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The Fokker–Planck Equation for the System "Brownian Particle in Thermostat" Based on the Presented Probability Approach

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A one-dimensional system "Brownian particle in thermostat" is considered. The Fokker–Planck equation describing dynamics of the particle system under consideration is derived on the basis of the presented probability approach. The solution of the derived equation is also obtained.

Key words: Brownian particle, thermostat, the Fokker–Planck equation, the probability approach.

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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. [1–5].

The system "Brownian particle in thermostat" is an important case of many-particle many kind system, and the studying of this system is of selfdependent interest [6].

In the present paper it is derived the Fokker–Planck equation describing the dynamics of particle system under consideration, and it is obtained the solution of the derived equation based on the probability approach used to describe the system.

2. Description of Thermostat

We consider a one-dimensional system "Brownian particle in thermostat". All particles of thermostat are identical and have the mass $m_0 = 1$. The velocity distribution of particles of thermostat is equilibrium, the Maxwellian [7]:

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

The coordinates of the particles are uniformly distributed along a straight line on the admissible configurations. Later we can neglect the particle sizes.

The probability of location of particle in the small segment dl is determined by the expression

$$P = n\,dl, \tag{2}$$

where n is the concentration of particles.

Indeed, let the length of rod, on which N particles are located, be equal to L. Taking into account that the coordinate distribution is equilibrium and passing to the thermodynamic limit we find the probability of location of k particles in this segment as the Poisson distribution

$$P_k = \frac{(n\,dl)^k}{k!} e^{-n\,dl}.$$

By remaining the first order of smallness over dl, we obtain (2).

We denote the concentration by $n = 1$. It is obvious that the probability of the particle to be located in the small segment dl and have a velocity in the interval $[v, v + dv)$ is equal to $dl\varphi(v)\,dv$.

In the thermostat considered, there is a massive Brownian particle with mass $m \gg 1$. The problem is to describe its behaviour, i.e., to find the distribution function of coordinate q and velocity u depending on time t.

Probability of the Brownian particle having velocity in the interval $[u_0, u_0 + du_0)$ to collide with the particle of thermostat having velocity in the interval $[v_0, v_0 + dv_0)$ during a little period of time dt is determined by the expression

$$\Phi(u_0, v_0)\,du_0 dv_0 dt = \varphi(v_0)|u_0 - v_0|\,du_0 dv_0 dt. \tag{3}$$

By the law of conservation of momentum and energy we obtain that the Brownian particle must collide with the particle having the velocity

$$v_0 = \frac{m+1}{2}u - \frac{m-1}{2}u_0. \tag{4}$$

Notice that collisions of particles do not change equilibrium distribution.

By (1), (3), (4) we can write the expression for $\Phi(u_0, u)\, du_0 du dt$, that is a probability of the fact that the Brownian particle having velocity in the interval $[u_0, u_0 + du_0)$, after collision with the particle of thermostat happened at the time dt, will have velocity in the interval $[u, u + du)$:

$$\Phi(u_0, u)\, du_0 du dt = \frac{1}{\sqrt{2\pi}} \left(\frac{m+1}{2}\right)^2 e^{-\frac{1}{2}\left(\frac{m+1}{2}u - \frac{m-1}{2}u_0\right)^2} |u - u_0|\, du_0 du dt. \quad (5)$$

We write the probability $P(u_0, t)$ of lacking of collisions of the Brownian particle moving with velocity u_0 at time t. The probability of lacking of collisions during a little period of time dt is determined by the expression

$$1 - f(u_0)\, dt, \quad (6)$$

where

$$f(u_0) = \int_{-\infty}^{\infty} \varphi(v_0) |u_0 - v_0|\, dv_0.$$

Then we write

$$P(u_0, t + dt) = P(u_0, t)(1 - f(u_0)\, dt),$$

hence

$$P(u_0, t) = e^{-f(u_0)t}.$$

3. The Kinetic Equation

We use the velocity part of distribution function since the coordinate of Brownian particle is included only into the initial distribution function determined as a product of velocity and configuration multipliers. The kinetic equation is derived directly from (5), (6).

