On Statistics and 1/f Noise of Brownian Motion
in Boltzmann-Grad Gas and Finite Gas on Torus. I. Infinite Gas

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An attempt is made to compare statistical properties of self-diffusion of particles constituting gases in infinite volume and on torus. In this first part, equations are derived which represent roughened but solvable variant of the collisional approximation to exact BBGKY equations. With their help, statistics of Brownian motion in infinite gas is considered, under the Boltzmann-Grad limit, and shown to be essentially non-Gaussian, involving 1/f fluctuations in diffusivity.

PACS numbers: 05.20.Dd, 05.40.-a, 05.40.Fb, 83.10.Mj

I. INTRODUCTION

In [1] (see also Part VII and then in [2]) it was argued that kinetics of statistically nonuniform (though may be thermodynamically equilibrium) gas does not reduce to the Boltzmann equation, even under the Boltzmann-Grad limit \((\nu \to \infty, \delta \to 0, \nu \delta^2 = \text{const.})\), with \(\nu\) being concentration of gas particles and \(\delta\) radius of their repulsive interaction. Moreover, just this limit makes clear why the Boltzmann’s “Stosschalanassatz” (“molecular chaos” hypothesis) fails and the Boltzmann equation becomes inadequate when the one-particle distribution function \(F_1(t, \mathbf{r}, \mathbf{v})\) really depends on spatial coordinate \(\mathbf{r}\). Instead, an infinite chain of kinetic equations (reproduced in Appendix B) arises, which involves, in addition to \(F_1\), specific \(n\)-particle distribution functions \(F_n(t, \mathbf{r}, \mathbf{v}_1, \ldots, \mathbf{v}_n)\) representing local (probability) densities of \(n\)-particle chains of collisions (strictly speaking, impact parameters and/or other internal parameters of the collisions also are arguments of the \(F_n\)). The resulting long-scale statistics of self-diffusion (Brownian motion) of gas particles displays low-frequency fluctuations (1/f-noise) of diffusivity, which correspond to not the Wiener process but essentially different, non-Gaussian and non-Marcovian, random walk (thus confirming earlier phenomenological considerations \([4, 5, 6]\)).

In contrary to that conjectures, the mathematical theory of dynamical systems with “hyperbolic behavior” (exponential instability and mixing of phase trajectories), in particular, such as \(N\) hard balls in a container or on torus (most interesting for me), succeeds in proof of various ergodic, Bernoullian and Marcovian properties of these systems (see e.g. \([6, 7, 8]\) and references therein). In respect to hard balls on torus, this implies, undoubtedly, that their Brownian motion along it reduces (at sufficiently rough time scales) to the usual Wiener process (one can easy make sure of this by numeric simulation of 3 hard balls on 2-D torus).

It would be interesting to reconcile these rigorous results with above mentioned non-rigorous results on the Boltzmann-Grad gas (which can be placed on torus as well). There is no contradiction, in principle, if maximal time scale, \(\tau_{ng}\), which still perceives “anomalous” non-Gaussian and non-Marcovian features of Brownian paths in \(N\)-particle system (or minimum time scale which still suppresses and loses these features), is a growing function of \(N\), for instance,

\[
\frac{\tau_{ng}(N)}{\tau_f(N)} \sim N^-1\quad (1)
\]

where \(\tau_f(N)\) is mean free flight time (we take in mind that \(1 \ll N < \infty\), of course).

I can suggest heuristic arguments in favour of this hypothesis. Indeed, consider Brownian path of some particle during some time interval \(\Delta t\). The corresponding fragment of the path consists of \(\sim n = \Delta t/\tau_f\) collisions and free flights and is fully characterized by \(N_\Delta \sim 2Dn\) details (\(D\) denotes torus dimension), namely, velocity vectors \(\mathbf{v}_i\) and flight times \(\tau_j\) \((\tau_j = 1/n\) and besides \((D-1)\)-dimensional impact parameters of collisions. Compare this quantity with a number \(N_c\) of initial conditions (parameters of the gas state at the beginning of the interval) which might have an influence on this fragment. It is natural to expect that statistics of the Brownian displacement \(\Delta R_s = \sum_{j} v_{i_1} \tau_{1_1} + \ldots + v_{i_s} \tau_{s} (s = 1 \div n)\) is sensitive to the ratio \(N_\Delta/N_c\). If \(N_\Delta/N_c \ll 1\) then a particular realization of \(\Delta R_s\) is hardly able to try all principal possibilities allowed by initial conditions, therefore, it can be essentially non-ergodic, in one or another sense. In opposite, if \(N_\ Delta/N_c \gg 1\) then any of qualitatively different possibilities will be sampled many times, which gives grounds for good ergodicity.

To estimate \(N_c\), notice that outside particle coming to \(j\)-th collision \((j = 1 \div n)\) previously had \(\sim j\) collisions with other particles, which in their turn also had collisions before, and so on. Therefore total number, \(N_p\), of particles whose initial states influence our fragment can be estimated as \(N_p \sim (n+1)^{(n+1)/(n+1)} \sim e^n/\sqrt{n}\). At \(\Delta t/\tau_f = n > \ln N\,_{\text{in torus}}\), in fact, initial state of the whole gas is important, \(N_p = N\). Correspondingly, \(N_c = 2DN_p \sim 2D\min(N, e^n/\sqrt{n})\).

