MOLECULAR RANDOM WALKS AND INVARIANCE GROUP OF THE BOGOLYUBOV EQUATION

YURIY E. KUZOVLEV

Abstract. Statistics of molecular random walks in a fluid is considered with the help of the Bogolyubov equation for generating functional of distribution functions. An invariance group of solutions to this equation as functions of the fluid density is discovered. It results in many exact relations between probability distribution of the path of a test particle and its irreducible correlations with the fluid. As the consequence, significant restrictions do arise on possible shapes of the path distribution. In particular, the hypothetical Gaussian form of its long-range asymptotic proves to be forbidden (even in the Boltzmann-Grad limit). Instead, a diffusive asymptotic is allowed which possesses power-law long tail (cut off by ballistic flight length).

1. Introduction

Random wandering of particles of the matter is mechanism of diffusion and many other transport processes as well as the source of various noises and fluctuations. What kind of statistics can rule over it? This important question never was considered in the framework of rigorous statistical mechanics. It may seem that anyway the answer is obvious: if in the Lorentz gas statistics of random walks is asymptotically Gaussian \[1\] then all the more it must be Gaussian in usual gas. However, such a reasoning loses its convincingness when one notices that it indirectly equates (i) chaotic nature of random walk in the sense of Hamiltonian dynamics and (ii) randomness of the walk in the sense of the probability theory. The first, as is well known, is characterized by the “mixing” of the system’s phase trajectories \[2\], whereas the second by the “statistical independence” or simply “independence” \[3\] of their constituent parts. But already

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Krylov [2] thoroughly explained that generally the first does not imply the second. Therefore the question remains in force.

It can be comprehended by the example of $N$ hard balls in a box or on torus if treating their motion as the motion of single ball in $3N$-dimensional billiard [4] which is formed by $N(N-1)/2$ convex scatterers and resembles the Lorentz gas. How much far in time should be apart different fragments of the trajectory of this ball in order to behave as statistically independent one on another? It appears that not less than by the time necessary for the ball to know about existence of all the scatterers and thus about organization of the billiard. Let us express this characteristic time through the mean free-flight time in the original three-dimensional system, $\tau \sim (\pi r_0^2 \nu v_0)^{-1}$, where $r_0$ is diameter of the balls, $v_0$ is their typical velocity, $\nu = N/\Omega$ their mean concentration, and $\Omega$ is volume of the original system. Since the collision rate in the $3N$-dimensional billiard is equal to summary rate of collisions between arbitrary balls in the three-dimensional system, approximately $N/2\tau$, then the mentioned characteristic time can be estimated as $[N(N-1)/2]/[N/2\tau] \sim N\tau \sim \Omega/\pi r_0^2 v_0$. Even for 1 cm$^3$ of the air that is time on order of 1000 years!

If so, then ergodicity of behavior of $N$-particle system can be expected not sooner than after observing it during time intervals $\gg N\tau$. From the point of view of real physical many-particle systems (let even closed ones), that is quite inaccessible time. As to reality, only more or less peculiar parts of the system’s phase trajectory are observable. Thus, it was true remark [5] that the role of ergodicity in physics is strongly exaggerated since there the limit $N \to \infty$ precedes the limit $t/\tau \to \infty$.

Similar conclusions follow from the fact that the number of initial conditions what determine trajectory of a particle of usual gas is not 6, as in the case of Lorentz gas, but $6N$. Correspondingly, the trajectory can display enough its individuality (and be recognized) only after $N$ free flights and $N$ collisions, which requires time $\sim N\tau$. All
the more, to disclose its ergodic properties and observe how it divides into statistically independent parts we need in time scales $\gg N\tau$.

To speak more specifically, the non-ergodicity of a system of (infinitely) many particles does mean that rates of relaxation and fluctuation processes in it are different at different phase trajectories, as well as at diverse parts of one and the same trajectory [6]. For instance, individual diffusivity of a gas particle undergoes low-frequency fluctuations [7] which manifest themselves in a substantial difference of asymptotic probability distribution of the particle’s displacement from the Gaussian distribution.

The theoretical tools for rigorous investigations of such a statistics were developed by N. Bogolyubov [8] and his followers. That are the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equations and the equivalent Bogolyubov’s equation for generating functional of many-particle distribution functions. But nobody have learned how to use them avoiding truncations of the hierarchy on the hypothesis about some “obvious” “statistical independence” adopted from the probability theory. Hence, there is necessity of methods which can treat the basic equations respectfully.

The present work is just caused by such the necessity. Here, we will find and describe an invariance group of solutions to the Bogolyubov equation, as applied to the problem about statistics of random walk of test particle in thermodynamically equilibrium fluid. Then we will discuss consequences from exact relations of the group. In particular, demonstrate that they imply non-Gaussian character of long-range asymptotic of the random walk. Importantly, in case of gas this asymptotic, along with above mentioned characteristic time $\sim N\tau$, is insensible to gas density and stays strongly non-Gaussian even in the Boltzmann-Grad limit.
2. EQUATIONS OF MOLECULAR RANDOM WALK

Let a box with volume $\Omega$ contains $N \gg 1$ identical atoms plus one more test particle. Atoms have mass $m$, coordinates $r_j$ and momenta $p_j$ ($j = 1, 2 \ldots N$) and interact with each other via potential $\Phi_a(r_j - r_k)$. The test particle has mass $M$, coordinate $R$, momentum $P$ and interacts with atoms via potential $\Phi_b(r_j - R)$. The potentials are spherically symmetric and short-range with impenetrable point core. Because of interactions the test particle is in chaotic motion, therefore let us name it “molecular Brownian particle” (BP).

We are interested in probability distribution of current position of BP, $R(t)$, under condition that at initial time moment $t = 0$ it was placed at certainly known position: $R(0) = R_0$, while personal positions of atoms all the times are unknown. The simplest statistical ensemble what satisfies this requirement is determined by the Liouville equation, \[ \frac{\partial D_N}{\partial t} = [H_N, D_N], \] for full normalized distribution function of the system, $D_N$, and the initial condition to it,

$$D_N(t = 0) = \frac{\delta(R - R_0) e^{-H_N/T}}{\int dR \int dP \int_1^{n+1} ... \int_N \delta(R - R_0) e^{-H_N/T}} \tag{2.1}$$

