

**THE EINSTEIN LAW FOR THE SYSTEM "BROWNIAN
PARTICLE IN THERMOSTAT" BASED ON
THE PRESENTED PROBABILITY APPROACH**

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Abstract: A one-dimensional system "Brownian particle in thermostat" is considered. The equation — the Einstein law for Brownian motion is derived on the basis of presented probability approach in the paper. The kinetic equation for space part of the distribution function is obtained.

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1. Introduction

The studying of simple models of particle systems such as systems of hard spheres allows us to solve a number of problems of description of dynamics of many-particle systems. The problems are rigorous justification of kinetic equations, justification of approximate methods of description of dynamics etc. [1], [2], [3], [4], [5] and [6].

The system "Brownian particle in thermostat" is an important case of many-particle many kind system, and the studying of this system is of self-dependent interest [7].

In the present paper it is derived the equation — the Einstein law for Brownian motion on the basis of the presented probability approach used to describe the considerable many-particle system. It is obtained the kinetic equation for space part of the distribution function of Brownian particle in thermostat.

2. Formulation of the Problem

We consider a one-dimensional system "Brownian particle in thermostat" of many particles. All particles of thermostat are identical and have the mass $m_0 = 1$. The velocity distribution of particles of thermostat is equilibrium, the Maxwellian:

$$\varphi(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}. \quad (1)$$

The coordinates of the particles are uniformly distributed along a straight line on the admissible configurations. In the thermostat considered there is a massive Brownian particle with mass $m \gg 1$. We can neglect the particle sizes. We assume collisions between particles be absolutely hard.

The aim of the present paper is the studying of massive Brownian particle motion, derivation of the equation — the Einstein law for the system "Brownian particle in thermostat", derivation of the kinetic equation for space part of the distribution function of Brownian particle on the basis of the presented probability approach used to describe the considerable many-particle system.

3. Statistical Characteristics of Brownian Particle Motion

We calculate the mean time and free path (displacement) of Brownian particle as functions of its initial velocity u_0 .

The probability $P(u_0, t)$ of lacking of collisions of the Brownian particle moving with velocity u_0 at time t is determined by the function [8]:

$$P(u_0, t) = e^{-f(u_0)t}, \quad (2)$$

where, taking into account that the velocity distribution function of particles in thermostat is equilibrium, the Maxwellian (1), function $f(u_0)$ can be determined in terms of special function $erf\left(\frac{u_0}{\sqrt{2}}\right)$, which is the erf integral, i.e.

$$f(u_0) = u_0 erf\left(\frac{u_0}{\sqrt{2}}\right) + \sqrt{\frac{2}{\pi}} e^{-\frac{u_0^2}{2}}.$$

Particles of thermostat, which collide with a massive Brownian particle with mass $m \gg 1$, have identical and vice versa, in comparison with Brownian particle, very small mass $m_0 = 1$. Then velocity of particles of thermostat after collision with Brownian particle will be much bigger than velocity of Brownian particle. If we assume mean modulus of velocity of particles of thermostat after collision with Brownian particle be unity then according to momentum and energy conservation laws we obtain that Brownian particle velocity $|u_0| \ll 1$. By this we conclude that the change of velocity of Brownian particle after collision with the particle of thermostat is a small quantity. Therefore, approximation of the function (2) results to expression

$$P(u_0, t) \approx e^{-\frac{2+u_0^2}{\sqrt{2\pi}}t}, \quad (3)$$

where $\frac{2+u_0^2}{\sqrt{2\pi}} \approx f(u_0)$.

It is obvious, that time t between collisions of the Brownian particle having velocity u_0 with particles of thermostat (mean free time of Brownian particle) is random variable with distribution function

$$\varphi(t) = -\frac{\partial P(u_0, t)}{\partial t} = f(u_0)e^{-f(u_0)t}. \quad (4)$$

By this function we conclude that mean time between collisions of Brownian particle with particles of thermostat (mean free time of Brownian particle) is equal to (by (3))

$$\langle t \rangle = \int_0^{\infty} t\varphi(t) dt = \frac{1}{f(u_0)} \approx \frac{\sqrt{2\pi}}{2+u_0^2}.$$

