ON THE EVALUATION OF COORDINATE PROBABILITIES FOR NONLINEAR SYSTEMS BY GIBBS' METHOD

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Using the general principles of Gibbs' statistical mechanics, we have developed a method which enables us to evaluate the transition probability density for any generalized coordinate in a system with a nonlinear relaxation mechanism. This method does not require a knowledge of the law of motion for the average value of the coordinate, but uses only the general form of the corresponding equation of motion.

THE method developed by Terletskiĭ and the author[5] using general results obtained earlier[1-4] enables us to evaulate the transition probability density for a generalized coordinate if the behavior of its average value is known when there are additional constant forces present (or included).

The averaged equation of motion contains, however, the average value of the coordinate (the first moment) only when the corresponding system is linear. In the case of a nonlinear system, however, the averaged equation contains also higher moments of the coordinates, the order of which is determined by the character of the nonlinearity.

This fact makes it difficult to use the known nonlinear equations of motion when one wants to find the transition probability density using the scheme given in reference 5, since in problems of Brownian motion one usually starts from the averaged equations of motion and the average dissipative forces produced by the interaction of the system with the medium.

The aim of the present paper consists of setting up a scheme which enables us to evaluate the transition probability density for nonlinear systems starting solely from the general form of the appropriate equation of motion.

1. THE CHARACTERISTIC FUNCTION

As in reference 5, we shall introduce for the generalized coordinate Q the transition probability density $W(Q, t; Q_0, t_0)$ and the characteristic function $Z(a, t; b, t_0)$ corresponding to it. Using the same notation as in reference 5, we have

$$W_0(Q_0)W(Q, t; Q_0, t_0) = (2\pi)^{-2}\iint\limits_{-\infty}^{+\infty}\{\exp(i\xi Q + i\eta Q_0)\}\, Z(a, t; b, t_0)\, d\xi\, d\eta, \tag{1}$$

where

$$a = i\xi\Theta, \quad b = i\eta\Theta, \quad \Theta = kT.$$

The following relations follow from the definition of Z (see reference 5)

$$\overline{\dot{Q}}^{a} = -(\Theta/a)\,\dot{Z}/Z\,|_{b=0}, \tag{2}$$

$$\overline{Q^j}^{a} = (-\Theta)^j \frac{1}{Z}\frac{\partial^j Z}{\partial a^j}\Big|_{b=0}, \tag{3}$$

where the index a denotes that we have taken an average over an auxiliary ensemble which is distinguished from the original, equilibrium one by the inclusion of an additional constant force $-a$, acting in the direction of the coordinate Q.

The equation of motion for Q averaged over the ensemble just mentioned connects $\overline{\dot{Q}}^{a}$ with the moments $\overline{Q^j}^{a}$ and, would according to (2) and (3) at the same time be a differential equation for the characteristic function Z. Using the inverse Fourier transformation one can from this equation go over to a differential equation for the probability density itself.

The transition probability density $W(Q, t; Q_0, t_0)$ is the solution of this equation which has a source for $t = t_0$.

2. A BROWNIAN PARTICLE IN AN EXTERNAL FIELD

The averaged equation of motion for a particle in the presence of an additional force $(-a)$ and neglecting the inertial forces is of the form

$$\gamma\overline{\dot{Q}}^{a} + \overline{F(Q)}^{a} = -a, \qquad (4)$$

where γ is the coefficient of viscosity and $F(Q) = -dU/dQ$ is the external force.

Expanding $F(Q)$ in a power series in Q and averaging (4) term by term we find

$$\gamma\overline{\dot{Q}}^{a} + \sum_j A_j \overline{Q^j}^{a} = -a,$$
$$A_j = (1/j!)\, d^{j+1}U/dQ^{j+1}|_{Q=0}. \qquad (4')$$

Substituting (2) and (3) into (4′) we find a differential equation for the characteristic function $Z(a, t)$:

$$\gamma\frac{\partial Z}{\partial t} - \frac{a}{\Theta}\sum_j A_j(-\Theta)^j\frac{\partial^j Z}{\partial a^j} = \frac{a^2}{\Theta}Z. \qquad (5)$$

Evaluating the Fourier components of this equation, according to (1), we find that $W(Q, t; Q_0, t_0)$ satisfies the Einstein-Fokker-Planck equation

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial Q}\left(D\frac{\partial W}{\partial Q} - \frac{1}{\gamma}\frac{\partial U}{\partial Q}W\right), \quad D = \frac{\Theta}{\gamma}, \qquad (6)$$

being its source function. One sees easily that the inclusion of an additional constant force $-a$ leads formally to the appearance of a diffusion current on the right hand side of Eq. (6).

