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# THE ANALYTIC ASPECTS OF THE BOGOLIUBOV GENERATING FUNCTIONAL EQUATIONS WITHIN THE BOBOLIUBOV CANONICAL TRANSFORMATION METHOD

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**Abstract**

The analytic aspects of the Bogoliubov generating functional equations and their transformation properties within the Bogoliubov canonical transformation method are studied. The classical Bogoliubov idea [2] to use the Wigner density operator transformation for studying the non equilibrium distribution functions within the Bogoliubov canonical transformation method is developed, a new analytic non-stationary solution to the classical N.N. Bogoliubov evolution functional equation is constructed.


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# 1 Introduction: The Bogoliubov functional equation and its analytical structure

We consider 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 $\Lambda \subset \mathbb{R}^3$ , which is specified by a quantum-mechanical Hamiltonian operator $\hat{H} : L_2^{(sym)}(\mathbb{R}^{3N};\mathbb{C}) \to L_2^{(sym)}(\mathbb{R}^{3N};\mathbb{C})$ 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 $\nabla_j := \partial/\partial x_j$, $j = \overline{1,N}$, $\hbar-$the Planck 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 a partition $V = V^{(l)} + V^{(s)}$, where $V^{(s)}-$ 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 [2, 10, 5, 6], 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

$$\mathbf{H}_0 := -\frac{\hbar^2}{2m}\int_{\mathbb{R}^3} d^3x \psi^+ \nabla_x^2 \psi, \tag{1.2}$$

$$\mathbf{V} := \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V(x-y)\psi^+(x)\psi^+(y)\psi(y)\psi(x),$$

and the operator $\mathbf{H} : \mathbf{\Phi} \to \mathbf{\Phi}$ acts in a suitable Fock space [10, 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 Bogoliubov $n-$particles distribution functions can be written down [2, 3, 1] as

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

where $n \in \mathbb{Z}_+$, $\rho(x) := \psi^+(x)\psi(x)-$the density operator at $x \in \mathbb{R}^3$, ": :"$-$ the usual [2, 10] 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 $\beta \to \infty$, normed by the condition

$(\Omega, \Omega) = 1$. Having introduced the Bogoliubov generating functional as

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

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

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

Here $x_j \in \mathbb{R}^3$, $j = \overline{1,n}$, $n \in \mathbb{Z}_+$, and the symbol ": $\frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}...$ $...\frac{1}{i}\frac{\delta}{\delta f(x_n)}$ :" imitates the normal ordering symbol ": :" action on operator expressions $\rho(x_1)\rho(x_1)...\rho(x_n)$, that is

$$\begin{aligned} &:\frac{1}{i}\frac{\delta}{\delta f(x_1)}: = \frac{1}{i}\frac{\delta}{\delta f(x_1)}, \\ &:\frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}: = \frac{1}{i}\frac{\delta}{\delta f(x_1)}[\frac{1}{i}\frac{\delta}{\delta f(x_2)} - \delta(x_1 - x_2)], \end{aligned} \tag{1.5}$$

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 $\mu \in \mathbb{R}$ being a suitable "chemical" potential:

$$\mathcal{L}(f) := tr(\mathcal{P}\exp[i\rho(f)]), \quad \mathcal{P} := \frac{\exp(-\beta\mathbf{H}^{(\mu)})}{tr\exp(-\beta\mathbf{H}^{(\mu)})}, \tag{1.6}$$

where "$tr$" means the operator trace-operation in the Fock space $\mathbf{\Phi}$. Keeping in mind within the task of studying distribution functions (1.3) in the classical statistical mechanics case, we need to calculate the trace in (1.6) as $\hbar \to 0$. The latter gives rise to the following expressions:

$$\begin{aligned} \mathcal{L}(f) &= Z(f)/Z(0), \quad Z(f) := \exp[-\beta V(\delta)]\mathcal{L}_0(f), \\ \mathcal{L}_0(f) &= \exp(z\int_{\mathbb{R}^3} d^3x\{\exp[if(x)] - 1\}), \end{aligned} \tag{1.7}$$

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

$$V(\delta) := \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : \ . \tag{1.8}$$

Based on expressions (1.7) and (1.8) we can formulate the following proposition.

