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## Abstract

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# TIME CORRELATIONS IN CLASSICAL STATISTICAL SYSTEMS CONSISTING OF A LARGE NUMBER OF INTERACTING PARTICLES

*(Presented by Academician N. N. Bogolyubov, 19 IX 1956)*

In certain problems of the statistical physics of classical systems consisting of a large number of interacting particles, it is necessary to know the correlation function $\Phi_1(t, x_1 \mid x_0)$, which gives the probability that, in time $t$, a particle of the system will pass into an infinitesimally small neighborhood $dx_1$ of the dynamical state $x_1$ from the dynamical state $x_0$. To determine this function it seems quite reasonable to use the representation of a Markov random process. The resulting equation for $\Phi_1(t, x_1 \mid x_0)$ will, of course, be an equation of the Fokker–Planck type. The problem of determining the coefficients entering it, which are connected with physical ideas about dynamical friction and diffusion in velocity space, can be solved by special methods ([1],[2]). However, such an approach—quite apart from the fact that it suffers from excessive phenomenological character, since it leaves aside the derivation of the equation of Fokker–Planck type*—breaks down completely in those cases where the representation of a Markov random process is inapplicable, for example, in the case of a real gas. In the present communication we shall present the results of applying another method—the method of the chain of linked distribution functions ([3]), which, from a unified point of view, gives both the derivation, for $\Phi_1(t, x_1 \mid x_0)$, of the Fokker–Planck equation in the case of systems with long-range interaction (systems of plasma type), and the derivation of an equation for systems with short-range interaction (a real gas), where the idea of a Fokker–Planck mechanism loses its force.

Our consideration will concern a system of $N$ identical classical particles, interacting pairwise with one another by a potential $\Phi(|q|)$ and enclosed in some macroscopic volume $V$.

Let us introduce into the discussion the following chain of one-, two-, etc. argument correlation functions:

$$\Phi_s(t, x_1, \dots, x_s \mid x_0) = V^{s-1} \frac{\left\langle \delta(x_1(0) - x_0) \prod_{(1 \le i \le s)} \delta(x_i(t) - x_i) \right\rangle}{\langle \delta(x_1(0) - x_0) \rangle}, \quad (1)$$

which give the conditional probability of finding, at time $t$, a complex of $s$ particles of the system, respectively, in infinitesimally small neighborhoods $dx_1, \dots, dx_s$ of the dynamical states $x_1, \dots, x_s$, if at the initial moment the particle of this complex with index 1 was in the dynamical state $x_0$. The symbol $\langle \dots \rangle$ denotes the usual statistical averaging over the initial states of the system; $x_1(0)$ and $x_i(t)$ are, respectively, the dynamical state of the first particle of the complex at the initial moment and of the $i$-th particle of the complex at the moment $t$. The factor $V^{s-1}$ is introduced to make it possible correctly to carry out the limiting transition $N \to \infty$, $V \to \infty$, $V/N = v = \text{const}$. The first of

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* A derivation is known ([4]) of an equation of Fokker-Planck type for a special model of coupled harmonic oscillators.

of the introduced functions $\Phi_1(t, x_1 \mid x_0)$ is precisely the probability of transition of a particle of the system in time $t$ into an infinitesimally small neighborhood $dx_1$ of the dynamical state $x_1$, if this particle was initially in the dynamical state $x_0$. To obtain another important correlation function $\Psi_1(t, x_1 \mid x_0)$, giving the probability of finding, at time $t$, a particle of the system in an infinitesimally small neighborhood $dx_1$ of the dynamical state $x_1$ under the condition that at $t = 0$ some other particle of the system was in the state $x_0$ (this function is a direct generalization of the ordinary pair distribution function and coincides with it at $t = 0$), it is necessary to know the function $\Phi_2(t, x_1, x_2 \mid x_0)$; its integral with respect to the first argument is equal to the function $\Psi_1$:

$$\Psi_1(t, x_1 \mid x_0) = \int \Phi_2(t, x, x_1 \mid x_0)\, dx. \quad (2)$$

It is not difficult, by differentiating (1), to establish the following chain of equations for the functions $\Phi_s(t, x_1, \dots, x_s \mid x_0)$:

