcal{L}(f_a)\mathcal{L}(g_{\lambda a})] = 0$, $a \in \mathbb{R}^3$, *for any* $f, g \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$;

vi) density condition, $\frac{1}{i}\frac{\delta\mathcal{L}(f)}{\delta f(x)}\Big|_{f=0} = \bar{\rho} \in \mathbb{R}_+$.

Then the functional (3.1) solves the Bogolubov type functional equation (1.10), giving the positive measure $d\bar{\mu}\exp$ *Fourier representation on the adjoint tempered generalized function space* $\mathcal{S}'(\mathbb{R}^3;\mathbb{R})$ *as*

$$\mathcal{L}(f) = \int\limits_{\mathcal{S}'(\mathbb{R}^3;\mathbb{R})} d\bar{\mu}(\xi)\exp[i(\xi, f), \tag{3.2}$$

where $(\xi, f) := \int_{\mathbb{R}^3} d^3x\xi(x)f(x)$ *for* $\xi \in \mathcal{S}'(\mathbb{R}^3;\mathbb{R})$ *and* $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$.

The obtained result makes it possible to find the many-particle distribution functions (1.5) and apply them for constructing different thermodynamic functions that are important [1, 9] in applications.

Below, following the Bogolubov method [3], we obtain, based on the expression (2.3), the important Kirkwood – Saltzbourg – Simansic functional equation for the Bogolubov generating functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$. Namely, making use of the expression (2.3) we can write the following relationship:

$$\frac{1}{i}\frac{\delta\mathcal{L}_{(N+1)}(f)}{\delta f(x)} = \exp[if(x)]\frac{(N+1)Z_N}{Z_{N+1}}\mathcal{L}_{(N)}(f(\cdot) + i\beta V(\cdot - x)) \tag{3.3}$$

for any $x \in \mathbb{R}^3$. Since, by definition,

$$\lim_{N\to\infty}\mathcal{L}_{(N)}(f) = \mathcal{L}(f), \quad f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R}), \quad \lim_{N\to\infty}\frac{(N+1)Z_N}{Z_{N+1}} := z \in \mathbb{R}_+,$$

from (3.3) one gets right away that

$$\exp[-if(x)]\frac{1}{i}\frac{\delta\mathcal{L}(f)}{\delta f(x)} = z\mathcal{L}(f(\cdot) + i\beta V(\cdot - x)), \tag{3.4}$$

which is called the Kirkwood – Saltzbourg – Symansic functional equation, which is very important for proving Proposition 3.1 by means of the classical Leray – Schauder fixed point theorem [1, 2, 10] in some suitably defined Banach space. In particular, at $f = 0$ from (3.4) one finds the following important relationship:

$$\bar{\rho} = z\mathcal{L}(i\beta V(\cdot - x)) \tag{3.5}$$

for any $x \in \mathbb{R}^3$.

4. The quantized Wigner operator and the N. N. Bogolubov generating functional method in nonequilibrium statistical mechanics. For studying nonequilibrium properties of a many-particle classical statistical system it was proposed [4, 6] to use the quasiclassical quantized Wigner density operator

$$w(x;p) := \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} d^3\alpha \exp(i\alpha p)\,\psi^+\left(x+\frac{\hbar\alpha}{2}\right)\psi(x-\frac{\hbar\alpha}{2}), \tag{4.1}$$

where the one-particle phase space variables satisfy $(x;p) \in T^*(\mathbb{R}^3)$. By means of simple calculations one can see that the Hamilton operator $\mathbf{H} : \mathbf{\Phi} \to \mathbf{\Phi}$ can be written as

$$\mathbf{H} = \int_{T^*(\mathbb{R}^3)} d^3p d^3x \frac{p^2}{2m} w(x;p) + \int_{T^*(\mathbb{R}^3)} d^3p d^3x \int_{T^*(\mathbb{R}^3)} d^3\xi d^3y V(x-y) : w(x;p)w(y;\xi) : \ , \tag{4.2}$$

where the symbol : : as before, denotes the usual Wick ordering of creation and annihilation operators on the Fock space $\mathbf{\Phi}$. With regard to the following applications, let us mention formulae for Wigner density operators (4.1) in the Wick sence,