**Proposition 1.1.** *The functional (1.4) satisfies [3, 2, 4] the following functional Bogoliubov type equation:*

$$\begin{aligned} &[\nabla_x - i\nabla_x f(x)]\frac{1}{i}\frac{\delta \mathcal{L}(f)}{\delta f(x)} \\ = \quad &-\beta \int_{\mathbb{R}^3} d^3y \nabla_x V(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : \mathcal{L}(f), \end{aligned} \tag{1.9}$$

*with the expression (1.7) being its exact functional-analytic solution.*

Below we will proceed to constructing effective analytic tools allowing to find exact functional-analytic solutions to the Bogoliubov functional equation (1.9), describing equilibrium many-particle dynamical systems, as well as, generalize the obtained results for the case of non-equilibrium dynamical many particle systems.

## 2 The "collective" variables representation within the Bogoliubov canonocal transformation method

Taking into account the two-particle potential energy partition $V = V^{(s)} + V^{(l)}$, owing to the representation (1.7) one can easily write down the following expression for the generating functional $Z(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$ :

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

where we put

$$
\begin{aligned}
V^{(l)}(\delta) \quad &:= \quad \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V^{(l)}(x-y) \times \qquad (2.2)\\
\times \quad &: \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)}:,\\
V^{(s)}(\delta) \quad &:= \quad \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V^{(s)}(x-y) \times\\
\times \quad &: \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)}:.
\end{aligned}
$$

Needing 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 analogue of Bogoliubov-Zubarev canonical transform [1, 3] to "collective" variables [12] within the grand canonical ensemble, suggested before in [4, 9, 8, 7]. Namely, denote by $\mathcal{L}^{(l)}_{(n)}(f)$, $n \in \mathbb{Z}_+$, $-$ a partial solution to the functional equation (1.9), possessing exactly $n \in \mathbb{Z}_+$ particles. Then, owing to the results of [3], for $\mathcal{L}^{(l)}(f)$, $n \in \mathbb{Z}_+$, there holds the following exact expression:

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

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

$$
\begin{aligned}
\mathcal{L}^{(l)}(f) &:= \sum_{n\in\mathbb{Z}_+} \frac{z^n}{n!}\mathcal{L}^{(l)}_{(n)}(f) Q^{-1}_{0,} \qquad (2.4)\\
Q_0 &:= (\sum_{n\in\mathbb{Z}_+} \frac{z^n}{n!}\mathcal{L}^{(l)}_{(n)}(0))^{-1}.
\end{aligned}
$$

The sum in (2.4) can be calculated exactly, taking into account the expression

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

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

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

$$J(\omega) := \exp\left[-\int\limits_{\mathbb{R}^3} d^3k\frac{2\pi^2}{\beta\nu(k)}\omega_k\omega_{-k} + \int\limits_{\mathbb{R}^3} d^3k\ln\frac{\pi}{\beta\nu(k)}\right] \quad (2.6)$$

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

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

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

$$J^{(l)}(\omega) := J(\omega)\exp\left[\int\limits_{\mathbb{R}^3} d^3xg(x;\omega)\right] = \quad (2.8)$$
$$= J(\omega)\exp\left[-\frac{(2\pi)^2}{2!}(2\pi)^3\int\limits_{\mathbb{R}^3} d^3k\omega_k\omega_{-k} + \right.$$
$$+\sum_{n\neq 2}\frac{(-2\pi i)^n}{n!}(2\pi)^3\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2 ... \int\limits_{\mathbb{R}^3} d^3k_n \times$$
$$\left.\times\prod_{j=1}^n \omega_{k_j}\delta\left(\sum_{J=1}^N k_j\right)\right].$$

