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AN EQUATION FOR THE DIFFUSION IN PHASE SPACE FOR NONLINEAR SYSTEMS

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We have generalized the method developed in references 1 and 2, which is based upon Gibbs' method, to the case of diffusion in phase space. Starting only from the general rules of statistical mechanics and an assumption about the form of the averaged nonlinear macroscopic equation of motion for the system, we derive a general space-velocity equation of motion for the probability density. In the particular case of a linear law of friction this equation is the same as the well-known Einstein-Fokker-Planck space-velocity equation. For a system with a non-linear frictional force which does not depend on the coordinates in a uniform external field we obtain the general solution of the diffusion equation obtained here.

INTRODUCTION

We have shown in previous papers[1,2] that one can derive by Gibbs' method not only the exact formulae of the theory of Brownian motion for fluctuations and correlations,[3,4] but also a general expression for the transition probability density in configuration space, and also equations for this probability density in the case of essentially nonlinear systems.

We shall show below that the general statistical method developed by us can also be applied to derive a general equation of motion for the probability density in the phase space of the coordinates and momenta (or velocities) for arbitrary nonlinear systems.

To obtain such a diffusion equation it is sufficient to make only an assumption about the form of the averaged macroscopic equation of motion for the coordinate and momentum of the particle and there is no necessity to introduce any assumption about the correlations of the random forces or about the character of the stochastic process.

TRANSITION PROBABILITY DENSITY IN PHASE SPACE

Let $Q(X)$ and $P(X)$ be the generalized coordinate and its conjugate generalized momentum of interest to us, where X is the totality of all canonical variables of the microsystem. We denote by $W(Q, P, t; Q_0, P_0, t_0)$ the probability density for a transition of the system from the state $Q(X) = Q_0$, $P(X) = P_0$ at the initial moment t_0 to the state $Q(X) = Q$, $P(X) = P$ at time t. The probability density for the equilibrium values of Q and P in a Gibbs ensemble

$$w(X) = \exp\{[\Psi - H(X)]/\Theta\}$$

will be denoted by $W_0(Q, P)$. We have then, in accordance with reference 5

$$W(Q, P, t; Q_0, P_0, t_0)$$
$$= \int_{(X^0)} \delta\{Q - Q(X^t)\}\,\delta\{P - P(X^t)\}\,\frac{\exp\{[\Psi - H(X^0)]/\Theta\}}{W_0(Q_0, P_0)}$$
$$\times\,\delta\{Q_0 - Q(X^0)\}\,\delta\{P_0 - P(X^0)\}\,dX^0, \tag{1}$$

where X^t and X^0 are the canonical variables of the system at times t and t_0, which are connected through the relations $X^t = x(t; X^0, t_0)$ which are solutions of the dynamical equations with a Hamiltonian $H(X)$. From (1) we have clearly, for $t = t_0$,

$$W(Q, P, t_0; Q_0, P_0, t_0) = \delta(Q - Q_0)\,\delta(P - P_0).$$

If initially, at $t = t_0$, Q and P are given not exactly, but corresponding to some probability density $\rho(Q, P)$ the probability density at an arbitrary moment t will be defined as

$$W(Q, P, t)$$
$$= \int_{(Q_0)}\int_{(P_0)} W(Q, P, t; Q_0, P_0, t_0)\,\rho(Q_0, P_0)\,dQ_0\,dP_0$$
$$= \int_{(X^0)} \delta\{Q - Q(X^t)\}\,\delta\{P - P(X^t)\}$$
$$\times \exp\left\{\frac{1}{\Theta}[\Psi - H(X^0)]\right\}\,\frac{\rho\{Q(X^0), P(X^0)\}}{W_0\{Q(X^0), P(X^0)\}}\,dX^0. \tag{2}$$

Expression (1) is obtained from (2) for $\rho(Q, P)$

$= \delta(Q - Q_0)\,\delta(P - P_0)$. Similarly to what was done in reference 1, Eq. (2) can be written in the form

$$W(Q,\ P;\ t) = (2\pi)^{-2} \iint\limits_{-\infty}^{+\infty} \exp\left[i(\xi Q + \eta P)\right] \varphi(\xi,\ \eta;\ t)\, d\xi\, d\eta, \tag{3}$$

where φ is the characteristic function:

$$\varphi(\xi,\ \eta;\ t) = \int\limits_{(X^0)} R\{Q(X^0),\ P(X^0)\} \exp\left\{-i\left[\xi Q(X^t) + \eta P(X^t)\right] + \frac{1}{\Theta}\left[\Psi - H(X^0)\right]\right\} dX^0, \tag{4}$$

$$R(Q,\ P) = \rho(Q,\ P) / W_0(Q,\ P). \tag{5}$$

It is obvious that the moments of the distribution (3) can be expressed in terms of φ as follows

$$\overline{Q^m P^n} = i^{m+n}\, \partial^{m+n}\varphi / \partial\xi^m \partial\eta^n \big|_{\xi,\,\eta=0}. \tag{6}$$