Since $|u_0| \ll 1$, then $\langle t \rangle$ weakly depends on Brownian particle velocity u_0 . Therefore, we can suppose

$$\begin{aligned} \langle t \rangle &\approx \sqrt{\frac{\pi}{2}}, \\ f(u_0) &\approx \sqrt{\frac{2}{\pi}}. \end{aligned} \quad (5)$$

We calculate relaxation time [8]-to-mean time between collisions of Brownian particle with particles of thermostat ratio (this is mean number of free paths of Brownian particle during relaxation time of its velocity):

$$\langle n \rangle = \frac{T_{rel.}}{\langle t \rangle} \approx \frac{m\sqrt{2\pi}}{8} \cdot \frac{2}{\sqrt{2\pi}} = \frac{m}{4}. \quad (6)$$

Mean free path (displacement) of Brownian particle according to (4) and (5):

$$\langle \lambda \rangle = \int_0^{\infty} |u_0| t \varphi(t) dt = |u_0| \frac{1}{f(u_0)} \approx \sqrt{\frac{\pi}{2}} |u_0|.$$

Denote $\langle \lambda \rangle$ by λ_0 , i.e.

$$\lambda_0 \approx \sqrt{\frac{\pi}{2}} |u_0|. \quad (7)$$

We calculate mean-square free path (displacement) of Brownian particle according to (4) and (5):

$$\langle \lambda^2 \rangle = \int_0^{\infty} u_0^2 t^2 \varphi(t) dt = u_0^2 \frac{2}{f^2(u_0)} \approx \pi u_0^2.$$

Denote $\langle \lambda^2 \rangle$ by λ_0^2 , i.e.

$$\lambda_0^2 \approx \pi u_0^2. \quad (8)$$

We calculate mean-square velocity u of Brownian particle:

$$\langle u^2 \rangle = \int_{-\infty}^{\infty} u^2 \varphi(u) du = \int_{-\infty}^{\infty} u^2 \sqrt{\frac{m}{2\pi}} e^{-\frac{mu^2}{2}} du = \frac{1}{m},$$

where $\varphi(u)$ is the Maxwell distribution function for Brownian particle. Analogously we denote $\langle u^2 \rangle$ by u_0^2 , i.e.

$$u_0^2 = \frac{1}{m}. \quad (9)$$

4. The Kinetic Equation for Space Part of the Distribution Function

Main problem of calculation space part of the distribution function is occurrence of strong correlations between neighboring free displacements of Brownian particle.

We calculate statistical characteristics of Brownian particle motion during relaxation time of its velocity. Introduce the following denotations:

λ_i is the i -th displacement of Brownian particle between the i -th and the $(i + 1)$ -th collisions;

$\langle L^2 \rangle = \left\langle \left(\sum_{i=0}^N \lambda_i \right)^2 \right\rangle$ is mean-square displacement of Brownian particle during relaxation time of its velocity, where $N = \langle n \rangle - 1$ ($\langle n \rangle$ is from formula (6)).

Averaging we take into account that λ_{i+1} depends on λ_i , i.e. there is correlation. Therefore, it is necessary to obtain conditional distribution functions and their characteristics.

Taking into account that $m \gg 1$ and according to formula (6), we have

$$N = \langle n \rangle - 1 \approx \frac{m}{4} - 1 \approx \frac{m}{4}. \tag{10}$$

According to equality (5) from [8] we write distribution function of velocity u of Brownian particle after collision under condition, that before collision this particle had velocity u_0 (i.e. conditional distribution function):

$$\varphi(u/u_0) = C |u - u_0| e^{-\frac{1}{2} \left(\frac{m+1}{2} u - \frac{m-1}{2} u_0 \right)^2}.$$

To calculate the normalization factor C we use the normalization condition:

$$\int_{-\infty}^{\infty} \varphi(u/u_0) du = 1.$$

Calculating this integral we obtain:

$$C = \left(\frac{m+1}{2} \right)^2 \cdot \frac{1}{G_0(u_0)},$$

where $G_k(u_0) = \int_{-\infty}^{\infty} z^k |z| e^{-\frac{(u_0-z)^2}{2}} dz$ is the function from [8]. Here $u_0 - u = \frac{2}{m+1}z$, and for $G_k(u)$ from [8] $u_0 - u = \frac{2}{m-1}z$. Since $m \gg 1$, then $\frac{2}{m+1} \approx \frac{2}{m-1}$.