The expression (2.7) can now be represented [9] in the following cluster Ursell form:

$$\mathcal{L}^{(l)}(f) = \exp\left(\sum_{n=1}^{\infty}\frac{\bar{z}^n}{n!}\int\limits_{\mathbb{R}^3} d^3x_1 \int\limits_{\mathbb{R}^3} d^3x_2 ... \int\limits_{\mathbb{R}^3} d^3x_n \times \right. \tag{2.9}$$

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

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

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

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

where $g_n(x_1, x_2, ..., x_n)$, $n \in \mathbb{Z}_+$, are called the $n-$particle Ursell cluster functions, $R_n(x_1, x_2, ..., x_n)$, $n \in \mathbb{Z}_+$, are suitable "correlation" functions [2, 4, 9, 1] and $\sigma[n]$ denotes a partition of the set $\{1, 2, ..., n\}$ into non-intersecting 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

$$g_1(x_1) = G(\xi_k^{(1)})/G(0), \tag{2.11}$$

$$g_2(x_1, x_2) = G(\xi_k^{(2)})/G(0) - g_1(x_1)g_1(x_2), ...,$$

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

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

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

$$g^{(l)}(\xi_k^{(n)};\omega) := \prod_{j=1}^{n} g(x_j;\omega). \tag{2.12}$$

Since the integrals $\int \mathcal{D}(\omega) g^{(l)}(\xi_k^{(n)};\omega) J^{(l)}(\omega),\ \ n \in \mathbb{Z}_+$, one can calculate exactly, the formulae (2.9) and (2.11) are sources of the so called "virial" variables for Ursell-Mayer "cluster" correlation functions $g_n(x_1, x_2, ...x_n),\ \ n \in \mathbb{Z}_+$, having 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 $g_n(x_1, x_2, ...x_n),\ n \in \mathbb{Z}_+$, are fulfilled by means of the "screened" potential function $\bar{V}^{(l)}(x-y)$, $x, y \in \mathbb{R}^3$, where

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

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

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

and

$$\begin{aligned} &F_2(x_1,x_2) = z^2\int \mathcal{D}(\omega)g(x_1;\omega)g(x_2;\omega)J^{(l)}(\omega)\left[\int \mathcal{D}(\omega)J^{(l)}(\omega)\right]^{-1} \simeq \\ &\simeq \bar{\rho}^2\exp[-\beta\bar{V}^{(l)}(x_2-x_1)]\left\{1+\bar{\rho}\int\limits_{\mathbb{R}^3} d^3x_3[\exp\left(-\beta\bar{V}^{(l)}(x_1-x_3)\right)-\right. \\ &-1+\beta\bar{V}^{(l)}(x_1-x_3)][\exp\left(-\beta\bar{V}^{(l)}(x_2-x_3)\right)-1+\beta\bar{V}^{(l)}(x_2-x_3)]+ \\ &+\bar{\rho}\int\limits_{\mathbb{R}^3} d^3x_3[-\beta\bar{V}^{(l)}(x_1-x_3)]\times \\ &\qquad\qquad\times[\exp(-\beta\bar{V}^{(l)}(x_2-x_3))-1+\beta\bar{V}^{(l)}(x_2-x_3)]+ \\ &+\bar{\rho}\int\limits_{\mathbb{R}^3} d^3x_3[-\beta\bar{V}^{(l)}(x_2-x_3)]\times \\ &\qquad\qquad\left.\times[\exp(-\beta\bar{V}^{(l)}(x_1-x_3))-1+\beta V^{(l)}(x_1-x_3)]+\right\}... \end{aligned} \tag{2.14}$$

and so on. The result, presented above, can be obtained by means of slightly formal calculations, based on generalized functions and operator theories [13, 4]. Really, as $\hbar\to 0$ one has that

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

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 (1.7) and (2.1) for the N.N. Bogoliubov type generating functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, satisfying the functional equation (1.9) of Proposition (1.1).