One can also give the funtions φ a different physical meaning. Let us introduce the quantity

$$Z(a,\ b;\ t) = \int\limits_{(X^0)} R\{Q(X^0),\ P(X^0)\} \times \exp\left\{-\frac{1}{\Theta}\left[H(X^0) + aQ(X^t) + bP(X^t)\right]\right\} dX^0. \tag{7}$$

It is clear that for $a = i\xi\Theta$, $b = i\eta\Theta$

$$\varphi = e^{\Psi/\Theta} Z. \tag{8}$$

In the integrand of Eq. (7) we can replace $H(X^0)$ by $H(X^\tau)$ because of the conservation of energy, and dX^0 by dX^τ by virtue of Liouville's theorem. We can then consider the expression

$$w(X^\tau, \tau) = \frac{1}{Z} R\{Q(X^0),\ P(X^0)\} \times \exp\left\{-\frac{1}{\Theta}\left[H(X^\tau) + aQ(X^t) + bP(X^t)\right]\right\} \tag{9}$$

where we take into account that $X^t = x(t;\ X^\tau,\ \tau)$ and $X^0 = x(t_0;\ X^\tau,\ \tau)$, as the microscopic probability density for some non-equilibrium process satisfying the equation of motion for a phase ensemble:

$$\frac{\partial w}{\partial \tau} = [H,\ w]. \tag{10}$$

The moments taken over the ensemble (9) are obviously defined by the relations

$$\overline{Q^m\, P^n}^{\,a,b} = \frac{(-\Theta)^{m+n}}{Z} \frac{\partial^{m+n} Z}{\partial a^m\, \partial b^n}. \tag{11}$$

For a, b = 0 Eq. (11) is the same as (6).

Differentiating Z with respect to t we get also the relation

$$a\overline{\dot{Q}}^{\,a,b} + b\overline{\dot{P}}^{\,a,b} = -\frac{\Theta}{Z}\frac{\partial Z}{\partial t}. \tag{12}$$

We can thus evaluated φ and consequently also W if we know the moments (11) evaluated with respect to the non-equilibrium ensemble (9). Any information about these moments can only be obtained from a macroscopic experiment. A macroscopic experiment cannot give us, however, all moments, but only information about the change of the average values of Q and P in well defined non-equilibrium processes or the averaged equations of motion for these quantities. The problem thus arises of determining the equations of motion for Z and then also for W from the macroscopic equations of motion for Q and P.

THE EQUATION OF MOTION FOR THE PROBABILITY DENSITY

We shall write Eq. (9) for the microscopic probability density at time $\tau = t$ in the form

$$w(X^t, t) = \frac{1}{Z} R\{Q(X^0),\ P(X^0)\} \times \exp\left\{-\frac{1}{\Theta}\left[H(X^t) + aQ(X^t) + bP(X^t)\right]\right\}, \tag{13}$$

where $X^0 = x(t_0;\ X^t,\ t)$. This expression can be considered to be the non-equilibrium probability for a phase ensemble which is formed from an equilibrium ensemble with a Hamiltonian $H(X^t) + aQ(X^t) + bP(X^t)$ through a well defined fixing of the canonical variables X^t at time t by a given function $R\{x(t_0;\ X^t,\ t)\}$.

If we take into account that the momentum P enters into the Hamiltonian H only in the form of a term $P^2/2M$, as usual, we can consider an equilibrium system with a Hamiltonian $H + aQ + bP$ as being under the action of an additional force $-a + M\dot{b}$, since

$$\begin{aligned} H + aQ + bP &= H_1 + P^2/2M + bP + aQ \\ &= H_1 + (P + Mb)^2/2M - Mb^2/2 + aQ, \end{aligned} \tag{14}$$

and hence

$$\dot{Q} = P/M + b, \quad \dot{P} = -\partial H_1/\partial Q - a,$$

or

$$M\dot{Q} = -\partial H_1/\partial Q - a + M\dot{b}. \tag{15}$$

If $\rho = W_0$, i.e., $R = 1$, the ensemble (13) with the Hamiltonian (14) is an equilibrium one and the average values of Q and P, determined from (15) are therefore equal to zero. If however, $\rho \neq W_0$, the averages $\overline{\dot{Q}}^{\,a,b}$ and $\overline{\dot{P}}^{\,a,b}$ are, clearly, different from zero since such an ensemble is not an equilibrium one. We shall determine these averages from a macroscopic experiment.