3. AN ELECTRICAL CIRCUIT WITH A NON-LINEAR RELAXATION MECHANISM

We shall consider an electrical circuit consisting of a capacity C and a resistance with a non-linear current-voltage characteristic of the form

$$i = f(u) = \sum A_j u^j.$$

The charge Q concentrated upon the capacity is the generalized coordinate and the voltage u the generalized force so that the averaged equation of motion for Q when there is an additional constant force $-a$ present is of the form

$$\overline{\dot{Q}}^{a} + \overline{f[(Q/C) + a]}^{a} = 0. \qquad (7)$$

By means of the procedure described in Sec. 2 we find the following differential equation for the characteristic function $Z(a, t)$:

$$\frac{\partial Z}{\partial t} = \frac{a}{\Theta}\sum_{j,k} A_j\binom{j}{k}(-\Theta/C)^k a^{j-k}\frac{\partial^k Z}{\partial a^k}. \qquad (8)$$

The corresponding equation for the probability density itself

$$W(q, \tau) = (2\pi\Theta i)^{-1}\int_{-i\infty}^{+i\infty} e^{aQ/\Theta}Z(a, t)\,da$$

is of the form

$$\partial W/\partial\tau = \partial J/\partial q;$$
$$J = \sum_{j,k} B_j\binom{j}{k}\frac{\partial^k}{\partial q^k}(q^{j-k}W) = \sum_k \frac{1}{k!}\frac{\partial^k}{\partial q^k}\left(W\frac{d^k G}{dq^k}\right), \qquad (9)$$

where we have introduced the notation

$$q = Q(C\Theta)^{-1/2}, \quad \tau = t(C\Theta)^{-1/2}, \quad B_j = A_j(\Theta/C)^{j/2},$$
$$G(q) = \sum_j B_j q^j = f(q\sqrt{\Theta/C}).$$

The solution of this equation can be obtained in the form of quadratures. The expression for the current J can be transformed to the form

$$J = \exp(-q^2/2)J_1, \quad J_1 = \sum_{j,k}\frac{B_j j!}{2^k k!(j-2k)!}\frac{d^{j-2k}W_1}{dq^{j-2k}}, \qquad (10)$$

$$W_1 = W\exp(q^2/2), \qquad (10')$$

after which (9) can be written as

$$\partial W_1/\partial\tau = \partial J_1/\partial q - qJ_1. \qquad (11)$$

writing after that

$$W_1(q, \tau) = (2\pi i)^{-1}\int_{-i\infty}^{+i\infty} e^{qs}\overline{W}_1(s, \tau)\,ds, \qquad (12)$$

we obtain for the Fourier component $\overline{W}_1$ the equation

$$\frac{\partial\overline{W}_1}{\partial\tau} = s\overline{J}_1(s)\overline{W}_1 + \frac{\partial}{\partial s}[\overline{J}_1(s)\overline{W}_1],$$

$$\overline{J}_1(s) = \sum_{j,k}\frac{B_j j!s^{j-2k}}{2^k k!(j-2k)!} = \sum_j \frac{B_j i^j}{2^{j/2}}H_j(s/i\sqrt{2})$$

$$= (2\pi)^{-1/2}\int_{\infty}^{+\infty} e^{-(q-s)^2/2}G(q)\,dq \qquad (13)$$

[$H_n(x)$ is a Hermite polynomial] which after the substitution

$$\overline{W}_2 = \overline{J}_1\overline{W}_1\exp(s^2/2) \qquad (14)$$

leads to

$$\partial\overline{W}_2/\partial\tau - \overline{J}_1\partial\overline{W}_2/\partial s = 0. \qquad (15)$$

The initial condition $\overline{W}_2(s, \tau_0) = \overline{W}_{20}(s)$ is connected with the initial condition of the original equation (9) $W(q, \tau_0) = W_0(q)$ through (10′), (12), and (14).

Solving (15) by the methods of characteristics we find $\overline{W}_2(s, \tau) = \Phi(\psi)$ where $\psi(s, \tau) = \int ds/\overline{J}_1(s) + \tau$ is the characteristic of Eq. (15).