where $H_N$ is full Hamiltonian of the system (including interactions with the box walls) and \[ \int_k ... = \int ... \int d\vec{r}_k d\vec{p}_k. \] Evidently, such the ensemble differs from the Gibbs canonic ensemble by the initial BP’s localization only. The latter does not prevent us to introduce the marginal distribution functions (DF) \[ F_n(t) = \Omega^n \int_{n+1}^{n,...} \int_D D_N(t) \] and then go to the thermodynamical limit $N \to \infty$, $\Omega \to \infty$, $\nu = N/\Omega = \text{const}$ in exact analogy with \[ S \]. If writing out all the arguments of DF, we have \[ F_n(t) = F_n(t, R, r^{(n)}, P, p^{(n)}| R_0; \nu) \], where \[ r^{(n)} = \{r_1, ... r_n \} \], \[ p^{(n)} = \{p_1, ... p_n \} \]. As in the Bogolyubov’s book, all DF are not normalized in respect to the atoms’ coordinates. Instead, they must obey the conditions of decoupling of inter-particle correlations under separation of particles (in essence, that are conditions of existence of thermodynamical
limit \([8, 9]\)). For our task, with taking into account complete symmetry of DF in respect to atoms, these conditions can be written as follows: \(F_n \rightarrow F_{n-1} G_m(p_n)\) at \(r_n \rightarrow \infty\), where \(G_m(p) = (2\pi T m)^{-3/2} \exp (-p^2 / 2T m)\) is the Maxwell momentum distribution of a particle with mass \(m\). The only, non-principal, difference from \([8]\) is that numeration of DF begins from zero, so that \(F_0(t, R, P | R_0; \nu)\) describes the state of BP, and in respect to BP’s coordinate all the DF are normalized. In particular, \(\int F_0 dR = G_M(P)\). The basic Liouville equation induces the BBGKY equations

\[
\frac{\partial F_n}{\partial t} = [H_n, F_n] + \nu \frac{\partial}{\partial P} \int_{n+1} \Phi'_b(R - r_{n+1}) F_{n+1} + \nu \sum_{j=1}^{n} \frac{\partial}{\partial p_j} \int_{n+1} \Phi'_a(r_j - r_{n+1}) F_{n+1} \tag{2.2}
\]

\((n = 0, 1, \ldots)\) with initial conditions

\[
F_n(t = 0) = \delta(R - R_0) F_n^{(eq)}(r^{(n)} | R; \nu) G_M(P) \prod_{j=1}^{n} G_m(p_j) , \tag{2.3}
\]

where \(H_n\) is Hamiltonian of subsystem “\(n\) atoms plus BP”, \(\Phi'_{a,b}(r) = \nabla \Phi_{a,b}(r)\), and \(F_n^{(eq)}(r^{(n)} | R; \nu)\) are usual thermodynamically equilibrium DF for \(n\) atoms in presence of BP occupying point \(R\).

In principle, all that will do for finding \(F_0(t, R, P | R_0; \nu)\) and thus probability distribution of BP’s path, \(\Delta R(t) = R(t) - R_0\), without any additional assumptions. At that, since our problem is expressed by the recurrent relations, it can be lighten, as usually, by use of generating functions. Such the approach to the BBGKY hierarchy was formulated and sampled already by Bogolyubov \([8]\). Here it will help us to visualize some properties of the hierarchy what are hardly seen directly from it. Following Bogolyubov, let us combine all DF into generating functional (GF)

\[
\mathcal{F}\{t, R, P, \psi | R_0; \nu\} = F_0 + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int_1^{\infty} \int \int F_n \prod_{j=1}^{n} \psi(r_j, p_j) \tag{2.4}
\]

and equations (2.2) into corresponding “generating equation” for it:

\[
\frac{\partial \mathcal{F}}{\partial t} + \frac{P}{M} \cdot \frac{\partial \mathcal{F}}{\partial R} = \mathcal{L}\left(\psi, \frac{\delta}{\delta \psi}\right) \mathcal{F} , \tag{2.5}
\]
where \( \hat{L} \) is operator composed of usual and variational derivatives,

\[
\hat{L} \left( \psi, \frac{\delta}{\delta \psi} \right) = -\int_1 \psi(x_1) \frac{p_1}{m} \cdot \frac{\partial}{\partial r_1} \frac{\delta}{\delta \psi(x_1)} + \\
+ \int_1 \left[ 1 + \psi(x_1) \right] \left[ \Phi_b(R - r_1), \frac{\delta}{\delta \psi(x_1)} \right] + \\
+ \frac{1}{2} \int_1 \int_2 \left[ 1 + \psi(x_1) \right] \left[ 1 + \psi(x_2) \right] \left[ \Phi_a(r_1 - r_2), \frac{\delta^2}{\delta \psi(x_1) \delta \psi(x_2)} \right],
\]

with \( x_j = \{r_j, p_j\} \). This is direct analogue of equation (7.9) from [8]. To make this evident, notice that \( \psi(x) = u(x)/\nu \), where \( u(x) \) is functional argument used in [8], and factor \( [1 + \psi(x_1)][1 + \psi(x_2)] \) can be replaced by \( [\psi(x_1) + \psi(x_2) + \psi(x_1)\psi(x_2)] \) due to the identity \( \int_1 \int_2 [\Phi_a(r_1 - r_2), \ldots] = 0 \).

Let us formulate the initial condition to equation (2.5). For that, it is convenient to introduce the generating functional of equilibrium DF in the configuration space,

\[
F^{(eq)}\{\phi|R; \nu\} = 1 + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int \ldots \int F_n^{(eq)}(r^{(n)}|R; \nu) \prod_{j=1}^n \phi(r_j) \, dr_j,
\]

where \( \phi(r) \) is corresponding functional variable. Besides, introduce linear mapping \( \phi\{\psi\} \) of functions \( \psi(r, p) \) to functions \( \phi(r) \) as follows:

\[
\phi\{\psi\}(r) = \int \psi(r, p) G_m(p) \, dp
\]

Then the initial conditions (2.3) do intend

\[
F\{0, R, P, \psi|R_0; \nu\} = \delta(R - R_0) G_M(P) F^{(eq)}\{\phi\{\psi\}|R; \nu\}
\]

It is easy to guess or verify that expression \( G_M(P) F^{(eq)}\{\phi\{\psi\}|R; \nu\} \) represents the stationary solution of equation (2.5), so that

\[
\left[ -(P/M) \cdot \partial / \partial R + \hat{L} \right] G_M(P) F^{(eq)}\{\phi\{\psi\}|R; \nu} = 0
\]

This equality yields

\[
\left[ \frac{\partial}{\partial r} + \frac{\Phi'_b(r - R)}{T} \right] \frac{\delta F^{(eq)}}{\delta \phi(r)} = \frac{1}{T} \int [1 + \phi(r')] \Phi'_a(r' - r) \frac{\delta^2 F^{(eq)}}{\delta \phi(r) \delta \phi(r')} \, dr',
\]
where, similarly to (2.7), \( \phi(r) \) appears as independent functional variable in the configuration space. The latter equation determines all the equilibrium DF and is analogue of equation (2.14) from [8].