Let the macroscopic equations of motion for the particle be of the form

$$\dot{P} = F(\dot{Q}, Q) - a, \qquad \dot{Q} = P/M + b, \tag{16}$$

where F is the sum of an external force of the potential type and a dissipative force, which depends in some arbitrary way on both $\dot{Q}$ and on Q. We shall assume that the motion averaged over the ensemble (13) is described by the Eqs. (16), i.e.,

$$\bar{\dot{P}}^{a,b} = \overline{F(Q,\dot{Q})}^{a,b} - a, \qquad \bar{\dot{Q}}^{a,b} = \bar{P}^{a,b}/M + b. \quad (17)$$

This is a natural physical assumption which is common to all theories developed so far, in any case for systems which are not too far from an equilibrium situation.

Combining (11), (12), and (17), using a transformation similar to the one used in reference 2, and introducing the velocity V = P/M instead of the momentum we get for W the equation

$$\frac{\partial W}{\partial t} + V\frac{\partial W}{\partial Q} = \frac{1}{M}\frac{\partial}{\partial V}\sum_{n=0}^{\infty}\frac{(\Theta/M)^n}{n!}\frac{\partial^n}{\partial V^n}\left[W\frac{\partial^n}{\partial V^n}F(Q,V)\right]. \quad (18)$$

We have thus obtained a more general equation for the diffusion in coordinate-velocity space for a system with an arbitrary form of the macroscopic dissipative and potential forces.

It is evident that the expression for the transition probability density W (Q, P, t; Q_0, P_0, t_0) can be obtained as a solution of Eq. (18) with the initial condition W (Q, P; t_0) = $\delta(Q - Q_0)\,\delta(P - P_0)$.

If

$$F(Q,V) = K(Q) + \gamma(Q)V, \quad (19)$$

Eq. (18) goes over into the usual Einstein-Fokker-Planck space-velocity equation of the form (see, e.g., reference 6)

$$\frac{\partial W}{\partial t} + V\frac{\partial W}{\partial Q} + \frac{K}{M}\frac{\partial W}{\partial V} = \frac{\gamma}{M}\frac{\partial}{\partial V}(VW) + \frac{\gamma\Theta}{M^2}\frac{\partial^2 W}{\partial V^2}. \quad (20)$$

In contradistinction to all known methods of deriving equations for the probability density, Eqs. (18) and (20) have been obtained by using only the general rules of statistical mechanics and a single assumption (17) about the averaged equations of motion. We have not made any assumptions about the Markov character of the random process or about the character of the correlations of the random collisional forces. We have thus obtained Eq. (18) starting from the most general assumptions.

THE GENERAL SOLUTION OF EQ. (18) FOR ONE PARTICULAR CASE

If the external force and the frictional force do not depend on the coordinates, i.e., F(Q, V) = K + G(V), then Eq. (18), like Eq. (9) in reference 2, can be integrated by quadratures. The corresponding formula for the source function is of the form

$$W(q, v, \tau;\ q_0, v_0, \tau_0)$$

$$= (2\pi i)^{-2}\iint\limits_{-i\infty}^{+i\infty}\exp\left\{\frac{1}{2}(p - v_0)^2 - \frac{1}{2}(s - v)^2 + \sigma\left[q - q_0 + \int_p^s\frac{\xi\,d\xi}{\bar{G}_1(\xi) + \sigma - K}\right]\right\}dp\,d\sigma,$$

$$\tau - \tau_0 + \int_p^{s(p,\sigma;\tau)} d\xi/[\bar{G}_1(\xi) + \sigma - K] = 0,$$

$$\bar{G}_1(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-(v-\xi)^2 2}\,G_1(v)\,dv, \quad (21)$$

where we have introduced the notation

$$\tau = t/\sqrt{M\Theta}, \qquad v = V\sqrt{M/\Theta},$$
$$q = Q/\Theta, \qquad G_1(v) = G(v\sqrt{\Theta/M});$$

the function s (p, σ; τ) is determined by the second of Eqs. (21).

Following the method given here one can easily obtain equations similar to Eq. (18) also for other, non-mechanical, physical systems by suitably choosing in each concrete case the generalized coordinates, velocities and forces.

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