Conditional value $\langle u \rangle$ under condition u_0 :

$$\begin{aligned} \langle u \rangle / u_0 &= \int_{-\infty}^{\infty} u \varphi(u/u_0) du = \\ &= \frac{1}{G_0(u_0)} \int_{-\infty}^{\infty} \left(u_0 - \frac{2}{m+1} z \right) |z| e^{-\frac{1}{2} (u_0-z)^2} dz = \\ &= u_0 - \frac{2}{m+1} \cdot \frac{G_1(u_0)}{G_0(u_0)}. \end{aligned}$$

Here we have performed above mentioned substitution $u_0 - u = \frac{2}{m+1}z$.

Since mass of Brownian particle is much bigger than mass of particle of thermostat, then the change of velocity of the Brownian particle is small after one collision. Therefore, we suppose $G_0(u_0) \approx G_0(u)$, $G_1(u_0) \approx G_1(u)$. Taking into account that $|u_0| \ll 1$ we approximate functions $G_0(u)$, $G_1(u)$ [8], then we obtain $G_0(u_0) \approx 2$, $G_1(u_0) \approx 4u_0$. Therefore,

$$\langle u \rangle / u_0 \approx u_0 \left(1 - \frac{4}{m+1} \right). \quad (11)$$

Analogously we write conditional value $\langle u^2 \rangle$ under condition u_0 :

$$\begin{aligned} \langle u^2 \rangle / u_0 &= \int_{-\infty}^{\infty} u^2 \varphi(u/u_0) du = \\ &= u_0^2 - \frac{4u_0}{m+1} \cdot \frac{G_1(u_0)}{G_0(u_0)} + \frac{4}{(m+1)^2} \cdot \frac{G_2(u_0)}{G_0(u_0)} \approx \\ &\approx u_0^2 \left(1 - \frac{8}{m+1} \right) + \frac{8}{(m+1)^2}, \end{aligned} \quad (12)$$

where $G_2(u_0) \approx 4$ [8].

Here u is Brownian particle velocity after collision, i.e. u is the following after u_0 velocity of Brownian particle. Analogously for λ and λ_0 . Then using formulas (7) and (8) we obtain:

$$\langle \lambda \rangle \approx \sqrt{\frac{\pi}{2}} \langle |u| \rangle, \quad (13)$$

$$\langle \lambda^2 \rangle \approx \pi \langle u^2 \rangle. \quad (14)$$

Here, for the sake of simplicity, we do not use indices 1 for u and λ .

Using expressions (13), (11), (7) and (14), (12), (8), we find mean characteristics of displacement of Brownian particle:

$$\langle \lambda \rangle / u_0 \approx \sqrt{\frac{\pi}{2}} \langle |u| \rangle / u_0 \approx \sqrt{\frac{\pi}{2}} |u_0| \left(1 - \frac{4}{m+1} \right) \approx \lambda_0 \left(1 - \frac{4}{m+1} \right)$$

or taking into account $\lambda = \lambda_1$

$$\langle \lambda_i \rangle / \lambda_{i-1} \approx \lambda_{i-1} \left(1 - \frac{4}{m+1} \right).$$

$$\begin{aligned} \langle \lambda^2 \rangle / u_0 &\approx \pi \langle u^2 \rangle / u_0 \approx \pi \left(u_0^2 \left(1 - \frac{8}{m+1} \right) + \frac{8}{(m+1)^2} \right) \approx \\ &\approx \lambda_0^2 \left(1 - \frac{8}{m+1} \right) + \frac{8\pi}{(m+1)^2} \end{aligned}$$

or taking into account $\lambda = \lambda_1$

$$\langle \lambda_i^2 \rangle / \lambda_{i-1} \approx \lambda_{i-1}^2 \left(1 - \frac{8}{m+1} \right) + \frac{8\pi}{(m+1)^2}.$$