## 3 A diagrammatic structure of functional-analytic solutions to the Bogolubof functional equation

Having considered (2.1) and (2.7) as starting expressions with just known functions $g_n(x_1, x_2, ...x_n)$, $n \in \mathbb{Z}_+$, for the functional

$\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, one can obtain the following expansion:

$$
\begin{aligned}
&\mathcal{L}(f) = Z(f)/Z(0),\\
&Z(f) = \exp[-\beta V^{(s)}(\delta)]\mathcal{L}^{(l)}(f) =\\
&= \exp[-\beta V^{(s)}(\delta)] \exp\left[\sum_{n=1}^{\infty}\frac{z^n}{n!}\int_{\mathbb{R}^3} d^3x_1 \int_{\mathbb{R}^3} d^3x_2 ... \int_{\mathbb{R}^3} d^3x_n \times\right.\\
&\left.\times \prod_{j=1}^{n}\{\exp[if(x_j)]-1\}g_n(x_1,x_2,...,x_n)\right] = \qquad (3.1)\\
&= \exp\left[\sum_{N=1}^{\infty}\frac{1}{N!}W(G_N^{(c)})\right],
\end{aligned}
$$

where functionals $W(G_N^{(c)})$, $N=\overline{1,\infty}$, are calculated via the following rule. Denote by $G_N^{(c)}$, $N=\overline{1,\infty}$, such a connected graph that: it 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. Moreover, each vertex $[y(n)]$ is necessary connected with $n$ vertices of type $[\alpha]$ by means of dashed lines each to other, and $[\alpha]$ vertices can be connected arbitrarily by means of uniform lines. If now to attribute to each generalized $[\gamma(n)]-$vertex - the factor $g_n(x_1,x_2,...x_n)$, to each simple $[\alpha]-$vertex - the factor $z\int_{\mathbb{R}^3} d^3x\exp[if(x)]$, and to the line connecting them - the factor $\{exp[-\beta V^{(s)}(x_{l_1}-x_{l_2})]-1\}$, 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 rise to the expression (2.15), where the factor $1/N!$ counts the symmetry order of the graph $G_N^{(c)}$ under the generalized vertices permutations. It is evident, that by representing the factor $\exp[if(x)]$, entering the vertex $[\alpha]$, as $\{\exp[if(x)]-1\}+1$, the expression (2.15) can easily be resumed into Ursell-Mayer type expressions but already with suitably other $g_n-$functions, replacing the former ones, giving rise to expansions similar to (2.14), based already on the "screened" potential (2.13).

Thereby we can formulate, taking into account the results of [4, 9], the next proposition, characterizing the Bogoliubov type generating functional $\mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, satisfying the functional equation (1.9).

**Proposition 3.1.** *Let the Bogoliubov 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 Bogoliubov 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:$\frac{1}{i}\frac{\delta\mathcal{L}(f)}{\delta f(x)}|_{f=0} = \bar{\rho} \in \mathbb{R}_+$.*

*Then the functional (3.1) solves the Bogoliubov type functional equation (1.9), allowing the positive measure $d\bar{\mu}$, whose Fourier representation on the adjoint tempered generalized functions space $\mathcal{S}'(\mathbb{R}^3;\mathbb{R})$ is exactly*

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

*where $(\xi, f) := \int\limits_{\mathbb{R}^3} d^3x\xi(x)f(x)$ 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 to constructing different thermodynamic functions important [2, 7] for applications.

Below, following the Bogoliubov method [3], we obtain, based on the expression (2.3), the important Kirkwood-Saltzbourg-Simansic functional equation for the Bogoliubov 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 down 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 $x \in \mathbb{R}^3$, where $Z_N := \int\limits_{\mathbb{R}^{3N}} dx_1 dx_2 ... dx_N \exp(-\beta V_N)$, $N \in \mathbb{Z}_+$.