Unfortunately, to the best of my knowledge, non-stationary solutions to equations like (2.5) above or (7.9) in [8] never were investigated by Bogolyubov or others. However, the experience of work with the BBGKY equations prompts (see e.g. [10]) the desirability of a change of variables, i.e. transition from DF to another functions which help to concentrate on inter-particle correlations and statistical dependencies. To make a suitable choice of such functions, let us discuss hypothetical equalities

\[
F_n(t, R, r^{(n)}, P, p^{(n)}| R_0; \nu) \overset{?}= F_0(t, R, P| R_0; \nu) F^{(eq)}(r^{(n)}| R; \nu) \prod_{j=1}^{n} G_m(p_j)
\]

or, equivalently,

\[
\mathcal{F}\{t, R, P, \psi| R_0; \nu\} \overset{?}= F_0(t, R, P| R_0; \nu) \mathcal{F}^{(eq)}\{\phi(\psi)| R; \nu\}.
\]

They state, evidently, that the conditional DF (conditional probability distributions) of atoms, i.e. \( F_n/F_0 \), do not depend on the past BP’s displacement \( R - R_0 \). This assumption seems natural as concerns thermodynamically equilibrium random walk when all possible positions of BP are equivalent. Nevertheless, this is certainly wrong assumption, since it is incompatible with the equations (2.2). Indeed, the substitution of \( F_1 \) in the first equation (for \( F_0 \)) by \( F_0(t, R, P| R_0; \nu) F^{(eq)}(r_1| R; \nu) G_m(p_1) \) turns the integral of BP’s interaction with atoms into zero:

\[
\int \Phi'_b(R - r_1) F_1 = 0 \quad \text{(at least because \( F^{(eq)}(r_1| R; \nu) \) is even function of the difference \( r_1 - R \) while \( \Phi'_b(R - r_1) \) is its odd function).}
\]

As the result, the first of equations (2.2) reduces to the equation of free BP’s flight, \( \partial F_0/\partial t = [H_0, F_0] \), as if BP does not interact with atoms at all.

The aforesaid implies that, first, the current state of the medium (system of atoms) is statistically dependent on the summary displacement of BP \( \Delta R(t) = R(t) - R_0 \) during all time of its observation. In other words, some essential and quantitatively significant correlations between the medium and the history of BP’s wandering are in existence.
We will name them “historical correlations”, in order to ideally separate them from the equilibrium correlations, as described by \( F_n^{(eq)}(r^{(n)}|R; \nu) \), between current coordinates of BP and atoms. Second, to perform an adequate formal separation of the two sorts of BP-atoms correlations, we can describe the historical correlations with functions \( V_n = V_n(t, R, r^{(n)}, P, p^{(n)}|R_0; \nu) \) defined by the generating relations as follow:

\[
\mathcal{F}\{t, R, P, \psi | R_0; \nu\} = \mathcal{V}\{t, R, P, \psi | R_0; \nu\} \mathcal{F}^{(eq)}\{\phi\{\psi\} | R; \nu\}, \tag{2.11}
\]

\[
\mathcal{V}\{t, R, P, \psi | R_0; \nu\} = V_0 + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int \cdots \int V_n \prod_{j=1}^{n} \psi(r_j, p_j) \]

In particular, \( V_0(t, R, P | R_0; \nu) = F_0(t, R, P | R_0; \nu) \) and

\[
F_1(t, R, r_1, P, p_1 | R_0; \nu) = F_0(t, R, P | R_0; \nu) F_1^{(eq)}(r_1 | R; \nu) G_m(p_1) + V_1(t, R, r_1, P, p_1 | R_0; \nu) \tag{2.12}
\]

It is clear from this definition that from the viewpoint of the probability theory the functions \( V_n \ (n > 0) \) represent a kind of cumulant functions (cumulants, or semi-invariants). Therefore we will name them “cumulant functions”. Notice that in physical literature (see e.g. [10]) similar objects frequently are called “correlation functions”.

In terms of the cumulant functions (CF) initial conditions \( (2.3) \) and \( (2.9) \) become strongly simplified:

\[
V_0(0, R, P | R_0; \nu) = \delta(R - R_0) G_M(P),
\]

\[
V_n(0, R, r^{(n)}, P, p^{(n)} | R_0; \nu) = 0 \ (n > 0),
\]

\[
\mathcal{V}\{0, R, P, \psi | R_0; \nu\} = \delta(R - R_0) G_M(P) \tag{2.13}
\]

The conditions of the decoupling of correlations at infinity also become simpler:

\[
V_n(t, R, r^{(n)}, P, p^{(n)} | R_0; \nu) \rightarrow 0 \text{ at } r_k \rightarrow \infty \tag{2.14}
\]

\((1 \leq k \leq n)\), that is CF tend to zero if at least one \( n \) atoms moves away from BP to infinity. In opposite, the generating equation \( (2.5) \) in terms of CF becomes more
complicated. Inserting (2.11) into (2.5) one can obtain
\[
\frac{\partial V}{\partial t} + \frac{P}{M} \cdot \frac{\partial V}{\partial R} = \tilde{L} \left( \psi, \frac{\delta}{\delta \psi} \right) V + \tilde{L}' \left( \nu, \psi, \frac{\delta}{\delta \psi} \right) V ,
\]  
(2.15)

where the new operator appears,
\[
\tilde{L}' \left( \nu, \psi, \frac{\delta}{\delta \psi} \right) = \left\{ \int \left[ 1 + \phi(r) \right] \Phi'_b(R - r) \nu C \{ r, \phi | R \} \, dr \right\} \left( \frac{P}{MT} + \frac{\partial}{\partial P} \right) + \int_{1}^{2} \left[ 1 + \psi(x_1) \right] \left[ 1 + \psi(x_2) \right] \left[ \Phi_a(r_1 - r_2) \nu C \{ r_2, \phi | R \} G_m(p_2) \frac{\delta}{\delta \psi(x_1)} \right]
\]

Here \( \phi(r) \) and \( \phi \) are mentioned as linear functionals of \( \psi(r, p) \) in the sense of the mapping \( \phi \{ \psi \}(r) \) defined by (2.8), and besides one more functional is introduced,
\[
C \{ r, \phi | R ; \nu \} = \frac{\delta \ln \mathcal{F}(eq) \{ \phi | R ; \nu \}}{\nu \delta \phi(r)}
\]  
(2.16)

Correspondingly, the BBGKY equations become more complicated. Therefore, here we write out them only for extreme but principally interest case of “BP in ideal gas” (when atoms do not interact with each other, i.e. \( \Phi_a(r) = 0 \) ). In this case,
\[
\frac{\partial V_0}{\partial t} = -\frac{P}{M} \cdot \frac{\partial V_0}{\partial R} + \nu \frac{\partial}{\partial P} \int_1 \Phi'_b(R - r_1) V_1 ,
\]
\[
\frac{\partial V_n}{\partial t} = [ H_n , V_n ] + \nu \frac{\partial}{\partial P} \int_{n+1} \Phi'_b(R - r_{n+1}) V_{n+1} + \]
\[
+ T \sum_{j=1}^{n} \mathcal{P}(j , n) \ G_m(p_n) \ E'(r_n - R) \left( \frac{P}{MT} + \frac{\partial}{\partial P} \right) V_{n-1} \quad (n > 0) ,
\]

where \( H_n = P^2/2M + \sum_{j=1}^{n} \left[ \frac{P_j^2}{2m} + \Phi_b(R - r_j) \right] , \ E(r) = \exp \left[ - \Phi(r) / T \right] , \ E'(r) = \nabla E(r) = - \Phi'(r) E(r) / T , \) and \( \mathcal{P}(j, n) \) denotes operation of transposition of arguments \( x_j = \{ r_j , p_j \} \) and \( x_n = \{ r_n , p_n \} \). Thus, the natively bidiagonal BBGKY hierarchy if being represented via CF becomes at least tridiagonal.
3. INVARIANCE GROUP OF THE EQUILIBRIUM GENERATING FUNCTIONAL