Denote

$$1 - \frac{4}{m} = \gamma, \tag{15}$$

$$\frac{8\pi}{m^2} = \delta, \tag{16}$$

then we obtain (taking into account that $m \gg 1$)

$$\langle \lambda_i \rangle / \lambda_{i-1} \approx \gamma \lambda_{i-1}, \tag{17}$$

$$\langle \lambda_i^2 \rangle / \lambda_{i-1} \approx \gamma^2 \lambda_{i-1}^2 + \delta. \tag{18}$$

We calculate mean square of displacement

$$\langle L^2 \rangle = \langle (\lambda_0 + \lambda_1 + \dots + \lambda_N)^2 \rangle$$

of Brownian particle during relaxation time of its velocity, starting from the last summand since this summand depends on previous ones. Therefore, numbering k ($k = 0, 1, 2, \dots, N$) of averaged quantities we perform from the end of the chain. We start, for example, from the k -th (from the end) summand.

Denote

$$S_k = \left(\sum_{j=0}^{N-k} \lambda_j \right)^2. \tag{19}$$

We average over the last summand (i.e. over the $(N-k)$ -th), using formulas (19), (17), (18):

$$\begin{aligned} \langle S_k \rangle_{N-k} &= \left\langle \left(\sum_{j=0}^{N-k-1} \lambda_j + \lambda_{N-k} \right)^2 \right\rangle_{N-k} = \\ &= \left(\sum_{j=0}^{N-k-1} \lambda_j \right)^2 + 2 \left(\sum_{j=0}^{N-k-1} \lambda_j \right) \langle \lambda_{N-k} \rangle_{N-k} + \langle \lambda_{N-k}^2 \rangle_{N-k} = \\ &= S_{k+1} + 2\gamma R_{k+1} + \gamma^2 \lambda_{N-k-1}^2 + \delta, \end{aligned} \tag{20}$$

where R_{k+1} is obtained from denotation

$$R_k = \left(\sum_{j=0}^{N-k} \lambda_j \right) \lambda_{N-k}. \tag{21}$$

Note, that in numbering $N - k - 1 = N - (k + 1)$.

$$\begin{aligned} \langle R_k \rangle_{N-k} &= \left\langle \left(\sum_{j=0}^{N-k-1} \lambda_j \right) \lambda_{N-k} + \lambda_{N-k}^2 \right\rangle_{N-k} = \\ &= \left(\sum_{j=0}^{N-k-1} \lambda_j \right) \langle \lambda_{N-k} \rangle_{N-k} + \langle \lambda_{N-k}^2 \rangle_{N-k} = \\ &= \gamma R_{k+1} + \gamma^2 \lambda_{N-k-1}^2 + \delta. \end{aligned} \tag{22}$$

It is obvious (formula (20)), that step-by-step averaging does not change the linear form

$$\mathcal{L}_k = S_k + a_k R_k + b_k \lambda_{N-k}^2 + c_k \delta, \tag{23}$$

where a_k, b_k, c_k are unknown coefficients. Under $k = 0$ $\mathcal{L}_0 = S_0$. Then from formula (23) $a_0 = b_0 = c_0 = 0$.

To determine coefficients a_k, b_k, c_k we perform the following averaging according to formulas (23), (20), (22) and (18):

$$\begin{aligned} \mathcal{L}_{k+1} &= \langle \mathcal{L}_k \rangle_{N-k} = (S_{k+1} + 2\gamma R_{k+1} + \gamma^2 \lambda_{N-k-1}^2 + \delta) + \\ &\quad + a_k (\gamma R_{k+1} + \gamma^2 \lambda_{N-k-1}^2 + \delta) + \\ &\quad + b_k (\gamma^2 \lambda_{N-k-1}^2 + \delta) + c_k \delta = \\ &= S_{k+1} + (\gamma a_k + 2\gamma) R_{k+1} + (\gamma^2 b_k + \gamma^2 a_k + \gamma^2) \lambda_{N-k-1}^2 + (1 + a_k + b_k + c_k) \delta. \end{aligned}$$