$$\frac{\partial \Phi_s(t, x_1, \dots, x_s \mid x_0)}{\partial t} = [H_s; \Phi_s(t, x_1, \dots, x_s \mid x_0)] + \frac{1}{v} \int \left[ \sum_{(1 \le i \le s)} \Phi(|q_i - q|);\ \Phi_{s+1}(t, x_1, \dots, x_s, x \mid x_0) \right] dx, \quad (3)$$

where $[\,;\,]$ denotes the Poisson brackets with respect to the variables $x_1, \dots, x_s$; $H_s$ is the Hamiltonian of the $s$-particle complex. The chain of equations (3) coincides with the chain of equations for the ordinary distribution functions $F_s(t, x_1, \dots, x_s)$, reducible to ([3]):

$$\frac{\partial F_s(t, x_1, \dots, x_s)}{\partial t} = [H_s; F_s(t, x_1, \dots, x_s)] + \frac{1}{v} \int \left[ \sum_{(1 \le i \le s)} \Phi(|q_i - q|);\ F_{s+1}(t, x_1, \dots, x_s, x) \right] dx. \tag{4}$$

In contrast to (4), the chain of equations (3) must be solved with the following initial conditions:

$$\Phi_s(t, x_1, \dots, x_s \mid x_0)|_{t=0} = \delta(x_1 - x_0) \frac{F_s(0, x_1, \dots, x_s)}{F_1(0, x_1)}, \tag{5}$$

where $F_s(0, x_1, \dots, x_s)$ are the initial conditions for the chain (4).

Methods for solving the chain (4) were developed by N. N. Bogolyubov ([3]). In our case, in view of the close connection of the introduced functions $\Phi_s(t, x_1, \dots, x_s \mid x_0)$ with the ordinary correlation functions $F_s(t, x_1, \dots, x_s)$, (3) and (4) must be solved jointly. In doing so, it proves possible to use a large part of the ideas from ([3]).

We shall seek a solution of (3) and (4), valid for times much larger than the free-path time, in a form in which time enters through the functional dependence on the first correlation functions:

$$\Phi_s(t, x_1, \dots, x_s \mid x_0) = \Phi_s(x_1, \dots, x_s \mid x_0;\ F_1, \Phi_1), \tag{6}$$

$$F_s(t, x_1, \dots, x_s) = F_s(x_1, \dots, x_s;\ F_1) \tag{7}$$

for the correlation functions for $s = 2, 3$, etc. The first correlation functions themselves are assumed to satisfy the equations

$$\frac{\partial \Phi_1(t, x_1 \mid x_0)}{\partial t} = B(x_1 \mid x_0;\ F_1, \Phi_1), \tag{8}$$

$$\frac{\partial F_1(t, x_1)}{\partial t} = A(x_1;\ F_1), \tag{9}$$

where $A(x_1; F_1)$ and $B(x_1 \mid x_0; F_1, \Phi_1)$ are functionals, respectively, of $F_1$ and of $F_1, \Phi_1$; these functionals are determined by means of the functionals $F_2(x_1, x_2; F_1)$

and $\Phi_2(x_1, x_2; F_1, \Phi_1)$ from the first equations of chains (3) and (4), respectively. From the subsequent equations of chains (3) and (4) we obtain equations relating the functionals $F_s(x_1, \dots, x_s; F_1)$ and $\Phi_s(x_1, \dots, x_s \mid x_0; F_1, \Phi_1)$ to the subsequent functionals $F_{s+1}(x_1, \dots, x_{s+1}; F_1)$ and $\Phi_{s+1}(x_1, \dots, x_{s+1} \mid x_0; F_1, \Phi_1)$, respectively ($s \ge 2$).