Further, let us consider the functional (2.16), which is interesting already because it enters the generating evolution equation (2.15), and expand it into a series:

\[ C\{\mathbf{r}, \phi \mid \mathbf{R}; \nu \} = F_1^{(eq)}(\mathbf{r} \mid \mathbf{R}; \nu) + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int \cdots \int C_{n+1}(\mathbf{r}, \mathbf{r}_1 \ldots \mathbf{r}_n \mid \mathbf{R}; \nu) \prod_{j=1}^{n} \phi(\mathbf{r}_j) \, d\mathbf{r}_j \quad (3.1) \]

According to (2.7), this expansion just defines the functions \( C_n(\mathbf{r}_1 \ldots \mathbf{r}_n \mid \mathbf{R}; \nu) \) \( (n > 1) \).

In particular,

\[ C_2(\mathbf{r}, \mathbf{r}_1 \mid \mathbf{R}; \nu) = F_2^{(eq)}(\mathbf{r}, \mathbf{r}_1 \mid \mathbf{R}; \nu) - F_1^{(eq)}(\mathbf{r} \mid \mathbf{R}; \nu) F_1^{(eq)}(\mathbf{r}_1 \mid \mathbf{R}; \nu), \]
\[ C_3(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) = F_3^{(eq)}(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) + 2 F_1^{(eq)}(\mathbf{r}) F_1^{(eq)}(\mathbf{r}_1) F_1^{(eq)}(\mathbf{r}_2) - F_1^{(eq)}(\mathbf{r}) F_2^{(eq)}(\mathbf{r}_1, \mathbf{r}_2) - F_1^{(eq)}(\mathbf{r}_1) F_1^{(eq)}(\mathbf{r}_2) - F_1^{(eq)}(\mathbf{r}_2) F_2^{(eq)}(\mathbf{r}, \mathbf{r}_1), \]

(for brevity in the second expression arguments \( \mathbf{R} \) and \( \nu \) are omitted). Clearly, from the viewpoint of the atoms’ coordinates, the functions \( C_n \) relate to the equilibrium DF \( F_n^{(eq)} \) like cumulants of a random field relate to its statistical moments.

The conditions of vanishing of inter-particle correlations at infinity mean that all these cumulants tend to zero if at least one atom is moved away from the others:

\[ C_n(\mathbf{r}_1 \ldots \mathbf{r}_n \mid \mathbf{R}; \nu) \to 0 \quad \text{at} \quad \mathbf{r}_j \to \infty \quad (3.2) \]

In case of mowing away BP from atoms we have:

\[ F_1^{(eq)}(\mathbf{r} \mid \mathbf{R}; \nu) \to 1 \quad \text{at} \quad \mathbf{R} \to \infty, \]
\[ C_n(\mathbf{r}_1 \ldots \mathbf{r}_n \mid \mathbf{R}; \nu) \to C_n(\mathbf{r}_1 \ldots \mathbf{r}_n; \nu) \quad \text{at} \quad \mathbf{R} \to \infty, \quad (3.3) \]

where \( C_n(\mathbf{r}_1 \ldots \mathbf{r}_n; \nu) \) are cumulant functions of equilibrium media taken in absence of BP. Moreover, under sufficiently short-range interaction potentials, all the limit transitions in (3.2)-(3.3) are absolutely integrable, which will be assumed below.

Next, consider equation (2.10) rewriting it in the form

\[ \left[ \frac{\partial}{\partial \mathbf{r}} + \frac{\Phi'(\mathbf{r} - \mathbf{R})}{T} \right] C\{\mathbf{r}, \phi \mid \mathbf{R}; \nu \} = \frac{1}{T} \int [1 + \phi(\mathbf{r}')] \Phi'_n(\mathbf{r}' - \mathbf{r}) \frac{\delta C\{\mathbf{r}', \phi \mid \mathbf{R}; \nu \}}{\delta \phi(\mathbf{r})} \, d\mathbf{r}' + \]
\[ + \frac{\nu}{T} \int [1 + \phi(\mathbf{r}')] \Phi'_n(\mathbf{r}' - \mathbf{r}) C\{\mathbf{r}', \phi \mid \mathbf{R}; \nu \} \, d\mathbf{r}', \quad (3.4) \]
and with its help let us ascertain (probably, for the first time) some important properties of the functional $C\{r, \phi | R; \nu \}$. Notice, first, that integrability of the asymptotic (3.2) makes it possible to extend this functional to bounded functions $\phi(r)$ which do not tend to zero at infinity, in particular, to constants. This fact allows to introduce such the objects as follow:

$$C(\sigma, \nu) = \lim_{\phi(r) \to \sigma, R \to \infty} C\{r, \phi | R; \nu \} = 1 + \sum_{n=1}^{\infty} \frac{\nu^n \sigma^n}{n!} \int_{1}^{\infty} \cdots \int_{1}^{\infty} C_{n+1}(r, r_1, \ldots, r_n; \nu) ,$$

$$C_{\sigma}\{r, \phi | R; \nu \} = \frac{C\{r, \sigma + \phi | R; \nu \}}{C(\sigma, \nu)} ,$$

where $\sigma = \text{const}$, $\int_{n}^{\infty} = \int \ldots \int dr_n$, and integrals in (3.5) are practically independent on $r$. Second, after the change $\phi(r) \to \sigma + \phi(r)$ the equation (3.4) can be transformed, through elementary algebraic manipulations, into equation for $C_{\sigma}\{r, \phi | R; \nu \}$:

$$\left[ \frac{\partial}{\partial r} + \frac{\Phi_b'(r - R)}{T} \right] C_{\sigma}\{r, \phi | R; \nu \} = \frac{1}{T} \int \left[ 1 + \frac{\phi(r')}{1 + \sigma} \right] \Phi_a'(r' - r) \frac{\delta C_{\sigma}\{r', \phi | R; \nu \}}{\delta [\phi(r)/(1 + \sigma)]} dr' +$$

$$+ C_{\sigma}\{r, \phi | R; \nu \} \frac{\nu C(\sigma, \nu)(1 + \sigma)}{T} \int \left[ 1 + \frac{\phi(r')}{1 + \sigma} \right] \Phi_a'(r' - r) C_{\sigma}\{r', \phi | R; \nu \} dr' \quad (3.7)$$