Thus, we obtain the recurrent relations:

$$\begin{cases} a_{k+1} = \gamma a_k + 2\gamma, \\ b_{k+1} = \gamma^2 b_k + \gamma^2 a_k + \gamma^2, \\ c_{k+1} = 1 + a_k + b_k + c_k, \end{cases}$$

from what, according to $a_0 = b_0 = c_0 = 0$, we obtain

$$\begin{aligned} a_1 &= 2\gamma, \\ a_2 &= 2\gamma^2 + 2\gamma, \\ a_3 &= 2\gamma^3 + 2\gamma^2 + 2\gamma, \\ &\dots\dots\dots \\ a_k &= 2\gamma(1 + \gamma + \gamma^2 + \dots + \gamma^{k-1}) = 2\gamma \frac{1-\gamma^k}{1-\gamma}; \end{aligned}$$

$$\begin{aligned}
 b_1 &= \gamma^2, \\
 b_2 &= \gamma^2(\gamma^2) + 2\gamma(\gamma^2) + \gamma^2 = \gamma^2(1 + \gamma)^2, \\
 &\dots\dots\dots \\
 b_k &= \gamma^2(1 + \gamma + \gamma^2 + \dots + \gamma^{k-1})^2 = \left(\frac{a_k}{2}\right)^2 = \left(\gamma \frac{1-\gamma^k}{1-\gamma}\right)^2; \\
 c_{k+1} &= 1 + a_k + b_k + c_k = 1 + 2\gamma \frac{1-\gamma^k}{1-\gamma} + \left(\gamma \frac{1-\gamma^k}{1-\gamma}\right)^2 + c_k = \\
 &= \left(1 + \gamma \frac{1-\gamma^k}{1-\gamma}\right)^2 + c_k.
 \end{aligned}$$

Therefore,

$$c_k = \sum_{j=0}^{k-1} \left(1 + \gamma \frac{1-\gamma^j}{1-\gamma}\right)^2 = \frac{1}{(1-\gamma)^2} \left(k - 2\gamma \frac{1-\gamma^k}{1-\gamma} + \gamma^2 \frac{1-\gamma^{2k}}{1-\gamma^2}\right).$$

Altogether, after all averagings for $k = N$ (i.e. before relaxation of velocity of Brownian particle), taking into account that numbering of averaged quantities was conducted from the end, i.e. $\lambda_{N-k} = \lambda_{N-N} = \lambda_0$ and according to formulas (19), (21) $S_N = \lambda_0^2$, $R_N = \lambda_0^2$, substituting a_N , b_N , c_N into formula (23), we obtain:

$$\begin{aligned}
 \mathcal{L}_N &= \lambda_0^2 \left(1 + 2\gamma \frac{1-\gamma^N}{1-\gamma} + \left(\gamma \frac{1-\gamma^N}{1-\gamma}\right)^2\right) + \\
 &\quad + \frac{1}{(1-\gamma)^2} \left(N - 2\gamma \frac{1-\gamma^N}{1-\gamma} + \gamma^2 \frac{1-\gamma^{2N}}{1-\gamma^2}\right) \delta = \\
 &= \lambda_0^2 \left(1 + \gamma \frac{1-\gamma^N}{1-\gamma}\right)^2 + \frac{1}{(1-\gamma)^2} \left(N - 2\gamma \frac{1-\gamma^N}{1-\gamma} + \gamma^2 \frac{1-\gamma^{2N}}{1-\gamma^2}\right) \delta.
 \end{aligned}$$

Substituting λ_0^2 , N , γ , δ according to formulas (8), (9), (10), (15), (16) and taking into account that $m \gg 1$ and $\mathcal{L}_N = \langle L^2 \rangle$ (since \mathcal{L}_N is calculated mean square of displacement of Brownian particle during relaxation time of its velocity), we obtain

$$\begin{aligned}
 \langle L^2 \rangle &\approx \frac{\pi}{m} \left(1 + \frac{m}{4}(1 - e^{-1})\right)^2 + \\
 &\quad + \frac{\pi}{2} \left(\frac{m}{4} - \frac{m}{2}(1 - e^{-1}) + \frac{m}{8}(1 - e^{-2})\right).
 \end{aligned}$$

Calculate

$$\left(1 + \frac{m}{4}(1 - e^{-1})\right)^2 = 1 + \frac{m}{2}(1 - e^{-1}) + \frac{m^2}{16}(1 - e^{-1})^2 \approx \frac{m^2}{16}(1 - e^{-1})^2,$$

since $m \gg 1$ and therefore the first and the second summands are much smaller than the third summand.