Since, by definition, $\lim_{N\to\infty} \mathcal{L}_{(N)}(f) = \mathcal{L}(f)$, $f \in \mathcal{S}(\mathbb{R}^3;\mathbb{R})$, $\lim_{N\to\infty} \frac{(N+1)Z_N}{Z_{N+1}} := z \in \mathbb{R}_+$, 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-Saltzburg-Symanzik functional equation, being very important for proving the Proposition (3.1) by means of the classical Leray-Schauder fixed point theorem [11, 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 Bogoliubov generating functional method in non-equilibrium statistical mechanics: the quantized Wigner transform

For the study of non-equilibrium properties of a many-particle classical statistical system it was proposed [4, 9] to use the quasi-classical quantized Wigner density operator

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

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

$$\mathbf{H} = \int\limits_{T^*(\mathbb{R}^3)} d^3p d^3x \frac{p^2}{2m} w(x;p) \tag{4.2}$$

$$+ \int\limits_{T^*(\mathbb{R}^3)} d^3p d^3x \int\limits_{T^*(\mathbb{R}^3)} d^3\xi d^3y V(x-y) : w(x;p) w(y;\xi) :,$$

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

$$
\begin{aligned}
&\left[\int_{\mathbb{R}^3} d^3x\psi^+(x)\nabla_x^2\psi(x), w(z;\vartheta)\right] \overset{\hbar\to 0}{\simeq} \\
&\frac{\hbar}{i}\left\{\frac{\vartheta^2}{2m}, w(z;\vartheta)\right\}, \\
&\left[\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y V(x-y) : \rho(x)\rho(y) :, w(z;\vartheta)\right] \overset{\hbar\to 0}{\simeq} \\
&\frac{2\hbar}{i}\int_{\mathbb{R}^3} d^3y \left\{V(z-y), : \rho(y)w(z;\vartheta) :\right\}, \\
&w(x;p)w(y,\xi) \overset{\hbar\to 0}{\simeq} \\
&: w(x;p)w(y,\xi) : + w(x;p)\delta(x-y)\delta(p-\xi),
\end{aligned} \tag{4.3}
$$

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 Bogoliubov ideas, we will define a Bogoliubov generating functional $\mathcal{L}(f),\ f \in \mathcal{S}(T(\mathbb{R}^3);\mathbb{R})$, as

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

where, by definition, $(w,f) := \int\limits_{T(\mathbb{R}^3)} d^3xd^3pw(x;p)f(x;p)$ and $\mathcal{P} : \mathbf{\Phi} \to \mathbf{\Phi}$ is the statistical operator, satisfying the following [2, 3, 8, 4, 1] evolution equation with respect to the time variable $t \in \mathbb{R}_+$ :

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

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

$$
F_n(x_1, x_2, ..., x_n; p_1, p_2, ..., p_n|t),
$$

$n \in \mathbb{Z}_+$, the following expressions

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

hold as $\hbar \to 0$, where

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

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

To find the distribution functions (4.6) we will derive, following N.N. Bogoliubov [3, 2], the corresponding evolution functional equation on the N.N. Bogoliubov generating functional (4.4). Making use of the relationship (4.4), one easily obtains that

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

Now, based on relationships (4.3), we finally obtain the following

Bogoliubov type evolution functional equation:

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

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

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

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

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

$$\Phi(\delta) = \sum_{n\in\mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 ... \times$$
$$\times \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \Phi_n(x_1, x_2, ..., x_n; p_1, p_2, ..., p_n|t) \times$$
$$\times : \frac{1}{i}\frac{\delta}{\delta f(x_1;p_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2;p_2)} ... \frac{1}{i}\frac{\delta}{\delta f(x_n;p_n)} :, \tag{4.11}$$
$$\mathcal{L}_0(f) = \sum_{n\in\mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \times$$
$$\times \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \bar{F}_{\int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 ... n} \times$$
$$\times (x_1 - \frac{p_1}{m}t, x_2 - \frac{p_2}{m}t, ..., x_n - \frac{p_n}{m}t; p_1, p_2, ..., p_n) \times$$
$$\times \prod_{j=1}^{n} \{\exp[if(x_j;p_j)] - 1\},$$