In case of the Boltzmann-Grad gas \(N = \infty\), and \(N_\Delta/N_c \sim n^{3/2}e^{-n}\) is certainly very small. Hence, non-ergodicity of \(\Delta R_n\) (more precisely, “anomalous” behav-

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ior of fourth and higher-order cumulants of $\Delta R_n$ is not surprising. At finite $N$ (and not too short time intervals, $\Delta t > \tau_f \ln N$), $N_s/N = \Delta t/N\tau_f$. Hence, the border between ergodic and non-ergodic behavior lies at $\Delta t/\tau_f \sim N$. That is nothing but our hypothesis (1).

In view of above reasonings, a system of large finite number of particles on torus is of special interest. Unfortunately, even in the much simpler case of infinite Boltzmann-Grad gas the chain of kinetic equations discussed in [1, 2] seems not solvable somehow except their more or less caricature roughening. Therefore, in the present paper I confine myself by two unpretentious tasks. In this first part of the paper, the mentioned equations are subjected to even more grotesque simplification but allowing for their formally exact solution. At that, their principal structure is preserved, therefore the solution is must be quite meaningful. In the next second part, modification of the roughened equations for finite $N$ will be derived and adapted to torus. Their analysis indeed demonstrates existence of characteristic time $\tau_{nd}$ which both formally and essentially corresponds to (1). Other results will be commented in final Conclusion.

II. EQUATIONS OF SELF-DIFFUSION IN INFINITE GAS

Our consideration will be based on equations of the collisional approximation (see Appendix B and [1, 2]), first of all, on equations [3,13] adapted for thermodynamically equilibrium but statistically non-uniform gas when Boltzmannian collision operator is replaced by the Boltzmann-Lorentz collision operator [13].

Recall that equations [1,3] deal with $n$-particle distribution functions $F_n(t, R, v_1...v_n)$ which describe close encounters of $n$ particles (with pair collisions between some of them) clustered in vicinity of given point $R$. The closeness means that the particles belong to a “collision box” defined by $|r_j - R| < d$, where $d$ is suitable scale much greater than interaction radius $\delta$ but much smaller than dimension $\sim (n/\nu)^{1/D}$ of volume typically needed to contain $n$ particles ($\nu$ and $D$ are mean number of particles per unit volume and space dimension of gas, respectively). At that, the general position $n$-particle distribution functions (DF) $F_n(t, r_1...r_n, v_1...v_n)$, for particles out of any encounter, are factored into product $\prod_{j=1}^{n} F_n(t, r_j, v_j)$, at least, under the Boltzmann-Grad limit $\nu \to \infty$, $\delta \to 0$, $\lambda \sim 1/\nu \delta^{D-1} = \text{const}$, where $\lambda$ is mean free path. These DF are normalized to gas volume $\Omega$: $\int F_n(t, r_1...r_n, v_1...v_n) dv_1...dv_n = \Omega^n$. Below it will be convenient to name $F_n(t, R, v_1...v_n)$ cluster distribution functions (CDF) while $F_n(t, r_1...r_n, v_1...v_n)$ volume distribution functions (VDF).

The stationary solution to the equations [3,13] is

$$F_n(R, v_1...v_n) = \prod_{j=1}^{n} F_0(v_j) = F^n_{eq}(v),$$

where $F_0(v) = (2\pi v_0^2)^{-D/2} \exp(-v^2/2v_0^2)$ is equilibrium velocity distribution, $v_0^2 = T/M$, and $T$ is gas temperature. Such DF represent statistical ensemble which tells nothing about positions of particles.

Now, consider more interesting ensemble which tells us that one of particles is localized, say, nearby coordinate origin, with coordinate probability distribution $W(r)$ ($\int W(r) dr = 1$, $\int rW(r) dr = 0$). To write this information on VDF, at first suppose that gas volume and total number of particles $N = n\Omega$ are finite. Then the highest VDF can be written as

$$F_N = F^n_{eq}(v) \frac{\Omega}{N} \sum_{j=1}^{N} W(r_j)$$

According to relation $F_n = \int F_{n+1} dv_{n+1} dr_{n+1}/\Omega$, the corresponding lower VDF are

$$F_n = F^n_{eq}(v) \left(1 + \frac{1}{\nu} \sum_{j=1}^{n} \left[W(r_j) - \frac{1}{\Omega}\right]\right)$$

(2)

Tending $\Omega$ to infinity and choosing the distribution $W(r)$ to have a suitable width (e.g. $\sim \lambda$), it is easy to see that corresponding CDF can be approximately represented by

$$F_n(R, v_1...v_n) = F^n_{eq}(v) \left[1 + \frac{n}{\nu} W(R)\right]$$

(3)

In the Boltzmann-Grad limit (when size of any “collision box” turns into zero in units of $\lambda$) this is formally exact expression.

Hence, in order to investigate self-diffusion of initially localized particle, we should solve equations [3,13] starting from statistically (but not thermodynamically) non-equilibrium initial conditions presented by (3). Obvious contribution of the first term on right-hand side of (3), that is uniform background of densities of particles and clusters, will be time-independent. Therefore we will omit it from solution, together with constant multiplier $1/\nu$ from its time-dependent part, but keep designation $F_n$ for the rest of it. Thus we come to the problem

$$\frac{\partial F_n}{\partial t} = -V^{(n)} \cdot \frac{\partial F_n}{\partial R} + \nu \sum_{j=1}^{n} \Lambda_j \int F_{n+1} dv_{n+1}$$

(4)

for infinite set of functions $F_n(t, R, v_1...v_n)$ under initial conditions

$$F_n(t = 0, R, v_1...v_n) = n W(R) \prod_{j=1}^{n} F_0(v_j)$$

(5)

with $V^{(n)} = (v_1 + ... + v_n)/n$ and $\Lambda_j$ being Boltzmann-Lorentz operator which acts onto $j$-th velocity.