Then

$$\langle L^2 \rangle \approx \frac{\pi m}{16} (1 - e^{-1}) ((1 - e^{-1}) - 4) + \frac{\pi m}{16} (2 + (1 - e^{-2})).$$

Taking out of context $\frac{\pi m}{16}$ and performing arithmetic operations we obtain:

$$\langle L^2 \rangle \approx \frac{\pi m}{8} e^{-1}.$$

Taking into account that relaxation time of velocity of Brownian particle [8] $T_{rel.} = \frac{m\sqrt{2\pi}}{8}$ we have

$$\langle L^2 \rangle \approx \frac{\sqrt{2\pi}}{2} e^{-1} T_{rel.}. \quad (24)$$

Thus, mean square of displacement $\langle L^2 \rangle$ of Brownian particle during large number of collisions of this particle with particles of thermostat is in proportion to time, i.e. we obtain the law, corresponding to diffusion motion. Therefore, the kinetic equation for space part of the distribution function of Brownian particle in thermostat has the form of the diffusion equation:

$$\frac{\partial F}{\partial t} = D \frac{\partial^2 F}{\partial x^2},$$

where x is the coordinate of Brownian particle, t is time, D is diffusion coefficient.

For this diffusion equation

$$\langle L^2 \rangle = 2D\tau \quad (\text{the Einstein law}), \quad (25)$$

where τ is observation time interval, sufficiently large for Brownian particle to collide many times with particles of thermostat.

The equation (25) represents the Einstein law. Derived equation (24) corresponds to the Einstein law.

Thus, we denote $T_{rel.} = \tau$.

Therefore, using formulas (25), (24), we obtain:

$$\langle L^2 \rangle = 2D\tau \approx \frac{\sqrt{2\pi}}{2} e^{-1} \tau.$$

Hence

$$D \approx \frac{\sqrt{2\pi}}{4} e^{-1},$$

i.e. D does not depend on mass of Brownian particle.

Thus, it is derived the equation — the Einstein law and obtained the kinetic equation for space part of the distribution function of Brownian particle, which has the form of diffusion equation, for the system "Brownian particle in thermostat".

References

- [1] N. N. Bogolyubov, *Problems of a dynamical theory in statistical physics*, Gostekhizdat, Moscow (1946) [in Russian].
- [2] M. A. Stashenko, G. N. Gubal', Existence theorems for the initial value problem for the Bogolyubov chain of equations in the space of sequences of bounded functions, *Sib. Mat. Zhurn.*, **47**, No. 1 (2006), 188–205 (English transl.: *Siberian Math. J.*, **47**, No. 1, Springer Verlag, New York (2006), 152–168), doi: <http://dx.doi.org/10.1007/s11202-006-0015-8>.
- [3] C. Cercignani, V. I. Gerasimenko, D. Ya. Petrina, *Many-particle dynamics and kinetic equations*, Kluwer Acad. Publ., Dordrecht (1997).
- [4] R. Illner, M. Pulvirenti, A derivation of the BBGKY hierarchy for the hard sphere particle systems, *Transp. Theory and Statist. Phys.*, **16**, No. 7 (1987), 997–1012.
- [5] M. A. Stashenko, G. N. Gubal', Boltzmann-Grad boundary path for one-measurable system, *Sci. Bull. Volyn. State Univ.*, No. 1 (2002), 5–13 [in Ukrainian].
- [6] N. Bellomo, M. Lachowics, J. Polewczak, G. Toscani, *Mathematical topics in nonlinear kinetic theory II: Enskog equation*, World Scientific, Singapore (1991).
- [7] D. Dürr, S. Goldstein, J. L. Lebowitz, A mechanical model of Brownian motion, *Commun. Math. Phys.*, **78**, No. 4 (1981), 507–530.
- [8] H. M. Hubal, The Fokker-Planck Equation for the System "Brownian Particle in Thermostat" Based on the Presented Probability Approach, *J. Math. Phys., Anal., Geom.*, **6**, No. 1 (2010), 48–55.