It is easy to see that its only difference from (3.4) is the scale transformation of the functional argument, $\phi(r) \to \phi(r)/(1 + \sigma)$, and besides transformation of the density argument $\nu$ into

$$\nu(\sigma, \nu) = \nu C(\sigma, \nu)(1 + \sigma) \quad (3.8)$$

Third, formal solution of equation (3.4) in the form of the series (3.1) is unambiguously determined by the conditions of decoupling of correlations (3.2)-(3.3). Fourth, by the definition (3.5)-(3.6) of functional $C_{\sigma}\{r, \phi | R; \nu \}$, the coefficients in its similar series expansion in terms of $\phi(r)$ satisfy the same conditions. To be exact, from (3.2)-(3.3)
it follows that
\[
C_n(r_1 \ldots r_n| R; \nu) + \sum_{k=1}^{\infty} \frac{\nu^k \sigma^k}{k!} \int_{n+1}^{\infty} \int_{n+k}^{\infty} C_{n+k}(r_1 \ldots r_{n+k}| R; \nu) \to 0 \quad \text{at} \quad r_j \to \infty ,
\]
\[
\frac{1}{C(\sigma, \nu)} \left[ F_1^{(\text{eq})}(r| R; \nu) + \sum_{k=1}^{\infty} \frac{\nu^k \sigma^k}{k!} \int_{1}^{\infty} \int_{1}^{\infty} C_{k+1}(r, r_1 \ldots r_k| R; \nu) \right] \to 1 \quad \text{at} \quad R \to \infty ,
\]
where \(1 \leq j \leq n\). At least, if we interpret the transitions (3.2)-(3.3) in the sense of absolute integrability and speak about not too large density values (useful information in this respect can be found in [9]).

Summarizing all the aforesaid, we can conclude that the solution to equation (3.7) is nothing but \(C_{\sigma}\{r, \phi| R; \nu\} = C\{r, \phi/(1 + \sigma)| R; \nu(\sigma, \nu)\}\). Combining this result with (3.6) and (3.8), we see that for arbitrary, in definite sense (see below), constant \(\sigma\) and bounded function \(\phi = \phi(r)\) the equality
\[
\nu C\{r, \sigma + \phi| R; \nu\} = \frac{\nu(\sigma, \nu)}{1 + \sigma} C\left\{r, \frac{\phi}{1 + \sigma}| R; \nu(\sigma, \nu)\right\}
\]
takes place. It can be rewritten also as
\[
\hat{T}(\sigma) C\{r, \phi| R; \nu\} = \frac{\nu(\sigma, \nu)}{(1 + \sigma) \nu} C\left\{r, \frac{1 + \phi}{1 + \sigma} - 1| R; \nu(\sigma, \nu)\right\} = C\{r, \phi| R; \nu\}
\]
(3.10)
The left equality here defines the one-parametric family of such transformations of the functional \(C\{r, \phi| R; \nu\}\) which, according to the right-hand equality, conserve its value. One can easy verify that this family is the Abelian group with composition rules
\[
\hat{T}(\sigma_2) \hat{T}(\sigma_1) = \hat{T}(\sigma_1 + \sigma_2 + \sigma_1 \sigma_2) ,
\]
\[
\nu(\sigma_2, \nu(\sigma_1, \nu)) = \nu(\sigma_1 + \sigma_2 + \sigma_1 \sigma_2, \nu)
\]
(3.11)
and with restrictions \(\sigma > -1\), \(\phi(r) > -1\). The latter are clear in view of the fact that functional \(\nu[1 + \phi(r)] C\{r, \phi| R; \nu\}\) represents mean concentration of atoms in presence of an external potential \(U(r)\) related to \(\phi(r)\) via \(\phi(r) = \exp[-U(r)/T] - 1\).
The substitution $\sigma = \exp(a) - 1$ yields $\hat{T}(a_2) \hat{T}(a_1) = \hat{T}(a_1 + a_2)$ and eliminates the restrictions.

The infinitesimal equivalent of the equalities (3.9) or (3.10) looks most convenient when expressed via particular CF:

$$\{ \kappa(\nu) + [1 + \kappa(\nu)] \nu \frac{\partial}{\partial \nu} \} F_1^{eq}(r|\mathbf{R};\nu) = \nu \int C_2(r, r'|\mathbf{R};\nu) \, dr' ,$$

$$\{ n\kappa(\nu) + [1 + \kappa(\nu)] \nu \frac{\partial}{\partial \nu} \} C_n(r_1...r_n|\mathbf{R};\nu) = \nu \int C_{n+1}(r_1...r_n, r'|\mathbf{R};\nu) \, dr' ,$$

$$\kappa(\nu) = \left[ \frac{\partial C(\sigma, \nu)}{\partial \sigma} \right]_{\sigma=0} = \nu \int C_2(r, 0; \nu) \, dr$$

The function $\kappa(\nu)$ defined just now is known (see e.g. [12]) to be directly concerning the state equation of the system: $1 + \kappa(\nu) = T(\partial\nu/\partial P)_T$, where $P$ denotes the pressure. Notice that in the framework of the grand canonical ensemble very similar relations can be easy derived by differentiation of DF in respect to the activity.

4. INVARIANCE GROUP OF THE GENERATING FUNCTIONAL OF HISTORICAL CORRELATIONS

We have approached to the substantiation of main results of the present work. Let us show that solution of the evolution equation (2.15) possesses invariance properties similar to (3.10). Since the initial condition to (2.15) (see (2.13)) does not depend on the variables $\psi = \psi(r, p)$ and $\nu$ at all, the solution to (2.15) is completely determined by the structure of operators $\hat{L}$ and $\hat{L}'$ and the conditions at infinity (2.14). The latter allow to extend the functional $\mathcal{V}\{t, \mathbf{R}, P, \psi|R_0;\nu\}$ (like the functional $\mathcal{C}$ before) to arguments $\sigma+\psi(r, p)$, with $\sigma = \text{const}$, in place of $\psi(r, p)$. The fact that the limit in (2.14) is achieved rapidly enough to indeed ensure this extension will become clear afterwards, from the relations (4.7) which will be obtained in this section. Next, thanks to (2.14) and besides to the definition (2.6) of operator $\hat{L}$, the variable $\psi(x_1)$ in the
first term of the expression \( \hat{L} V \) can be shifted by arbitrary constant:

\[
\int_1 \psi(x_1) \frac{p_1}{m} \frac{\partial}{\partial r_1} \frac{\delta V}{\delta \psi(x_1)} = \int_1 [a + \psi(x_1)] \frac{p_1}{m} \frac{\partial}{\partial r_1} \frac{\delta V}{\delta \psi(x_1)},
\]

where \( a = \text{const} \), for instance, \( a = 1 \). That is important difference of \( \hat{L} V \) from \( \hat{L} F \). Consequently, taking in mind the action of \( \hat{L} \) onto \( V \), one can write

\[
\hat{L} \left( \sigma + \psi, \delta \frac{\delta}{\delta \psi} \right) = \hat{L} \left( \frac{\psi}{1 + \sigma}, \delta \frac{\delta}{\delta \psi/(1 + \sigma)} \right) \quad (4.1)
\]