Eventually we are interested in spatial distributions

$$W_n(t, R) = \int F_n(t, R, v_1...v_n) dv_1...dv_n$$
In view of their definition and normalization of VDF, their statistical sense is quite clear: \( W_n(t, \mathbf{R})/N \) is density of probability that at time moment \( t > 0 \) an \( n \)-particle cluster at point \( \mathbf{R} \) contains (or at \( n = 1 \) coincides with) those unknown particle which at \( t = 0 \) was localized near point \( \mathbf{R} = 0 \). Naturally, the larger is cluster the greater is this probability. Equivalently, \( W_1(t, \mathbf{R}) \) is conditional density of probability that well-known particle, at \( t = 0 \) positioned near \( \mathbf{R} = 0 \), later will be registered at given point \( \mathbf{R} \). In other words, \( W_1(t, \mathbf{R}) \) presents probability distribution of Brownian displacement of any gas particle during time interval \( t \).

Of course, clusters (encounters) of \( n > 1 \) particles are ephemeral objects whose lifetime \( \sim d/v_0 \) is much smaller than mean free flight time \( \tau_f \). But they form constantly living “gas of encounters” under description by second and higher of equations (4). The latter have no principal difference from the first equation since it also describes statistics of gas but not individual particles.

III. ROUGHENED DESCRIPTION OF BROWNIAN MOTION

1. In the Boltzmannian kinetics, instead of (4) one has the single equation for one-particle DF \( F_1(t, \mathbf{r}, \mathbf{v}) \),

\[
\frac{\partial F_1}{\partial t} = -\mathbf{v} \cdot \frac{\partial F_1}{\partial \mathbf{r}} + \nu \Lambda F_1 ,
\]

where the Boltzmann-Lorentz operator \( \Lambda \) tends velocity distribution of gas particles to equilibrium one, \( F_0(\mathbf{v}) \). As above, we can treat \( F_1(t, \mathbf{r}, \mathbf{v}) \) as (small) non-stationary non-uniform addition to uniform background due to a priori information about initial position of one of particles. After solving (6) with corresponding initial condition \( F_1(t = 0, \mathbf{r}, \mathbf{v}) = W(\mathbf{r})F_0(\mathbf{v}) \), the distribution \( W_1(t, \mathbf{r}) = \int F_1(t, \mathbf{r}, \mathbf{v}) \, d\mathbf{v} \) will present us information about a law of Brownian motion of the selected particle.

Undoubtedly, in respect to large time scales, \( t \gg \tau_f \), that will be nothing but the Gaussian law, which can be expressed in several equivalent forms:

\[
\lim_{s \to \infty} W_1(s^2t, s\mathbf{r}) = (4\pi Dt)^{-D/2} \exp(-r^2/4Dt) ,
\]

\[
\lim_{s \to 0} \Xi_1(t/s, \sqrt{s} \mathbf{k}) = \exp(-Dt\mathbf{k}^2) ,
\]

\[
\lim_{s \to 0} s \Phi_1(sp, \sqrt{s} \mathbf{k}) = 1/(p + Dk^2) \]

Here \( \Xi_1(t, \mathbf{k}) \) is characteristic function of Brownian motion and \( \Xi_1(p, \mathbf{k}) \) its Laplace transform:

\[
\Xi_1(t, \mathbf{k}) = \int \exp(i \mathbf{k} \cdot \mathbf{r}) W_1(t, \mathbf{r}) \, d\mathbf{r} ,
\]

\[
\Phi_1(p, \mathbf{k}) = \int_0^\infty \exp(-p t) \Xi_1(t, \mathbf{k}) \, dt
\]

Such long-time asymptotic is insensitive to concrete form of operator \( \Lambda \). Therefore, let us learn to obtain it in most simple way, and then apply this our experience to equations (4).

The Boltzmann-Lorentz equation (4) directly yields

\[
\frac{\partial W_1(t, \mathbf{r})}{\partial t} = -\frac{\partial J_1(t, \mathbf{r})}{\partial \mathbf{r}} ,
\]

\[
J_1(t, \mathbf{r}) = \int \mathbf{v} F_1(t, \mathbf{r}, \mathbf{v}) \, d\mathbf{v} = \Phi_1(t) W_1(t, \mathbf{r}) ,
\]

\[
\frac{\partial (J_1(t, \mathbf{r}))_\alpha}{\partial t} = -\frac{\partial}{\partial \mathbf{r}} \int v_\alpha F_1 \, d\mathbf{v} + \nu \int v_\alpha \Lambda F_1 \, d\mathbf{v}
\]

Here, evidently, \( J_1(t, \mathbf{r}) \) represents probability flow and \( \Phi_1(t, \mathbf{r}) \) conditional mean function of velocity under given position of the particle.