We consider a change of distribution function $F(u, t)$ for infinitely little period of time dt:

- velocity of particle may not change (if there is no collision);
- velocity of particle may change after one collision (probabilities of two, three collisions should be neglected).

Therefore we have the following equality:

$$F(u, t + dt)\, du = F(u, t)\, du(1 - dt \int_{-\infty}^{\infty} \Phi(u, u_1)\, du_1) + du \int_{-\infty}^{\infty} F(u_0, t)\Phi(u_0, u)\, du_0 dt,$$

hence there follows

$$\frac{\partial F(u,t)}{\partial t} = -F(u,t)\int\limits_{-\infty}^{\infty}\Phi(u,u_1)\,du_1 + \int\limits_{-\infty}^{\infty}F(u_0,t)\Phi(u_0,u)\,du_0. \tag{7}$$

To pass to the Fokker–Planck equation we act in the following way. Since $m \gg 1$, then the change of velocity of the Brownian particle is small after one collision, therefore we represent $F(u_0,t)$ as the series over powers of difference (u_0-u) and substitute into (7). As a result, we obtain the equation

$$\begin{aligned}\frac{\partial F(u,t)}{\partial t} = F(u,t)&\left(\int\limits_{-\infty}^{\infty}\Phi(u_0,u)\,du_0 - \int\limits_{-\infty}^{\infty}\Phi(u,u_1)\,du_1\right)\\ &+\frac{\partial F(u,t)}{\partial u}\int\limits_{-\infty}^{\infty}(u_0-u)\Phi(u_0,u)\,du_0\\ &+\frac{1}{2!}\frac{\partial^2 F(u,t)}{\partial u^2}\int\limits_{-\infty}^{\infty}(u_0-u)^2\Phi(u_0,u)\,du_0\\ &+\frac{1}{3!}\frac{\partial^3 F(u,t)}{\partial u^3}\int\limits_{-\infty}^{\infty}(u_0-u)^3\Phi(u_0,u)\,du_0+\dots.\end{aligned} \tag{8}$$

The integrals in (8) have the form

$$\begin{aligned}\int\limits_{-\infty}^{\infty}(u_0-u)^k\frac{1}{\sqrt{2\pi}}\left(\frac{m+1}{2}\right)^2 e^{-\frac{1}{2}\left(\frac{m+1}{2}u-\frac{m-1}{2}u_0\right)^2}|u_0-u|\,du_0\\ = \frac{1}{\sqrt{2\pi}}\left(\frac{m+1}{m-1}\right)^2\left(\frac{2}{m-1}\right)^k\int\limits_{-\infty}^{\infty}z^k|z|e^{-\frac{(u-z)^2}{2}}\,dz,\end{aligned}$$

where the substitution $u_0-u=\frac{2}{m-1}z$ is performed.

We introduce the following functions:

$$G_k(u)=\int\limits_{-\infty}^{\infty}z^k|z|e^{-\frac{(u-z)^2}{2}}\,dz$$

and consider their conditions.

Differentiating $G_k(u)$, we obtain the recurrent relation

$$G_{k+1}(u)=uG_k(u)+\frac{dG_k(u)}{du},$$

which allows us to express $G_k(u)$ by $G_0(u)$, besides the explicit expression for $G_0(u)$ has the form

$$G_0(u) = 2e^{-\frac{u^2}{2}} + \sqrt{2\pi}u\, erf\left(\frac{u}{\sqrt{2}}\right),$$

where $erf(x)$ is the erf integral.

