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Abstract

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PHYSICS

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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 $\Phi_1(t, x_1 | x_0)$, 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 $\Phi_1(t, x_1 | x_0)$ 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 $\Phi_1(t, x_1 | x_0)$, 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:

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

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 $N \rightarrow \infty$, $V \rightarrow \infty$, $V/N = v = \text{const}$. The first of

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

of the introduced functions $\Phi_1(t, x_1 | x_0)$ 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 $\Psi_1(t, x_1 | x_0)$, 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 $\Phi_2(t, x_1, x_2 | x_0)$; its integral with respect to the first argument is equal to the function Ψ_1 :

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

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

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

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⁾:

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

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

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

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 $\Phi_s(t, x_1, \dots, x_s | x_0)$ 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:

$$\Phi_s(t, x_1, \dots, x_s | x_0) = \Phi_s(x_1, \dots, x_s | x_0; F_1, \Phi_1), \quad (6)$$

$$F_s(t, x_1, \dots, x_s) = F_s(x_1, \dots, x_s; F_1) \quad (7)$$

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

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

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

where $A(x_1; F_1)$ and $B(x_1 | x_0; F_1, \Phi_1)$ are functionals, respectively, of F_1 and of F_1, Φ_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 $\Phi_s(x_1, \dots, x_s | x_0; F_1, \Phi_1)$ to the subsequent functionals $F_{s+1}(x_1, \dots, x_{s+1}; F_1)$ and $\Phi_{s+1}(x_1, \dots, x_{s+1} | x_0; F_1, \Phi_1)$, respectively ($s \geq 2$).

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 $\Phi_s(x_1, \dots, x_s | x_0; F_1, \Phi_1)$ the following additional conditions, which have the physical meaning of conditions of weakening of correlations:

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

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

$$\text{as } t \rightarrow +\infty \quad (s \geq 2), \quad (11)$$

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

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

satisfying the initial condition

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

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 ε is a small parameter, and expand the desired functionals in its powers:

$$B(x_1 | x_0; F_1, \Phi_1) = B_0(x_1 | x_0; F_1, \Phi_1) + \varepsilon B_1(x_1 | x_0; F_1, \Phi_1) + \dots, \quad (14)$$

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

$$\begin{aligned} \Phi_s(x_1, \dots, x_s | x_0; F_1, \Phi_1) &= \Phi_s^0(x_1, \dots, x_s | x_0; F_1, \Phi_1) + \\ &+ \varepsilon \Phi_s^1(x_1, \dots, x_s | x_0; F_1, \Phi_1) + \dots \quad (s \geq 2), \end{aligned} \quad (16)$$

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

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 $\Phi_1(t, x_1 | x_0)$

$$\begin{aligned} \frac{\partial \Phi_1(t, x_1 | x_0)}{\partial t} = & - \sum_{(1 \leq \alpha \leq 3)} \frac{p_1^\alpha}{m} \frac{\partial \Phi_1(t, x_1 | x_0)}{\partial q_1^\alpha} + \\ & + \frac{1}{2} \sum_{\substack{(1 \leq \alpha \leq 3) \\ (1 \leq \beta \leq 3)}} \frac{\partial^2}{\partial p_1^\alpha \partial p_1^\beta} (\langle \Delta p_1^\alpha \Delta p_1^\beta \rangle \Phi_1(t, x_1 | x_0)) - \\ & - \sum_{(1 \leq \alpha \leq 3)} \frac{\partial}{\partial p_1^\alpha} (\langle \Delta p_1^\alpha \rangle \Phi_1(t, x_1 | x_0)), \end{aligned} \quad (18)$$

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

where

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

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

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

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 λ_D ; then for K , in the case of a pure Coulomb potential, we obtain

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

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:

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

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

$$\begin{aligned} \Phi_s(x_1, \dots, x_s|x_0; F_1, \Phi_1) &= \Phi_s^0(x_1, \dots, x_s|x_0; F_1, \Phi_1) + \\ &+ \frac{1}{v}\Phi_s^1(x_1, \dots, x_s|x_0; F_1, \Phi_1) + \dots \quad (s \geq 2), \end{aligned} \quad (26)$$

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

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

$$\begin{aligned} \frac{\partial \Phi_1(t, q_1, p_1|x_0)}{\partial t} &= - \sum_{(1 \leq \alpha \leq 3)} \frac{p_1^\alpha}{m} \frac{\partial \Phi_1(t, q_1, p_1|x_0)}{\partial q_1^\alpha} + \\ &+ \frac{1}{v} \int_0^{2\pi} \int_0^\infty \int_{(p_2)} \frac{|p_1 - p_2|}{m} \left\{ \Phi_1(t, q_1, p_1^*|x_0) \frac{e^{-\frac{p_2^{*2}}{2m\theta}}}{(2\pi m\theta)^{3/2}} \right. \\ &\quad \left. - \Phi_1(t, q_1, p_1|x_0) \frac{e^{-\frac{p_2^2}{2m\theta}}}{(2\pi m\theta)^{3/2}} \right\} dp_2 a da d\varphi, \end{aligned} \quad (28)$$

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

where p_1^* and p_2^* are the momenta of the particles after the collision, for which a is the impact parameter and φ 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.

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