In order to single out a unique solution of the problem it proves necessary to impose on the functionals $F_s(x_1, \dots, x_s; F_1)$ and $\Phi_s(x_1, \dots, x_s \mid x_0; F_1, \Phi_1)$ the following additional conditions, which have the physical meaning of conditions of weakening of correlations:

$$S_{-t}^{(s)} \left\{ F_s(x_1, \dots, x_s; S_t^{(1)} F_1) - \prod_{(1 \le i \le s)} S_t^{(1)} F_1 \right\} \to 0 \quad \text{as } t \to +\infty \quad (s \ge 2), \tag{10}$$

$$S_{-t}^{(s)} \left\{ \Phi_s(x_1, \dots, x_s \mid x_0; S_t^{(1)} F_1, S_t^{(1)} \Phi_1) - S_t^{(1)} \Phi_1 \prod_{(2 \le i \le s)} S_t^{(1)} F_1 \right\} \to 0$$

$$\text{as } t \to +\infty \quad (s \ge 2), \tag{11}$$

in which the operator $S_{-t}^{(s)}$ is defined as follows: it transforms an arbitrary function $\varphi(x_1, \dots, x_s)$ into the function $\varphi(t, x_1, \dots, x_s)$, which is a solution of the equation

$$\frac{\partial \varphi(t, x_1, \dots, x_s)}{\partial t} = [H_s; \varphi(t, x_1, \dots, x_s)], \tag{12}$$

satisfying the initial condition

$$\varphi(t, x_1, \dots, x_s)\big|_{t=0} = \varphi(x_1, \dots, x_s); \tag{13}$$

$H_s$ is the Hamiltonian of the $s$-particle complex.

Bearing in mind systems with long-range interaction, we assume that the potential energy $\Phi(|q_i - q|) = \varepsilon \psi(|q_i - q|)$, where $\varepsilon$ is a small parameter, and expand the desired functionals in its powers:

$$B(x_1 \mid x_0; F_1, \Phi_1) = B_0(x_1 \mid x_0; F_1, \Phi_1) + \varepsilon B_1(x_1 \mid x_0; F_1, \Phi_1) + \dots, \tag{14}$$

$$A(x_1; F_1) = A_0(x_1; F_1) + \varepsilon A_1(x_1; F_1) + \dots, \tag{15}$$

$$\Phi_s(x_1, \dots, x_s \mid x_0; F_1, \Phi_1) = \Phi_s^0(x_1, \dots, x_s \mid x_0; F_1, \Phi_1) +$$

$$+ \varepsilon \Phi_s^1(x_1, \dots, x_s \mid x_0; F_1, \Phi_1) + \dots \quad (s \ge 2), \tag{16}$$

$$F_s(x_1, \dots, x_s; F_1) = F_s^0(x_1, \dots, x_s; F_1) + \varepsilon F_s^1(x_1, \dots, x_s; F_1) + \dots \quad (s \geq 2). \tag{17}$$

In this case, after some calculations, it turns out to be possible to obtain, in the second approximation, in the case of statistical equilibrium, the following Fokker–Planck-type equation for $\Phi_1(t, x_1 \mid x_0)$

$$\frac{\partial \Phi_1(t, x_1 \mid x_0)}{\partial t} = -\sum_{(1\leq\alpha\leq 3)} \frac{p_1^\alpha}{m} \frac{\partial \Phi_1(t, x_1 \mid x_0)}{\partial q_1^\alpha} +$$

$$+\frac{1}{2} \sum_{\substack{(1\leq\alpha\leq 3)\\(1\leq\beta\leq 3)}} \frac{\partial^2}{\partial p_1^\alpha \partial p_1^\beta} \left( \langle \Delta p_1^\alpha \Delta p_1^\beta \rangle \Phi_1(t, x_1 \mid x_0) \right) -$$

$$-\sum_{(1\leq\alpha\leq 3)} \frac{\partial}{\partial p_1^\alpha} \left( \langle \Delta p_1^\alpha \rangle \Phi_1(t, x_1 \mid x_0) \right), \tag{18}$$

$$\Phi_1(t, x_1 \mid x_0)\big|_{t=0} = \delta(x_1 - x_0), \tag{19}$$

where

$$\langle \Delta p_1^\alpha \rangle = -\frac{1}{m\theta} \sum_{(1\leq\beta\leq 3)} \langle \Delta p_1^\alpha \Delta p_1^\beta \rangle, \tag{20}$$