At last, let us look at the operator \( \hat{L}' \) (the formula next to (2.15)). In contrast to \( \hat{L} \), it depends on the density \( \nu \). Nevertheless, with the help of equality (3.9) it is easy to make sure that it obeys a relation like (4.1) if the transformation of argument \( \psi(r, p) \) is accompanied by transformation of argument \( \nu \) in accordance with (3.8):

\[
\hat{L}' \left( \nu, \sigma + \psi, \delta \frac{\delta}{\delta \psi} \right) = \hat{L}' \left( \nu(\sigma, \nu), \frac{\psi}{1 + \sigma}, \delta \frac{\delta}{\delta \psi/(1 + \sigma)} \right) \quad (4.2)
\]

The combination of all these observations implies the invariance property

\[
V\{t, R, P, \sigma + \psi | R_0; \nu\} = V\left\{t, R, P, \frac{\psi}{1 + \sigma} | R_0; \nu(\sigma, \nu)\right\} \quad (4.3)
\]

or, equivalently and similarly to (3.10),

\[
\tilde{T}(\sigma) V\{t, R, P, \psi | R_0; \nu\} \equiv V\{t, R, P, \frac{1 + \psi}{1 + \sigma} - 1 | R_0; \nu(\sigma, \nu)\} = \quad (4.4)
\]

where the left equality, together with (3.5), (3.8), (3.10) and (3.11), defines action of the above characterized group of transformations onto functional \( V\{t, R, P, \psi | R_0; \nu\} \). Apparently, in respect to this functional that are such the transformations of its arguments which do not change its value. The expansion of the equality (4.3) into series in
terms of $\psi$ yields

$$V_0(t, R, P|R_0; \nu(\sigma, \nu)) = V_0(t, R, P|R_0; \nu) +$$

$$+ \sum_{n=1}^{\infty} \frac{\nu^n \sigma^n}{n!} \int_1^{\infty} \ldots \int_n V_n(t, R, r^{(n)}, P, p^{(n)}|R_0; \nu) ,$$

$$\int \frac{v(\sigma, \nu)}{(1 + \sigma)\nu}^k V_k(t, R, r^{(k)}, P, p^{(k)}|R_0; \nu(\sigma, \nu)) = V_k(t, R, r^{(k)}, P, p^{(k)}|R_0; \nu) +$$

$$+ \sum_{n=1}^{\infty} \frac{\nu^n \sigma^n}{n!} \int_{k+1}^{\infty} \ldots \int_{k+n} V_{k+n}(t, R, r^{(k+n)}, P, p^{(k+n)}|R_0; \nu)$$

(4.6)

Corresponding infinitesimal (in respect to $\sigma$) relations are similar to (3.12):

$$\left\{ n \zeta(\nu) + [1 + \zeta(\nu)] \nu \frac{\partial}{\partial \nu} \right\} V_n(t, R, r^{(n)}, P, p^{(n)}|R_0; \nu) =$$

$$= \nu \int_{n+1}^{\infty} V_{n+1}(t, R, r^{(n+1)}, P, p^{(n+1)}|R_0; \nu),$$

(4.7)

Formulas (4.5) and (4.6) can be interpreted as “virial expansions” of the probabilistic law of BP’s random wandering and statistical correlations between BP and medium, with those difference from the usual virial expansions of thermodynamic quantities [12] or kinetic coefficients [13] that here some decrements of the density do appear instead of its full value. However, in the limit when $\nu \to 0$ and $\sigma \to \infty$ with $\nu \sigma = \text{const}$ our relations take quite usual form. For instance, (4.5) transforms into

$$V_0(t, R, P|R_0; \nu(\nu)) = V_0(t, R, P|R_0; 0) + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int_1^{\infty} \ldots \int_n C_{n+1}(r, r_1 \ldots r_n|0) ,$$

(4.8)

$$v(\nu) \equiv \nu \left[ 1 + \sum_{n=1}^{\infty} \frac{\nu^n}{n!} \int_1^{\infty} \ldots \int_n C_{n+1}(r, r_1 \ldots r_n|0) \right],$$

where $\int$ in the first row means integration over all the atoms’ variables. It should be noted that formula (4.5) was obtained earlier in [11, 14, 15] on the base of the “generalized fluctuation-dissipation relations” [16, 17]. Up to that time, as far as I know, such kind of exact relations was not in use in statistical physics. It would be rather hard to extract them directly from the BBGKY hierarchy (2.2) or equivalent equations for CF. The only exclusion is the special case of BP in ideal gas [18, 19], when
\[ C_n = 0 \], and readers of this paper can easily derive relations (4.7) (with \( \kappa(\nu) = 0 \)) by means of differentiation of equations (2.17) in respect to gas density.

5. ON PRINCIPAL CONSEQUENCES FROM THE INVARIANCE RELATIONS

An exact solution of the BBGKY hierarchy automatically satisfies all the exact “virial expansions” (4.5)-(4.8) resulting from the above-stated invariance group. Moreover, expansion (4.8) itself gives explicit formal solution to the BBGKY hierarchy (since at \( \nu = 0 \) the corresponding equations for CF can be solved by means of direct successive quadratures, like equations (2.17) at \( \nu = 0 \)). Therefore it is natural to apply our above results to “testing of statistical hypotheses” about the BP’s wandering.

In this respect it is important to emphasize that formulas (4.5)-(4.6) interconnect two different random walks in two media with arbitrarily assigned densities ratio, \( \nu(\sigma, \nu)/\nu \). Consequently, all the terms in series (4.5) or (4.6), as well as in (4.8), are equally necessary for correct summation of the series, and its truncation would produce not an approximative but wrong result. Even in the “dilute gas limit” (when gas parameters tend to zero, \( 4\pi r^3 a/3 \rightarrow 0 \), \( 4\pi r^3 b/3 \rightarrow 0 \) with \( r_{a, b} \) being characteristic radii if atom-atom and BP-atom interactions) or in the so called “Boltzmann-Grad limit” (when simultaneously the mean free paths, \( \Lambda_b = (\pi r^2 b\nu)^{-1} \) and \( \Lambda_a = (\pi r^2 a\nu)^{-1} \), are fixed), as well as in the case of ideal gas (when \( \Lambda_a = \infty \) but \( \Lambda_b \) is finite). In all these cases, formulas (4.5)-(4.7) reduce to

\[
\frac{\partial^k V_n(t, R, r^{(n)}, P, p^{(n)}|R_0; \nu)}{\partial \nu^k} = \int_{n+1} \cdots \int_{n+k} V_{n+k}(t, R, r^{(n+k)}, P, p^{(n+k)}|R_0; \nu), \quad (5.1)
\]

thus making it quite obvious that from the point of view of rigorous theory all the historical correlations are equally substantial.

Meanwhile, it is the convention in physical literature to reject third- and higher-order inter-particle correlations when deriving closed equations (kinetic equations) for one-particle DF (for examples, see [8, 10, 13, 20]). Sometimes, as in the case of hard sphere
gas \cite{20,21}, these correlations get lost even insensibly for authors (see \cite{18} about that).