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

$$\begin{aligned} &\bar{F}_n(x_1, x_2, ..., x_n; p_1, p_2, ..., p_n) := \\ &tr(\bar{\mathcal{P}} : w(x_1; p_1)w(x_2; p_2)...w(x_n; p_n) :) = \\ &: \frac{1}{i}\frac{\delta}{\delta f(x_1; p_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2; p_2)}...\frac{1}{i}\frac{\delta}{\delta f(x_n; p_n)} : \mathcal{L}(f)|_{t=0, f=0}, \end{aligned} \tag{4.12}$$

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

$$\begin{aligned} \log(\mathcal{P}_0^{-1}\mathcal{P}) &:= \sum_{n \in \mathbb{Z}_+} \frac{1}{n!} \int\limits_{T(\mathbb{R}^3)} d^3x_1 d^3p_1 \int\limits_{T(\mathbb{R}^3)} d^3x_2 d^3p_2 ... \times \\ &\times \int\limits_{T(\mathbb{R}^3)} d^3x_n d^3p_n \Phi_n(x_1, x_2, ..., x_n; p_1, p_2, ..., p_n|t) \times \\ &\times : w(x_1; p_1)w(x_2; p_2)...w(x_n; p_n) : \end{aligned} \tag{4.13}$$

with

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

being the statistical operator of the non-interacting particle system.

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

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

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

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

If the "chaotic" condition is not fulfilled, we can proceed to the usual cluster Ursell-Mayer type representation [9, 4] for the Bogoliubov generating functional (4.10), where

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

$$
\times \int_{T(\mathbb{R}^3)} d^3x_n d^3p_n \times \tag{4.17}
$$

$$
\times \bar{g}_n \ \ (x_1 - \frac{p_1}{m}t, x_2 - \frac{p_2}{m}t, ..., x_n - \frac{p_n}{m}t; p_1, p_2, ..., p_n) \times
$$

$$
\left. \times \prod_{j=1}^{n} \{\exp[if(x_j;p_j)] - 1\} \right),
$$

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

$$
\bar{g}_n(x_1, x_2, ..., x_n; p_1, p_2, ..., p_n) := \tag{4.18}
$$

$$
= \sum_{\sigma[n]} (-1)^{m+1}(m-1)! \prod_{j=1}^{m} \bar{F}_{\sigma[j]}((x_k; p_k) \in \sigma[j]),
$$

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

and $\sigma[n]$ denotes a partition of the set $\{1, 2, ..., n\}$ into non-intersecting 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,

$$
\begin{aligned}
\bar{g}_1(x_1; p_1) &= \bar{F}_1(x_1; p_1), \\
\bar{g}_2(x_1, x_2; p_1, p_2) &= \bar{F}_2(x_1, x_2; p_1, p_2) - \bar{F}_1(x_1; p_1)\bar{F}_1(x_2; p_2), ...,
\end{aligned} \tag{4.19}
$$

and so on. The N.N. Bogoliubov 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 definitely showed, that the Bogoliubov generating functional equations with the canonical Bogoliubov transformation method are very effective tools for studying distribution functions of both equilibrium and non equilibrium states of classical many-particle dynamical systems. In some cases the Bogoliubov generating functionals can be represented by means of infinite Ursell-Mayer diagram expansions, whose convergence holds under some additional constraints on a statistical system. We also have shown that the Bogoliubov idea [3, 1] to use the Wigner density operator transformation to study the non equilibrium distribution functions proved to be very effective, having proposed a new analytic form of non-stationary solutions to the classical Bogoliubov evolution functional equation.

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