Notice that soon after start there is some correlation between current velocity of the particle and its displacement from initial position. But then, at \( t \gg \tau_f \), this correlation decreases down to zero for any thermodynamically equilibrium, and hence symmetrical, random walk (otherwise it would behave like ballistic flight). In other words, the conditional mean velocity is much smaller than above defined mean-square thermal velocity \( v_0 \):

\[
\Phi_1(t)/v_0 \to 0
\]
Corresponding Laplace transform \([11]\) of the characteristic function \([10]\) looks as
\[
\Phi_1(p, k) = \Xi_1(0, k) \left[ p + v_0^2 k^2 \right]^{-1} \tag{19}
\]
and evidently possesses Gaussian asymptotic \([9]\), with diffusivity \(D = v_0^2 / \gamma \). At that, velocity relaxation rate \(\gamma\) can be identified with \(\tau_f^{-1}\).

Let us compare \([10]\) with formally exact answer when \(\Lambda\) is Fokker-Planck operator \([1, 2]\) governing random process with Gaussian velocity fluctuations (the Ornstein-Uhlenbeck process),
\[
\frac{\Phi_1(p, k)}{\Xi_1(0, k)} = \left[ p + v_0^2 k^2 \right] \left( p + \gamma + \frac{2v_0^2 k^2}{p + 2\gamma + \ldots} \right)^{-1} \tag{19}
\]
This is infinite continued fraction with \(nv_0^2 k^2\) in denominators and \(n\gamma\) in denominators \((n = 1, 2, \ldots)\). As for equations \([15]\) and \([18]\), it can be shown that formally they correspond to a random process with dichotomic velocity fluctuations. However, from the point of view of large time scales both random walks are identical. Realistic \(\Lambda\)’s account for multi-state velocity hopping but lead to same random walks. This example gives hope of that similar approach to system \([3]\) will imitate its long-time behavior without principal losses.

2. In addition to distributions \(W_n(t, \mathbf{R})\), introduced in Sec.2, consider the “flows”
\[
J_n(t, \mathbf{R}) = \int V^{(n)} F_n(t, \mathbf{R}, \mathbf{v}_1, \ldots, \mathbf{v}_n) \; d\mathbf{v}_1 \ldots d\mathbf{v}_n
\]
In essence, equations \([4]\) describe the same physics as equation \([6]\). Hence, all above reasonings about decay (at \(t \gg \tau_f\) ) of correlations between velocities and positions of particles remain valid. And all they can be confirmed by direct analysis of \([7]\). Therefore, by analogy with \([10]\) we can write
\[
\nabla \int V^{(n)} V^{(n)} F_n(t, \mathbf{R}, \mathbf{v}_1, \ldots, \mathbf{v}_n) \; d\mathbf{v} \rightarrow
\rightarrow \int V^{(n)} V^{(n)} F_n \nabla W_n(t, \mathbf{R}) =
= \frac{v_0^2}{n} \nabla \alpha W_n(t, \mathbf{R}) \tag{20}
\]
(here and below \(d\mathbf{v} = d\mathbf{v}_1 \ldots d\mathbf{v}_n\) and \(\nabla\) replaces \(\partial / \partial \mathbf{R}\)). Analogue of formula \([17]\) is
\[
\nu \int V^{(n)} \left( \sum_{j=1}^n \Lambda_j F_{n+1} \right) d^{n+1} \mathbf{v} =
= \nu \int F_{n+1} \left[ \sum_{j=1}^n \frac{n}{n+1} \Lambda_j v_j \right] d^{n+1} \mathbf{v} =
= \nu \int F_{n+1} \left[ \frac{n+1}{n+1} \Lambda_j v_j \right] d^{n+1} \mathbf{v} =
= \frac{v_0^2}{n} \nabla \alpha W_n(t, \mathbf{R}) \tag{21}
\]
The last row is obtained with the help of integration by parts. Integration by parts “in opposite direction” gives
\[
\lim_{s \to 0} s \Phi_1(s, \sqrt{s} k) = 2 \int_0^\infty \exp(-DK^2t) \frac{d\tau}{(1 + p \tau)^3}
\] (29)
Performing here inverse Laplace transform, we obtain
\[
\lim_{s \to 0} \Xi_1(t/s, \sqrt{s} k) = \int_0^\infty \exp(-xDK^2t) \exp\left(-\frac{1}{x}\right) \frac{dx}{x^3}
\] (30)
with \(\Xi_1\) defined by (10). Then the inverse Fourier transform of (30) produces
\[
\lim_{s \to \infty} W_1(s^2t, sR) = \frac{\Gamma(2 + D/2)}{(4\pi Dt)^{D/2} (1 + R^2/4Dt)^{2+D/2}}
\] (31)
This probability distribution describe random walk which has the same characteristic scaling property \(R^2 \sim t\) as Gaussian random walk (Wiener process), but at that obeys extremely non-Gaussian statistics. Formula (30) shows that this walk can be represented as Wiener process with random but time-independent diffusivity \(\tilde{D}\) distributed with probability density \(w(D/D)/D\), where \(w(x) = x^{-3} \exp(-1/x)\). That is absolutely non-ergodic process. Besides, as it is evident from (31), the fourth and higher statistical moments of this process are infinite. Apparently, non-Gaussian and non-ergodic peculiarities of our random walk was too exaggerated by the considered limiting procedure, and we have to return to equation (27) which demonstrates that in fact all the moments are finite.