Expanding these functions into series, we obtain the following equalities:

$$\begin{aligned} G_0(u) &= 2 + u^2 - \frac{1}{12}u^4 + \cdots ; \\ G_1(u) &= 4u + \frac{2}{3}u^3 + \cdots ; \\ G_2(u) &= 4 + 6u^2 + \frac{2}{3}u^4 + \cdots ; \\ G_3(u) &= 16u + 8\frac{2}{3}u^3 + \cdots . \end{aligned}$$

The second integral in (8) has the form

$$\begin{aligned} \int_{-\infty}^{\infty} \Phi(u, u_1)\, du_1 &= \left(\frac{m+1}{2}\right)^2 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(\frac{m+1}{2}u_1 - \frac{m-1}{2}u\right)^2} |u_1 - u|\, du_1 \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |z| e^{-\frac{(u-z)^2}{2}}\, dz = \frac{1}{\sqrt{2\pi}} G_0(u), \end{aligned}$$

where the substitution $u_1 = u - \frac{2}{m+1}z$ is performed.

Equation (8) in the terms of the functions $G_k(u)$ has the form

$$\begin{aligned} \frac{\partial F(u,t)}{\partial t} &= a(u)F(u,t) + b(u)\frac{\partial F(u,t)}{\partial u} \\ &\quad + D(u)\frac{\partial^2 F(u,t)}{\partial u^2} + S(u)\frac{\partial^3 F(u,t)}{\partial u^3} + \ldots , \end{aligned} \tag{9}$$

where

$$\begin{aligned} a(u) &= \frac{4m}{(m-1)^2}\frac{1}{\sqrt{2\pi}}G_0(u); \\ b(u) &= \left(\frac{m+1}{m-1}\right)^2 \frac{2}{m-1}\frac{1}{\sqrt{2\pi}}G_1(u); \\ D(u) &= \frac{1}{2}\left(\frac{m+1}{m-1}\right)^2 \left(\frac{2}{m-1}\right)^2 \frac{1}{\sqrt{2\pi}}G_2(u); \\ S(u) &= \frac{1}{6}\left(\frac{m+1}{m-1}\right)^2 \left(\frac{2}{m-1}\right)^3 \frac{1}{\sqrt{2\pi}}G_3(u). \end{aligned}$$

From the choice of system of units we have that the root-mean-square velocity of particles of thermostat is equal to one. By the theorem on equidistribution of energy we conclude that the velocity of Brownian particle has the order $m^{-\frac{1}{2}}$. This fact allows us to find the order of smallness of all summands included into equation (9).

We estimate the order of smallness of all summands in (9):

$$\begin{aligned}
\sqrt{2\pi}a(u)F(u,t) &= \frac{8}{m}F(u,t) + \left(\frac{4}{m}u^2 + \frac{16}{m^2}\right)F(u,t) + \cdots;\\
\sqrt{2\pi}b(u)\frac{\partial F(u,t)}{\partial u} &= \frac{8}{m}u\frac{\partial F(u,t)}{\partial u} + \left(\frac{4}{3m}u^3 + \frac{40}{m^2}u\right)\frac{\partial F(u,t)}{\partial u} + \cdots;\\
\sqrt{2\pi}D(u)\frac{\partial^2 F(u,t)}{\partial u^2} &= \frac{8}{m^2}\frac{\partial^2 F(u,t)}{\partial u^2} + \left(\frac{12}{m^2}u^2 + \frac{48}{m^3}\right)\frac{\partial^2 F(u,t)}{\partial u^2} + \cdots;\\
\sqrt{2\pi}S(u)\frac{\partial^3 F(u,t)}{\partial u^3} &= \frac{64}{3m^3}u\frac{\partial^3 F(u,t)}{\partial u^3} + \cdots.
\end{aligned} \tag{10}$$

By the formulae of (10) we obtain the equation

$$\begin{aligned}
\sqrt{2\pi}\frac{\partial F(u,t)}{\partial t} &= \frac{8}{m}F(u,t) + \frac{8}{m}u\frac{\partial F(u,t)}{\partial u} + \frac{8}{m^2}\frac{\partial^2 F(u,t)}{\partial u^2}\\
&+ \frac{4}{m^2}(mu^2+4)F(u,t) + \frac{4u}{3m^2}(mu^2+30)\frac{\partial F(u,t)}{\partial u}\\
&+ \frac{12}{m^3}(mu^2+4)\frac{\partial^2 F(u,t)}{\partial u^2} + \frac{64}{3m^3}u\frac{\partial^3 F(u,t)}{\partial u^3} + \cdots.
\end{aligned}$$