$$\left[\int_{\mathbb{R}^3} d^3x\psi^+(x)\nabla_x^2\psi(x), w(z;\vartheta)\right] \overset{\hbar\to 0}{\simeq} \frac{\hbar}{i}\left\{\frac{\vartheta^2}{2m}, w(z;\vartheta)\right\},$$

$$\left[\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V(x-y) : \rho(x)\rho(y) :, w(z;\vartheta)\right] \overset{\hbar\to 0}{\simeq} \frac{2\hbar}{i}\int_{\mathbb{R}^3} d^3y \left\{V(z-y), : \rho(y)w(z;\vartheta) :\right\}, \tag{4.3}$$

$$w(x;p)w(y,\xi) \overset{\hbar\to 0}{\simeq} : w(x;p)w(y,\xi) : + w(x;p)\delta(x-y)\delta(p-\xi),$$

where the bracket $[\cdot,\cdot]$ means the usual commutator of operators in the Fock space $\mathbf{\Phi}$ and $\{\cdot,\cdot\}$ means the classical canonical Poisson bracket on the phase space $T^*(\mathbb{R}^3)$. Following the Bogolubov ideas, we will define a Bogolubov generating functional $\mathcal{L}(f),\ f \in \mathcal{S}(T(\mathbb{R}^3);\mathbb{R})$, as

$$\mathcal{L}(f) := \operatorname{tr}(\mathcal{P}\exp[i(w,f)], \tag{4.4}$$

where, by definition, $(w,f) := \int_{T(\mathbb{R}^3)} d^3x d^3p w(x;p) f(x;p)$ and $\mathcal{P} : \mathbf{\Phi} \to \mathbf{\Phi}$ is the statistical operator satisfying the following [1, 3, 4, 7] evolution equation with respect to the time variable $t \in \mathbb{R}_+$:

$$\frac{\partial\mathcal{P}}{\partial t} = \frac{i}{\hbar}[\mathcal{P},\mathbf{H}], \quad \operatorname{tr}\mathcal{P} = 1, \ \ \mathcal{P}|_{t=0} = \bar{\mathcal{P}}, \tag{4.5}$$

where the initial operator $\bar{\mathcal{P}} : \mathbf{\Phi} \to \mathbf{\Phi}$ is assumed to be given a priori.

Concerning the n-particle distribution functions $F_n(x_1, x_2, \ldots, x_n; p_1, p_2, \ldots, p_n|t)$, $n \in \mathbb{Z}_+$, the expressions

$$
\begin{aligned}
F_n(x_1, x_2, \ldots, x_n; p_1, p_2, \ldots, p_n|t) \,:=& \\
&= \operatorname{tr}(\mathcal{P} \,:\, w(x_1;p_1)w(x_2;p_2)\ldots w(x_n;p_n) \,:) = \\
&=: \frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2;p_2)}\ldots\frac{1}{i}\frac{\delta}{\delta f(x_n;p_n)} \,:\, \mathcal{L}(f)|_{f=0},
\end{aligned}
\tag{4.6}
$$

hold as $\hbar \to 0$, where

$$
\begin{gathered}
:\frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)} := \frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)}, \\
:\frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2;p_2)} := \frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)}\left(\frac{1}{i}\frac{\delta}{\delta f(x_2;p_2)} - \delta(x_1-x_2)\delta(p_1-p_2)\right), \\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots
\end{gathered}
\tag{4.7}
$$

and so on, owing to the last expression of (4.3).