3. Let \(R(t)\) denotes projection of \(D\)-dimensional Brownian displacement \(R(t)\) during time \(t\) onto some fixed direction, and vector \(k\) is oriented in parallel to it. Since the direction is fixed, we can treat \(k\) as scalar. Then compare expansions of both sides of (27) into series over \(k^2\):
\[
\Phi_1(p, k) - \frac{1}{p} = \sum_{n=1}^{\infty} \frac{(-k^2)^n}{(2n)!} \int_0^\infty e^{-pt} (R^{2n}(t)) dt = \frac{1}{p} \sum_{n=1}^{\infty} \left[ \frac{-\gamma Dk^2}{p^2} \right]^n \frac{1}{(n-1)!} \int_0^1 \frac{-\ln(1-x)}{(1 + \gamma x/p)^2} dx
\]
At \(p/\gamma \ll 1\), which correspond to large time, the comparison yields
\[
\int_0^\infty e^{-pt} (R^2(t)) dt = \frac{2D}{p^2}
\] (32)
\[
\int_0^\infty e^{-pt} (R^4(t)) dt = \frac{24D^2}{p^3} \ln \left(1 + \frac{\gamma}{p}\right)
\] (33)
\[
\int_0^\infty e^{-pt} (R^{2n}(t)) dt = (2n)! \zeta(n-1) \frac{D^2 v_0^{2n-4}}{p^{2n-1}} (n > 2)
\] (34)
Here \(\zeta(...)\) is the Riemann zeta function, and we used the integrals
\[
\int_0^1 \frac{-\ln(1-x)^n}{x^2} dx = n! \zeta(n) (n > 1),
\]
\[
\int_0^1 \frac{\ln(1-x)}{(1 + ax)^2} dx = -\frac{\ln(1 + a)}{a(1 + a)}
\]
Correspondingly to (32)-(34).
\[
\langle R^2(t) \rangle = 2Dt,
\]
\[
\langle R^4(t) \rangle = 12D^2t^2 \ln \gamma t,
\]
\[
\langle R^{2n}(t) \rangle = 2n(2n-1)\zeta(n-1) \times (Dt)^2 (v_0 t)^{2n-4} (n > 2)
\]
(35)
(36)
(37)
at \(\gamma t \gg 1\). Thus, except mean square of the displacement, all its higher-order moments are anomalously large from the point of view of Gaussian random walk (which has \(\langle R^{2n}(t) \rangle = (2n)! (2Dt)^n\)).

Comparing formulas (35) and (37) and distribution (31) at \(D = 1\), which also describes the projection \(R(t)\), we notice that these asymptotic formulas can be agreed with probability distribution (31) if the latter is supplemented by its cut off at \(\langle R(t) \rangle \sim v_0 t\). Hence, we can improve (31) if replace it, in asymptotical sense, by
\[
W_1(t, R) \approx \frac{\Gamma(5/2) G(R/v_0)}{(4\pi Dt)^{1/2} (1 + R^2/4Dt)^{5/2}}
\] (38)
where \(G(0) = 1\) and \(G(x)\) is extremely fast decaying function at \(x \to \pm \infty\) (this statement certainly follows from very slow growth of coefficients on right-hand side of (37)). Thus we come to conclusions as follow.

(i) In respect to probabilistic characteristics of out random walk, formula (38) practically coincides with (31), that is (31) is quite satisfactory. However, in respect to higher statistical moments, \(\langle R^{2n}(t) \rangle\) with \(n > 1\), there is not only strong quantative difference between (31) and (38) but also at least two principal differences.

(ii) The first difference is presented by fourth \(\langle R^4(t) \rangle\) moment. Such behavior of \(\langle R^4(t) \rangle\) as prescribed by (38) means that our Brownian motion indeed can be represented as Gaussian one with random diffusivity. However, diffusivity is not a “static” random value (as (38) implies) but (as (38) implies) a random process with characteristic low-frequency power spectrum \(\sim \ln(f)^3/f\) (where \(f \ll \gamma\) is frequency and \(\beta\) can be both positive and negative). In other words, the diffusivity fluctuates like 1/f-noise. This theme was already discussed not a once in [1, 2, 3, 4, 5].

(iii) The second peculiarity of our Brownian motion is presented by moments \(\langle R^{2n}(t) \rangle\) with \(n > 2\) which turn out to be dependent on not only (average) diffusivity \(D\) but also on the thermal velocity \(v_0\), i.e. characteristics of separate free flights. This formal result can be interpreted as evidence of that probability distribution of free flight time has a power-law tail. Comparing (38) and moments corresponding to purely free flight,
\[ \langle R^{2n}(t) \rangle = (2n)! (v_0 t)^{2n} \] (on \( \langle R^{2n}(t) \rangle = (v_0 t)^{2n} \) for dichotomic velocity), we can suppose that probability of anomalously long flights comparable with \( t \) behaves as \( \sim (\Delta t)^2/(v_0 t)^4 = 1/(\gamma t)^2 \) (i.e. is inversely proportional to square of mean number of collisions during the observation time). But, strictly speaking, this issue needs in investigation of many-time statistics of our Brownian motion. In any case, on the whole it appears to be rather rather non-ergodic process.