By the widely accepted opinion, under the Boltzmann-Grad limit the theory based on the BBGKY hierarchy should reduce to the classical kinetic theory of gases (where the BP’s probability distribution, $F_0 = V_0$, would obey either the linearized Boltzmann equation or similar Boltzmann-Lorentz equation \cite{20,21,23}). However, really from the aforesaid it follows that such is not the case: the classical kinetics is not an extreme case of the statistical-mechanical theory.

As an illustration, consider the BP in ideal gas. If rejecting all the higher-order correlations, i.e. putting on $V_2 = 0$ in the second of equations (2.17) (with $n = 1$) and then inserting its quadrature into the first equation, we come to a closed equation for $V_0$. An asymptotic of solution of this equation at $t \gg \tau = \Lambda_b/v_0$ (where $v_0 \sim \sqrt{T/M}$ is characteristic thermal velocity of BP) is certainly Gaussian:

$$V_0(t, \Delta R; \nu) \equiv \int V_0(t, R, P|R_0; \nu) dP \to \exp \left(-\frac{\Delta R^2}{4Dt}\right) \left(\frac{4\pi Dt}{3/2}\right), \quad (5.2)$$

where $\Delta R = R - R_0$, and $D \sim v_0\Lambda_b$ is the BP’s diffusivity. For a rarefied gas, $\Lambda_b = (\pi r_b^2 \nu)^{-1}$ and $D \propto \nu^{-1}$. Anyway, (5.2) is some rather complicated function of $\nu$. At the same time, from the point of view of the exact relations (5.1), the equality $V_2 = 0$ immediately implies that $V_0(t, \Delta R; \nu)$ is purely linear function of $\nu$!

So strong discrepancy does mean that asymptotic (5.2) is incorrect, and we have to get back to the complete BBGKY hierarchy. An approximate approach to its correct analysis was suggested already in [17] (or see \cite{22}) and developed in \cite{23}. In \cite{23}, for particular situation when the role of BP is played by a marked gas atom, the following asymptotic was found:

$$V_0(t, \Delta R; \nu) \to \frac{\Gamma(7/2)}{[4\pi D t]^{3/2}} \left[1 + \frac{\Delta R^2}{4Dt}\right]^{-7/2} \Theta \left(\frac{|\Delta R|}{v_0 t}\right), \quad (5.3)$$
Here, $\Theta(x)$ is definite function which turns to unit at $x = 0$ and rapidly goes to zero at $x \to \infty$. The characteristic feature of this probability distribution is that its fourth-order cumulants grow with time not linearly (as it would be in the case of Gaussian asymptotic) but under the law $\propto (Dt)^2 \ln(t/\tau)$, that is nearly proportionally to the square of time.

Empirically, such the statistical property of the random walk is taken for the fluctuations in current diffusivity of BP [6, 7, 24] whose power spectral density at frequencies $f \ll 1/\tau$ is approximately inversely proportional to the frequency (so called “1/f-noise” [6]; thus, results of [7, 23] confirmed the conjectures about origin of 1/f-noise stated for the first time in [24]). From the physical viewpoint, the origin of these fluctuations and corresponding “historical” statistical correlations described by CF $V_n$ ($n > 0$) is mere indifference of the system to the pre-history of BP’s collisions, i.e. to their total number and their time-average rate, as well as to ratios of numbers of collisions with different impact parameters [7]. Thus, the historical correlations are caused by complicity of particles in their collision rate fluctuations rather than by their interactions as such.

Let us demonstrate that quite similar conclusions can be deduced basing on only the virial expansions and the trivial non-negativeness of all the DF $F_n$.

From the non-negativity of $F_1$ and identity (2.12) we have

$$V_0(t, \Delta R; \nu) \int_{\Omega} F_1^{(eq)}(r|R; \nu) \, dr + \int_{\Omega} V_1(t, R, r|R_0; \nu) \, dr \geq 0 ,$$

(5.4)

where $V_1(t, R, r|R_0; \nu) \equiv \int \int V_1(t, R, r, p, p|R_0; \nu) \, dp \, dP$, and $\Omega$ is any region in the space of vectors $r - R$. At given $0 < \delta < 1$, let $\Omega(\delta, t, \Delta R; \nu) \equiv \Omega(\delta)$ be the minimum (in the sense of volume) among all regions $\Omega$ which satisfy the condition

$$\left| \int_{\Omega} V_1 \, dr - \int V_1 \, dr \right| \leq \delta \left| \int V_1 \, dr \right|$$

(5.5)
From this definition it follows that
\[
\Omega \max_r |V_1| \geq \left| \int_{\Omega} V_1 \, dr \right| \geq (1 - \delta) \left| \int V_1 \, dr \right| \tag{5.6}
\]
(spatial region and its volume are denoted by the same letter). In the aggregate the inequalities (5.4) and (5.5) produce, as can be easily verified, inequality
\[
V_0(t, \Delta R; \nu) \int_{\Omega(\delta)} F_1^{(eq)}(r | R; \nu) \, dr + (1 - \delta) \int_{\Omega} V_1(t, R, r | R_0; \nu) \, dr \geq 0 \tag{5.7}
\]
Combining it with the first of the virial expansions (4.7) (with \(n = 0\)) and taking into account that in the case under consideration \(z(\nu) \to 0\) and \(F_1^{(eq)}(r | R, \nu) \leq 1\), after quite obvious reasonings one obtains
\[
\Omega(t, \Delta R; \nu) V_0(t, \Delta R; \nu) + \frac{\partial V_0(t, \Delta R; \nu)}{\partial \nu} \geq 0 ,
\]
where the quantity \(\Omega(t, \Delta R; \nu)\) if defined as follows:
\[
\Omega(t, \Delta R; \nu) = \min_{0 < \delta < 1} \Omega(\delta, t, \Delta R; \nu) = \frac{\Omega(\delta, t, \Delta R; \nu)}{1 - \delta} \tag{5.9}
\]
Next, discuss a meaning of the latter quantity. Notice, first, that \(\Omega(\delta) \to 0\) when \(\delta \to 1\), merely by the definition of \(\Omega(\delta, t, \Delta R; \nu) = \Omega(\delta)\). Second, if the function \(V_1(t, R, r | R_0; \nu)\) does not change its sign when changing argument \(r - R\) (but keeping other arguments fixed) then at \(\delta \to 1\) the region \(\Omega(\delta)\) shrinks into infinitely small neighborhood of the point of maximum of \(|V_1|\) (or union of such neighborhoods), so that one can write
\[
\left| \int_{\Omega(\delta)} V_1 \, dr - \int V_1 \, dr \right| \to \left| \int V_1 \, dr \right| - \Omega(\delta) \max_r |V_1| ,
\]
Consequently, \(\Omega(t, \Delta R; \nu) \leq |\int V_1 \, dr|/(\max_r |V_1|)\). From the other hand, because of the inequality (5.6) definitely \(\Omega(t, \Delta R; \nu) \geq |\int V_1 \, dr|/(\max_r |V_1|)\). From here (recalling the constancy of \(V_1\)’s sign) we conclude that
\[
\Omega(t, \Delta R; \nu) = \frac{\int |V_1(t, R, r | R_0; \nu)| \, dr}{\max_r |V_1(t, R, r | R_0; \nu)|} \tag{5.10}
\]
This is nothing but the effective volume of a region in \((r - R)\)-space on which the two-particle correlation spreads out. Now, let our assumption about the sign constancy of \(V_1(t, R, r|R_0; \nu)\) in respect to \(r - R\) is not satisfied, and \(D\) denote those part of the \((r - R)\)-space where \(V_1\) has dominating sign, that is coinciding with sign of integral \(\int V_1 \, dr\). Then the analogous reasonings yield