By remaining only the summands of order of smallness $m^{-\frac{1}{2}}$ in this equation, we obtain the Fokker–Planck equation

$$\frac{m}{8}\sqrt{2\pi}\frac{\partial F(u,t)}{\partial t} = F(u,t) + u\frac{\partial F(u,t)}{\partial u} + \frac{1}{m}\frac{\partial^2 F(u,t)}{\partial u^2}. \tag{11}$$

4. On a Solution of the Fokker-Planck Equation

After substituting $\xi = \sqrt{\frac{m}{2}}u$ and $\tau = \frac{4t}{m\sqrt{2\pi}}$ equation (11) has the form

$$\frac{\partial F(\xi,\tau)}{\partial \tau} = 2F(\xi,\tau) + 2\xi\frac{\partial F(\xi,\tau)}{\partial \xi} + \frac{\partial^2 F(\xi,\tau)}{\partial \xi^2}. \tag{12}$$

The solution of equation (12) satisfies the conditions of boundedness and integrability, and it is represented as the formula

$$F(\xi,\tau) = \sum_{k=0}^{\infty} C_k e^{-\xi^2} H_k(\xi) e^{-2k\tau}, \tag{13}$$

where $H_k(\xi)$ are the Hermite polynomials. Taking into account the condition of orthogonality of polynomials and the initial data $F(\xi,\tau)|_{\tau=0} = F_0(\xi)$, we determine the coefficients C_k of the series (13)

$$C_k = \frac{\int\limits_{-\infty}^{\infty} F_0(\xi) H_k(\xi)\, d\xi}{2^k k! \sqrt{\pi}} .$$

We denote $F_0(\xi) = \delta(\xi - \xi_0)$. Then the solution (13) of equation (12) has the form

$$F(\xi,\tau) = \sum_{k=0}^{\infty} \frac{H_k(\xi_0)}{2^k k! \sqrt{\pi}} e^{-\xi^2} H_k(\xi) e^{-2k\tau}. \tag{14}$$

Notice that as $\tau \to \infty$ the first term of the series (14) remains only, i.e., there is a limiting distribution

$$\overline{F}(\xi) = \frac{1}{\sqrt{\pi}} e^{-\xi^2},$$

or in the terms of variables u

$$\overline{F}(u) = \sqrt{\frac{m}{2\pi}} e^{-\frac{mu^2}{2}}$$

the distribution passes to the Maxwell distribution (there is a relaxation).

Characteristic relaxation time is determined by the formula

$$T_{rel.} = \frac{m\sqrt{2\pi}}{8}.$$

By (14) we obtain that the mean velocity of Brownian particle changes according to the law

$$\langle \xi \rangle = \int\limits_{-\infty}^{\infty} \xi F(\xi,\tau)\, d\xi = \xi_0 e^{-2\tau},$$

or in initial system of units

$$\langle u \rangle = u_0 e^{-\frac{8t}{m\sqrt{2\pi}}}.$$

The dispersion of velocity of Brownian particle has the form

$$\sigma_\xi^2 = \langle \xi^2 \rangle - \langle \xi \rangle^2 = \langle \frac{H_2}{4} + \frac{H_0}{2} \rangle - (\xi_0 e^{-2\tau})^2 =$$
$$= \left(\xi_0^2 - \frac{1}{2} \right) e^{-4\tau} + \frac{1}{2} - (\xi_0 e^{-2\tau})^2 = \frac{1}{2}(1 - e^{-4\tau}),$$

or in the initial system of units

$$\sigma_u^2 = \frac{1}{m}(1 - e^{-\frac{16t}{m\sqrt{2\pi}}}).$$

Thus, it is obtained the Fokker–Planck equation for the system "Brownian particle in thermostat" and its solution in the form of the series over the Hermite polynomials.

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