V. RESUME

In this paper, previously constructed equations of the collisional approximation to kinetics of statistically nonuniform gas were applied to analysis of self-diffusion (Brownian motion) of particles of infinite-volume gas in its thermodynamical equilibrium, under the Boltzmann-Grad limit. With this purpose, a roughened version of the equations was derived which allowed for their almost complete solution. The latter demonstrated that statistics of the Brownian motion is essentially non-Gaussian, not obeying the central limit theorem, and hence essentially non-ergodic. It looks as if diffusivity of the Brownian path had no definite value but instead underwent low-frequency fluctuations with spectral properties similar to that of 1/f-noise and with probability distribution possessing power-law long tail. These results are in abrupt contradiction to what follows from standard kinetic approximations, but agree with Krylov’s doubts \[10\] about obligatory ergodicity of mixing dynamics.

APPENDIX A: BASIC EQUATIONS

Our start point are the Liouville equation for \( N \) particles in container \( 0 \leq r_\alpha \leq l \) (\( \alpha = 1 \div D \)):

\[ \frac{\partial F_N}{\partial t} = L^{(N)} F_N , \quad (A1) \]

\[ L^{(N)} \equiv - \sum_{j=1}^{N} p_j \cdot \frac{\partial}{\partial r_j} + \sum_{1 \leq j < m \leq N} L_{jm} , \]

\[ L_{jm} \equiv -\nabla U(r_j - r_m) \cdot \left( \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_m} \right) , \]

with \( U(r) \) being interaction potential, \( p_j = M v_j \) momentums, and \( F_N = F_N(t, r_1, r_2, r_N, v_1, v_2, v_N) \) normalized probability density of phase point of the system, and the corresponding Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) equations

\[ \frac{\partial F_1}{\partial t} = -v_1 \cdot \frac{\partial F_1}{\partial r_1} + (N - 1) \int_2 L_{12} F_2 , \quad (A2) \]

\[ \frac{\partial F_2}{\partial t} = L^{(2)} F_2 + (N - 2) \int_3 (L_{13} + L_{23}) F_3 , \quad (A3) \]

\[ \frac{\partial F_n}{\partial t} = L^{(n)} F_2 + (N - n) \int_{n+1}^N \sum_{j=1}^{n+1} L_{jn} F_{n+1} , \quad (A4) \]

where \[ \int_2 ... = \int ... d\nu_d dr_s \] and \( F_n = \int_{n+1}^N \sum_{j=1}^{n+1} L_{jn} F_{n+1} \). In the limit of infinitely big container, \( N \to \infty, l \to \infty \), \( \nu = N/\Omega = \text{const} (\Omega \equiv l^D) \), one must consider non-normalized distribution functions \( \Omega^n F_n \). If designate them again as \( F_n \) then (A3) turns into

\[ \frac{\partial F_n}{\partial t} = L^{(n)} F_2 + \nu \int_{n+1}^N \sum_{j=1}^{n+1} L_{jn} F_{n+1} \quad (A5) \]

The equations (A1)-(A5) hold also for particles on torus with equal dimensions, \( 0 \leq r_a \leq l \), if only supplement them with the periodic boundary conditions and replace \( U(r) \) by \( U(\rho) \), where \( \rho = \rho(r) \) is factual distance between two particles on torus: \( \rho_a = r_a \) when \( |r_a| \leq l/2 \) and \( \rho_a = -\text{sign}(r_a)(l-|r_a|) \) when \( |r_a| > l/2 \). However, if we want to consider unbounded Brownian motion of particles along the torus, we should introduce more rich distribution functions which keep count of their rotations. This is subject of second part of the paper.

APPENDIX B: COLLISIONAL APPROXIMATION

Assuming that our gas is sufficiently rarefied, that is \( \delta/l \ll 1 \), with \( a = l/\sqrt{N}\) being typical distance between neighbour particles and \( \delta \) interaction radius, we want to describe it approximately in terms of Boltzmannian pair collision operators (“collision integrals”). With this purpose, basing on the exact BBGKY equations (see Appendix A) consider \( F_2(t, r_1, r_2, v_1, v_2) \) at \( |r_2 - r_1| < d \) where \( \delta \ll d \ll a \). Any such configuration can be interpreted as a snapshot of certain process of collision of two particles or, may be, their close encounter without significant interaction. Therefore let us name the region \( |r_2 - r_1| < d \) “collision box” and characterize states inside it by inner time \( \Theta \) of corresponding collision plus relative velocity and \( (D-1) \)-dimensional impact parameter at its incoming stage. We can choose \( \Theta = 0 \) at perigee of the collision or encounter. If using these new variables, (A3) can be rewritten in the form

\[ \frac{\partial F_2}{\partial t} = -V^{(2)} \cdot \frac{\partial F_2}{\partial R} - \frac{\partial F_2}{\partial \Theta} + (N - 2) \int_3 (L_{13} + L_{23}) F_3 \quad (B1) \]

with \( R = (r_1 + r_2)/2 \) and \( V^{(2)} = (v_1 + v_2)/2 \) being position and velocity of center of gravity of the pair. At that, by definition of the inner time,

\[ -\frac{\partial F_2}{\partial \Theta} = -v_{12} \cdot \frac{\partial F_2}{\partial r_{12}} + L_{12} F_2 \quad (B2) \]
where \( r_{12} = r_2 - r_1 \) and \( v_{12} = v_2 - v_1 \).