$$\left\langle \Delta p_1^\alpha \Delta p_1^\beta \right\rangle = 2K \frac{\partial^2}{\partial p_1^\alpha \partial p_1^\beta} \int_{(p_2)} |p_2 - p_1| \frac{1}{(2\pi m\theta)^{3/2}} e^{-\frac{p_2^2}{2m\theta}} \, dp_2, \tag{21}$$

$$K = \frac{\pi m}{2v} \int_0^\infty r^3 F^2(r)\, dr, \qquad F(r) = \int_{-\infty}^{+\infty} \frac{\Phi'\left(\sqrt{x^2 + r^2}\right)}{\sqrt{x^2 + r^2}}\, dx. \tag{22}$$

In the case of a pure Coulomb potential, the integral for $F(r)$ is divergent, and it is necessary to resort to the usual procedure of cutting it off below at the interparticle distance $d$ and above at the Debye length $\lambda_D$; then for $K$, in the case of a pure Coulomb potential, we obtain

$$K = \frac{2\pi m e^4}{v} \ln \frac{\lambda_D}{d}. \tag{23}$$

After this, the expressions obtained for the coefficients (20), (21) of the Fokker–Planck equation can be compared with those calculated by Chandrasekhar [1] and by Gasiorowicz, Neuman, and Riddell [2]. The expressions obtained by us are in complete agreement with the results of the authors cited.

An interesting equation is obtained in the case of systems with short-range interaction. In this case we regard the parameter $1/v$ as small. We seek the required functionals in the form of expansions in powers of the small parameter:

$$B(x_1|x_0;\, F_1, \Phi_1) = B_0(x_1|x_0;\, F_1, \Phi_1) + \frac{1}{v} B_1(x_1|x_0;\, F_1, \Phi_1) + \cdots, \tag{24}$$

$$A(x_1;\, F_1) = A_0(x_1;\, F_1) + \frac{1}{v} A_1(x_1;\, F_1) + \cdots, \tag{25}$$

$$\Phi_s(x_1, \dots, x_s|x_0;\, F_1, \Phi_1) = \Phi_s^0(x_1, \dots, x_s|x_0;\, F_1, \Phi_1) +$$

$$+ \frac{1}{v} \Phi_s^1(x_1, \dots, x_s|x_0;\, F_1, \Phi_1) + \cdots \quad (s \geqslant 2), \tag{26}$$

$$F_s(x_1, \dots, x_s;\, F_1) = F_s^0(x_1, \dots, x_s;\, F_1) + \frac{1}{v} F_s^1(x_1, \dots, x_s;\, F_1) + \cdots \quad (s \geqslant 2). \tag{27}$$

After some calculations, in the case of statistical equilibrium, in the special case of absolutely hard spheres, we obtain the equation for $\Phi_1(t, x_1|x_0)$:

$$\frac{\partial \Phi_1(t, q_1, p_1|x_0)}{\partial t} = - \sum_{(1 \le \alpha \le 3)} \frac{p_1^\alpha}{m} \frac{\partial \Phi_1(t, q_1, p_1|x_0)}{\partial q_1^\alpha} +$$

$$+ \frac{1}{v} \int_0^{2\pi} \int_0^{\infty} \int_{(p_2)} \frac{|p_1 - p_2|}{m} \left\{ \Phi_1(t, q_1, p_1^*|x_0) \frac{e^{-\frac{p_2^{*2}}{2m\theta}}}{(2\pi m\theta)^{3/2}} \right.$$

$$\left. - \Phi_1(t, q_1, p_1|x_0) \frac{e^{-\frac{p_2^2}{2m\theta}}}{(2\pi m\theta)^{3/2}} \right\} dp_2\, a\, da\, d\varphi, \tag{28}$$

$$\Phi_1(t, q_1, p_1|x_0)\big|_{t=0} = \delta(q_1 - q_0)\delta(p_1 - p_0), \tag{29}$$

where $p_1^*$ and $p_2^*$ are the momenta of the particles after the collision, for which $a$ is the impact parameter and $\varphi$ the azimuthal angle; $p_1$ and $p_2$ are the momenta of these particles before the collision.

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*Note: Figure translations are in progress. See original paper for figures.*