For finding the distribution functions (4.6) we will derive, following N. N. Bogolubov [1, 3], the corresponding evolution functional equation on the N. N. Bogolubov generating functional (4.4). Making use of the relationship (4.4), one obtains easily that

$$
\begin{aligned}
\frac{\partial \mathcal{L}(f)}{\partial t} &= \operatorname{tr}\left(\frac{\partial \mathcal{P}}{\partial t}\exp[i(w,f)]\right) = \operatorname{tr}\left(\mathcal{P}\frac{i}{\hbar}[\mathbf{H}, \exp[i(w,f)]]\right) = \\
&= \operatorname{tr}\left(\mathcal{P}\int\limits_{T(\mathbb{R}^3)} d^3x d^3p \left\{\frac{p^2}{2m}, w(x;p)\exp[i(w,f)]\right\}\right) + \\
&\quad + \frac{1}{2}\operatorname{tr}\left(\mathcal{P}\int\limits_{T(\mathbb{R}^3)} d^3x d^3p \int\limits_{T(\mathbb{R}^3)} d^3y d^3\xi \left\{V(x-y), : w(x;p)w(y;\xi) : \exp[i(w,f)]\right\}\right).
\end{aligned}
\tag{4.8}
$$

Now, based on relationships (4.3), we finally obtain the following Bogolubov type evolution functional equation:

$$\frac{\partial \mathcal{L}(f)}{\partial t} = \int\limits_{T(\mathbb{R}^3)} d^3x d^3p \left\{ T(p), \frac{1}{i} \frac{\delta \mathcal{L}(f)}{\delta f(x;p} \right\} +$$

$$+ \frac{1}{2} \int\limits_{T(\mathbb{R}^3)} d^3x d^3p \int\limits_{T(\mathbb{R}^3)} d^3y d^3\xi \left\{ V(x-y), : \frac{1}{i} \frac{\delta}{\delta f(x;p)} \frac{1}{i} \frac{\delta}{\delta f(y;\xi)} : \mathcal{L}(f \right\}, \tag{4.9}$$

where, by definition, $T(p) := \frac{p^2}{2m}$, $p \in \mathbb{R}^3$, is the kinetic free particle energy.

Having analyzed the Bogolubov generating functional (4.4) within the quasiclassical Wigner density operator representation (4.1), one can obtain an exact functional-operator solution to the evolution Bogolubov functional equation (4.9):

$$\mathcal{L}(f) = \frac{Z(f)}{Z(0)}, \qquad Z(f) = \exp[\Phi(\delta)]\mathcal{L}_0(f) \tag{4.10}$$

for $f \in \mathcal{S}(T(\mathbb{R}^3); \mathbb{R})$. Here we denoted

$$\Phi(\delta) = \sum_{n \in \mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 \ldots \times$$

$$\times \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \Phi_n(x_1, x_2, \ldots, x_n; p_1, p_2, \ldots, p_n | t) \times$$

$$\times : \frac{1}{i} \frac{\delta}{\delta f(x_1;p_1)} \frac{1}{i} \frac{\delta}{\delta f(x_2;p_2)} \ldots \frac{1}{i} \frac{\delta}{\delta f(x_n;p_n)} :, \tag{4.11}$$

$$\mathcal{L}_0(f) = \sum_{n \in \mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 \ldots \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \times$$

$$\times \bar{F}_n \left(x_1 - \frac{p_1}{m}t, x_2 - \frac{p_2}{m}t, \ldots, x_n - \frac{p_n}{m}t; p_1, p_2, \ldots, p_n \right) \prod_{j=1}^{n} \{\exp[if(x_j;p_j)] - 1\},$$

where $\bar{F}_n(x_1, x_2, \ldots, x_n; p_1, p_2, \ldots, p_n)$, $n \in \mathbb{Z}_+$, are given n-particle distribution functions at $t = 0$, that is, owing to the definition (4.6),

$$\bar{F}_n(x_1, x_2, \ldots, x_n; p_1, p_2, \ldots, p_n) := \operatorname{tr}(\bar{\mathcal{P}} : w(x_1;p_1) w(x_2;p_2) \ldots w(x_n;p_n) :) =$$

$$=: \frac{1}{i} \frac{\delta}{\delta f(x_1;p_1)} \frac{1}{i} \frac{\delta}{\delta f(x_2;p_2)} \ldots \frac{1}{i} \frac{\delta}{\delta f(x_n;p_n)} : \mathcal{L}(f)|_{t=0, f=0}, \tag{4.12}$$

and $\Phi_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n|t),\ n \in \mathbb{Z}_+$, are so called cluster potential functions determined recursively by means of the following functional-operator relationships:

$$\log(\mathcal{P}_0^{-1}\mathcal{P}) := \sum_{n\in\mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 \dots \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \times$$

$$\times\, \Phi_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n|t) : w(x_1;p_1)w(x_2;p_2)\dots w(x_n;p_n) : \tag{4.13}$$

with

$$\mathcal{P}_0 = \exp\left(-\frac{it}{\hbar}\mathbf{H}_0\right)\bar{\mathcal{P}}\exp\left(\frac{it}{\hbar}\mathbf{H}_0\right) \tag{4.14}$$

being the statistical operator of a noninteracting particle system.

If the initial distribution at $t = 0$ is “chaotic”, that is, for all $n \in \mathbb{Z}_+$ the relationships

$$\bar{F}_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n) = \prod_{j=1}^{n} \bar{F}_1(x_j; p_j) \tag{4.15}$$

hold, one gets easily from (4.11) and (4.15) that

$$\mathcal{L}_0(f) = \exp\left(\int\limits_{T(\mathbb{R}^3)} d^3x d^3p \bar{F}_1\left(x - \frac{p}{m}t; p\right)\{\exp[if(x;p)] - 1\}\right). \tag{4.16}$$

If the “chaotic” condition is not fulfilled, we can proceed to the usual cluster Ursell–Mayer type representation [4, 6] for the Bogolubov generating functional (4.10),

$$\mathcal{L}_0(f) = \exp\left(\sum_{n\in\mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 \dots \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \times\right.$$

$$\left.\times \bar{g}_n\left(x_1 - \frac{p_1}{m}t, x_2 - \frac{p_2}{m}t, \dots, x_n - \frac{p_n}{m}t; p_1, p_2, \dots, p_n\right)\prod_{j=1}^{n}\{\exp[if(x_j;p_j)] - 1\}\right), \tag{4.17}$$

where the “cluster” distribution functions $\bar{g}_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n),\ n \in \mathbb{Z}_+$, have the form

$$\bar{g}_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n) := \sum_{\sigma[n]} (-1)^{m+1}(m-1)! \prod_{j=1}^{m} \bar{F}_{\sigma[j]}((x_k; p_k) \in \sigma[j]),$$

$$\bar{F}_n(x_1, x_2, \dots, x_n; p_1, p_2, \dots, p_n) := \sum_{\sigma[n]} \prod_{j=1}^{m} \bar{g}_{\sigma[j]}((x_k; p_k) \in \sigma[j]),$$

and $\sigma[n]$ denotes a partition of the set $\{1, 2, \ldots, n\}$ into nonintersecting subsets $\{\sigma[j] : j = \overline{1, m}\}$, that is, $\sigma[j] \cap \sigma[k] = \varnothing$ for $j \neq k = \overline{1, m}$, and $\sigma[n] = \cup_{j=1}^{m} \sigma[j]$. In particular,

$$\bar{g}_1(x_1; p_1) = \bar{F}_1(x_1; p_1),$$

$$\bar{g}_2(x_1, x_2; p_1, p_2) = \bar{F}_2(x_1, x_2; p_1, p_2) - \bar{F}_1(x_1; p_1)\bar{F}_1(x_2; p_2), \ldots,$$

and so on. The N. N. Bogolubov generating functional (4.10), owing to (4.11) and (4.17), allows a natural infinite series expansion whose coefficients can be represented as above by means of the usual Ursell – Mayer type diagram expressions, which can be effectively used for studying kinetic properties of our many-particle statistical system.

5. Conclusions. In the article we showed that the N. N. Bogolubov generating functional method is a very effective tool for studying distribution functions of both equilibrium and nonequilibrium states of classical many-particle dynamical systems. In some cases the N. N. Bogolubov generating functionals can be represented by means of infinite Ursell – Mayer diagram expansions that converge under some additional constraints on the statistical system under consideration. We show for the first time that the Bogolubov idea [1] to use the Wigner density operator transformation for studying the nonequilibrium distribution functions proved to be very effective, having proposed a new analytic form of a nonstationary solution to the classical N. N. Bogoliubov evolution functional equation.

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