Any dependence of \( F_2 \) on \( \Theta \), at least at \( |\Theta| \sim \) typical duration of collisions \( \tau_c \), does mean that at statistical ensemble under consideration a number (or probability of realization) of pairs coming into \( (\Theta < 0) \) a given sort of collisions differs from a number (or probability of realization) of pairs leaving \( (\Theta > 0) \) the same collision. Generally such is the case, and such difference obstructs collisional approximation, because collision operator must conserve probability (just as collision conserves number of particles). Or alternatively we should neglect this difference and postulate that

\[
\frac{\partial F_2}{\partial \Theta} = 0 \quad \text{when} \quad r_{12} \in \text{collision box} \tag{B3}
\]

in (A2), thus ensuring conservation of probability in the course of collisions. The destination of (B3) is correct transition from separate dynamic states to coherent collision as the whole.

According to (A2), relative displacement of colliding particles is included into collision. Consequently, it drops out of outward characterization of collision as the whole, and the latter obeys the equation

\[
\frac{\partial F_2}{\partial t} = -V^{(2)} \cdot \frac{\partial F_2}{\partial R} + (N - 2) \int_3 (L_{13} + L_{23}) F_3 \tag{B4}
\]

At that, equation (A2), which is probabilistic equivalent of Hamilton dynamics inside collision box,

\[
\frac{dr_{12}}{d\Theta} = v_{12} , \quad M \frac{dv_{12}}{d\Theta} = -\partial U(r_{12}) \tag{B5}
\]

together with (A3) serves for transformation of last term in (A2) into usual Boltzmann collision integral (1, 2).

Here we detect principal difference from Boltzmann’s theory: equation (A3) certainly forbids Boltzmann’s Stosseslawansatz (except trivial situation when \( F_1 \) is exactly spatially uniform). “Molecular chaos” fails in collision box, just where it was most wanted. However, nothing prevents “molecular chaos” outside collision box, and it really holds there (at least in the Boltzmann-Grad limit).

Clearly, the function \( F_2 \) governed by equation (A4) presents probability measure (ensemble-average density) of one or another sort of collisions (differentiated e.g. by their impact parameters and relative velocity \( v_{12} \)). Notice that it becomes normalized to unit, in respect to \( R^{(2)} \) and both velocities, if multiply \( F_2 \) by gas volume \( \Omega \). The first term on right-hand side of (A4) describes drift of collisions in spatially non-uniform gas while the second their redistribution over sorts due to intervention of a third outer particle.

Hence, next we should consider clusters of three close particles belonging to a reasonable “collision box”, e.g. \(|r_i - r_j| < d\), and again connect instant dynamic states inside it into 3-particle collision as a single whole. Of course, that is not literally 3-particle collision but sooner 3-particle encounters with possibility of pair collisions among some of the particles. Again, distribution of such 3-particle events over their sorts can change under influence by a fourth exterior particle. Continuing such scheme to \( n \)-particle encounters, we decompose the \( n \)-particle Liouville operator similarly to (B1):

\[
L^{(n)} F_n = -V^{(n)} \cdot \frac{\partial F_n}{\partial R} - \frac{\partial F_n}{\partial \Theta} , \tag{B6}
\]

with \( R = (r_1 + ... + r_n)/n \), \( V^{(n)} = (v_1 + ... + v_n)/n \), and \( \Theta \) being inner time of an encounter. Then again it is necessary to postulate conservation of probability in collision box:

\[
\frac{\partial F_n}{\partial \Theta} = 0 \quad \text{when} \quad r_i - r_j \in \text{collision box} \tag{B7}
\]

which simplifies (A4) into equation

\[
\frac{\partial F_n}{\partial t} = -V^{(n)} \cdot \frac{\partial F_n}{\partial R} + (N - n) \int_{n+1}^n \sum_{j=1}^n L_{jn} F_{n+1} \tag{B8}
\]

similar to (A5). At the same time, (A5) helps to transform the last term in similar equation for \( F_{n-1} \) into sum of \( n - 1 \) collision integrals.

Thus we come to a chain of coupled kinetic equations:

\[
\frac{\partial F_n}{\partial t} = -V^{(n)} \cdot \frac{\partial F_n}{\partial R} + (N - n) \sum_{j=1}^n S_{jn} F_{n+1} \tag{B9}
\]

where \( n = 1...N \) and \( S_{jn} \) is Boltzmannian collision operator describing collision between \( j \)-th particle from the \( n \)-particle cluster and one more “ \((n + 1)\)-th” particle from its exterior. Functions \( F_{n+1} \) represent \( F_{n+1} \) at boundary of \( (n + 1) \)-particle collision box, more precisely, at those parts of the boundary which correspond to incoming stage of these collisions. At that, differences \( \sim d < a \) between centers of gravity of successive collision boxes are neglected because of smallness in comparison with the mean free path \( \lambda \sim a/\partial r^{D-1} \). In the limit of infinite gas, after normalization to its volume, \( \Omega^n F_n \to F_n \), equations (B9) turn to infinite chain of equations from (1, 2).