\[
\frac{\left| \int V_1 \, dr \right|}{\max_{r} |V_1|} \leq \Omega(t, \Delta R; \nu) \leq \frac{\left| \int V_1 \, dr \right|}{\max_{r \in D} |V_1|} \leq \frac{\int_D |V_1| \, dr}{\max_{r \in D} |V_1|} \quad (5.11)
\]

Hence, in such the case we can say that \(\Omega(t, \Delta R; \nu)\) is even less than effective volume of a region where significant two-particle correlation takes place.

Further, let us confront inequality (5.8) with the hypothesis that the asymptotic of \(V_0(t, \Delta R; \nu)\) has Gaussian shape (5.2). From (5.8) it follows that this hypothesis can be true only if

\[
\Omega(t, \Delta R; \nu) \geq - \frac{\partial \ln D}{\partial \nu} \left( \frac{\Delta R^2}{4Dt} - \frac{3}{2} \right) = \frac{1}{\nu} \left( \frac{\Delta R^2}{4Dt} - \frac{3}{2} \right) \quad (5.12)
\]

(we took into account that in gas \(D \propto \nu^{-1}\)). In other words, if the mentioned effective volume, occupied by the two-particle correlation, is not bounded above under variations of \(t\) and \(\Delta R\). In opposite, if this volume is bounded above, and

\[
\nu \Omega(t, \Delta R; \nu) \leq c_1 = \text{const} , \quad (5.13)
\]

then the Gaussian asymptotic (5.2) is forbidden. Instead of it, inequality (5.8) allows the asymptotic like

\[
V_0(t, \Delta R; \nu) \rightarrow \frac{1}{(4\pi Dt)^{3/2}} \Psi \left( \frac{\Delta R^2}{4Dt} \right) \Theta \left( \frac{|\Delta R|}{v_0 t} \right) , \quad (5.14)
\]

where function \(\Psi(z)\) should satisfy the inequality

\[
z \frac{d\Psi(z)}{dz} + \alpha \Psi(z) \geq 0 , \quad \alpha \equiv \frac{3}{2} + c_1 \left[ - \frac{\partial \ln D}{\partial \ln \nu} \right]^{-1} = \frac{3}{2} + c_1 \quad (5.15)
\]

Consequently, \(\Psi(z)\) can not decrease at infinity faster than under the power law: \(\Psi(z \rightarrow \infty) \propto 1/z^{\alpha}\). The formula (5.3) in [23] corresponds to \(c_1 = \nu \Omega = 2\).
Thus, the theory inevitably leads to the statistical correlations whose length appears unbounded if not in space, as at variant (5.12), then in time, as at variant (5.13). It remains to ascertain what of these variants is more close to exact solution of the BBGKY hierarchy. From the physical viewpoint, the second is undoubtedly preferable. Indeed, according to equations (2.17), the source of the correlations between BP and atoms is their collisions. A collision intends such relative disposition of BP and an atom when the vector \( \rho = r - R \) belongs to the “collision cylinder” which is oriented in parallel to the relative velocity \( u = p/m - P/M \) and has radius \( \approx r_b \). At the same time, the particles should not be separated by a distance much larger than \( \Lambda = \min(\Lambda_a, \Lambda_b) \), since otherwise their collision most likely would be prevented by an encounter of one of them with other gas particles. Hence, the two-particle correlations are concentrated in the middle of the collision cylinder, at \( -\Lambda \lesssim u \cdot \rho / |u| \lesssim \Lambda \). The volume of this space region does not depend on the particles’ momenta, therefore it gives natural estimate of the volume \( \Omega(t, \Delta R; \nu) \). Obviously, it does not depend also on \( t \) and \( \Delta R \). Thus, \( \Omega \approx 2\Lambda_b \pi r_b^2 = 2/\nu \) (if, like on [23], BP is merely one of atoms). As the result, we come to (5.15) with \( c_1 = \nu \Omega \approx 2 \).

6. Conclusion

To resume, the problem about thermodynamically equilibrium random walk of a test “Brownian” particle (BP) in a fluid was formulated as a problem of classical statistical mechanics in the framework of the Gibbs canonic statistical ensemble of initial conditions. The corresponding BBGKY equations for distribution functions (DF) and the Bogolyubov equation for their generating functional were considered in terms of the cumulant functions (CF) introduced in order to extract statistical correlations between current state of the fluid and total displacement, or path, of the BP during all the time of its observation (“historical correlations”). It is shown
that the generating functionals of equilibrium DF and time-dependent DF both possess invariance in respect to definite continuous group of transformations of their arguments, including the density of the fluid (mean concentration of atoms).

The obtained invariance group produces the exact “virial expansions” (“virial relations”) which connect full sets of CF taken at different values of the density. With the help of these relations it was shown that all the many-particle correlations play equally important roles, regardless of the gas parameter value, and therefore the standard “Botzmannian” approach to kinetics of BP, which rejects third- and higher-order correlations, is incorrect even in the low-density or Boltzmann-Grad limit. Correspondingly, the virial relations quite certainly forbid the Gaussian asymptotic of the BP’s path probability density distribution inherent to the Boltzmann’s kinetics. Instead, such an asymptotic is allowed only which has power-law long tails (cut off at the BP’s path values on order of the ballistic flight path). This conclusion agrees with the results of approximative solving of the BBGKY equations \[7, 23\]. It means that all the constituent parts of trajectories (random walks) of BP are statistically dependent one on another. Therefore, the trajectories cannot be imitated by sequences of mutually independent, in the sense of the probability theory, random trials (speaking figuratively and in the Einstein words, “God does not play dice”). In this sense, any real molecular random walk, in contract to the random walk in the Lorentz gas, is non-ergodic.

It should be noted that results of the present paper can be easily extended to thermodynamically non-equilibrium random walks under influence of an external force (in this respect see \[11, 15, 22\]). It would be interesting also to generalize the considered invariance group to another problems focused on not selected particles only but sooner on collective and hydrodynamical variables.
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DONETSK INSTITUTE FOR PHYSICS AND TECHNOLOGY OF NASU, UL. R. LUXEMBURG 72, DONETSK 83114, UKRAINE
E-mail address: kuzovlev@kinetic.ac.donetsk.ua

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