Importantly, the boundary functions \( F_{n+1}^{in} \) in (B9) and (B10) in no way are ruled by these equations themselves. In essence, \( F_{n+1}^{in} \) supply initial conditions to equations (B5), as well as similar \( n \)-particle equations, and must be determined independently, by lacing \( F_{n+1}^{in} \)’s with probability distributions at exterior of the collision box. But its boundary is just border between violation and observance of “molecular chaos” (see Italic text above). Therefore, here somewhat mediate must be expected. For example,

\[
F_2^{in}(t, R, v_1, v_2) = F_1^{in}(t, R, v_1)F_1^{in}(t, R, v_2)
\]
where generally neither \( F_n'(t, R, v) \) nor \( F_\nu''(t, R, v) \) coincide with the one-particle distribution \( F_1(t, R, v) \). Thus Stosshalansatz is valid with respect to velocities of colliding particles only but not to their positions! More concrete formulation of such “weakened molecular chaos” follows again from conditions of conservation of probability (now at the border of “molecular chaos”) [1, 2]:

\[
F_{n+1}^{in}(t, R, v_1...v_n, v_{n+1}) = \tilde{F}_1(t, R, v_{n+1}) \times \\
\times \int F_{n+1}(t, R, v_1...v_n, v') dv' ,
\]

where \( \tilde{F}_1 \) is local one-particle velocity distribution,

\[
\tilde{F}_1(t, R, v) \equiv \frac{F_1(t, R, v)}{\int F_1(t, R, v') dv'} ,
\]

normalized to unit.

But what about \( D(n-1)-1 \) those arguments of \( F_n \) at \( n > 1 \) (in particular, impact parameters) which concretize geometry of \( n \)-particle encounters but not written out above? If we made attempt to take them into account, our theory would be not simpler than underlying BBGKY equations. Therefore we suppose that \( F_n \) in (B9) and (B10) represent distributions averaged over all sorts of the encounters. This roughening of the theory looks be caricature, but it can be legalized in many respects under the Boltzmann-Grad limit (\( \nu \rightarrow \infty, \delta \rightarrow 0, \lambda \sim 1/\nu^2D^{-1} = \text{const} \)). What is the chief thing, at that the theory keeps principal open-chain structure of its equations. By this reasons, in Sec.2 we venture to roughen the theory yet stronger.

Additional simplification appears when we want to investigate Brownian motion (self-diffusion) of gas particles in absence of their collective hydrodynamic motion, that is in thermodynamically equilibrium gas. This purpose can be achieved if apply the trick well known in classical kinetic theory of gases [4], namely, if treat “outside (\( n+1 \))-th particle” in (B11)-(B12) as a particle of equilibrium thermostat: \( \tilde{F}_1(t, R, v) \rightarrow F_0(v) \), where \( F_0(v) \) is equilibrium velocity distribution (standard Gaussian at \( N \rightarrow \infty \)). Correspondingly, the Boltzmann collision operator \( S_{j+1} \) transforms into the Boltzmann-Lorentz operator \( \lambda_j \), defined by

\[
S_{j+1} [F(v_j...v_j)W_0(v_{n+1})] = \lambda_j F(v_j...v_j)
\]

Equations (B10)-(B12) take the form [1, 2]

\[
\partial F_n/\partial t = -\nu^{(n)} \partial F_n/\partial R + \nu \sum_{j=1}^{n} \lambda_j \int F_{n+1} dv_{n+1} \tag{B13}
\]

and similarly equations (B9) do change. Thus we find ourselves in situation when spatial non-uniformity of distribution functions \( F_n \) has purely statistical origin: it describes not a thermodynamic perturbation but information about positions of some particles only (even may be a single particle).

[1] Yu. E. Kuzovlev, “Bogolyubov-Born-Green-Kirkwood-Yvon equations, self-diffusion and 1/f-noise in a slightly nonideal gas”, Sov.Phys.-JETP, 67 (12), 2469 (1988) [in Russian: Zh.Eksp.Teor.Fiz., 94, No.12, 140 (1988)].
[2] Yuriy E. Kuzovlev, “Kinetical theory beyond conventional approximations and 1/f-noise”, arXiv: cond-mat/9903350
[3] Yu. E. Kuzovlev and G.N.Bochkov, “On the origin and statistical characteristics of 1/f-noise”, “Radiophysics and Quantum Electronics”, No.3 (1983) [in Russian: Izv.VUZov.-Radiofizika, 26, 310 (1983)].
[4] G.N.Bochkov and Yu.E.Kuzovlev, “On the probabilistic characteristics of 1/f-noise”, “Radiophysics and Quantum Electronics”, No.9 (1984) [in Russian: Izv.VUZov.-Radiofizika, 27, 1511 (1984)].
[5] G.N.Bochkov and Yu.E.Kuzovlev, “New in 1/f-noise studies”, Sov.Phys.-Usp., 26, 829 (1983) [in Russian: UFN, 141, 151 (1983)].
[6] D.V.Anosov et al., “Dynamical systems with hyperbolic behaviour”, in “Modern problems of mathematics. Fundamentals. Vol.66”, ed. R.V.Gamkrelidze, VINITI, Moscow, 1991 (in Russian).
[7] N. Chernov and L.-S. Young, “Decay of correlations for Lorentz gases and hard balls”, in “Hard Ball Systems and the Lorentz Gas”, ed. D.Szasz, Encyclopaedia of Mathematical Sciences 101, pp. 89-120, Springer, 2000 [http://www.math.uab.edu/chernov].
[8] N. Simányi, “The Boltzmann-Sinai ergodic hypothesis in full generality”, arXiv: math.DS/0510022
[9] P. Resibois and M.de Leener. Classical kinetic theory of fluids. Wiley, New-York, 1977.
[10] N.S.Krylov. Works on the foundation of statistical physics. Princeton Univ. Press, Princeton, 1979.