Taking the initial condition into account we get $\overline{W}_2(s, \tau) = \overline{W}_{20}[p(s, \tau)]$ while $p(s, \tau)$ is determined from the condition

$$\int_s^p d\xi/\overline{J}_1(\xi) = \tau - \tau_0.$$

If we now use (10′), (12), and (14) to go from $\overline{W}_2$ to W, we get

$$W(q,\tau) = (2\pi i)^{-1} \int_{-i\infty}^{+i\infty}\int_{-\infty}^{+\infty} \exp\left\{\tfrac{1}{2}\left[(q'-p)^2-(q-s)^2\right]\right\}$$

$$\times W_0(q')\frac{\overline{J_1}(p)}{\overline{J_1}(s)}\,ds\,dq' = (2\pi i)^{-1}$$

$$\times \int_{-i\infty}^{+i\infty}\int_{-\infty}^{+\infty} W_0(q')\exp\left\{\tfrac{1}{2}\left[(q'-p)^2-(q-s)^2\right]\right\}dp\,dq'. \quad (16)$$

Substituting $W_0(q') = \delta(q'-q_0)$ into (16) we find the source function of Eq. (9).

$$W(q,\tau;\,q_0,\tau_0) = (2\pi i)^{-1}\int_{-i\infty}^{+i\infty}\exp\left\{\frac{1}{2}\left[(q_0-p)^2-(q-s)^2\right]\right\}dp,$$

$$\int_{p}^{s(p,\tau)} d\xi/\overline{J_1}(\xi) + \tau - \tau_0 = 0,$$

$$\overline{J_1}(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-(q-\xi)^2/2}G(q)\,dq, \quad (17)$$

which also gives the probability density for a transition of the circuit from a state Q_0 at time t_0 to a state Q at time t, if the current-voltage characteristic $i = f(q\sqrt{\Theta/C}) = G(q)$ of the non-linear resistance which enters into the circuit is known.

To study Eq. (17) further we perform a change of variables, putting

$$p - q_0 = \xi(C\Theta)^{-1/2},$$

$$W(q,\tau;\,q_0,\tau_0)\,dq = W(Q,t;\,Q_0,t_0)\,dQ,$$

after which we get, shifting the contour over which we integrate,

$$W(Q,t;\,Q_0,t_0) = \frac{1}{2\pi i C\Theta}\int_{-i\infty}^{+i\infty}\exp\left\{\frac{1}{2C\Theta}\left[\xi^2-(Q-\eta(\xi,t))^2\right]\right\}d\xi,$$

$$\int_{Q_0+\xi}^{\eta(\xi,t)} d\rho/F_\Theta(\rho) + t - t_0 = 0,$$

$$F_\Theta(\rho) = \frac{1}{\sqrt{2\pi C\Theta}}\int_{-\infty}^{+\infty}\exp\left[-\frac{(Q'-\rho)^2}{2C\Theta}\right]F(Q')\,dQ',$$

$$F(Q') = f(Q'/C). \quad (17')$$

We shall investigate the behavior of W as $\Theta \to 0$. In that case

$$(2\pi C\Theta)^{-1/2}\exp(\xi^2/2C\Theta) \to \delta(x),$$

where $x = -i\xi$ so that

$$W(Q,t;\,Q_0,t_0)$$

$$\to (2\pi C\Theta)^{-1/2}\exp\{-[Q-Q_\Theta(Q_0,t)]^2/2C\Theta\}, \quad (18)$$

while $Q_\Theta(Q_0,t)$ is determined by the condition

$$\int_{Q_0}^{Q_\Theta} d\rho/F_\Theta(\rho) + t - t_0 = 0, \quad (19)$$

i.e., satisfies the differential equation

$$\dot{Q}_\Theta + F_\Theta(Q_\Theta) = 0. \quad (20)$$

If we also take into account that as $\Theta \to 0$, $F_\Theta(Q_\Theta) \to F(Q_\Theta)$, according to its definition, while (18) goes over into a δ-function, we get in the limit $\Theta = 0$

$$W(Q,t;\,Q_0,t_0) = \delta[Q - Q(Q_0,t)], \quad (21)$$

where $Q(Q_0,t)$ is the solution of the original non-averaged equation

$$\dot{Q} + f(Q/C) = 0 \quad (7')$$

a result which we should have expected.

If we now go over to the case $\Theta \neq 0$ we shall "spread out" the original δ-shaped distribution (21) over the neighborhood of the trajectory given by (7′).

Putting $\eta(\xi,t) = Q_\Theta(Q_0,t) + \eta'(\xi,t)$ we find η' from the condition

$$\int_{Q_0+\xi}^{Q_\Theta+\eta'} d\rho/F_\Theta(\rho) + t - t_0 = 0. \quad (22)$$

Expanding (22) in the neighborhood of $\xi = 0$ in powers of ξ, η' and using (19) we get

$$\eta' = \varepsilon(Q_0,t)\,\xi,$$

$$\varepsilon(Q_0,t) = F_\Theta(Q_\Theta)/F_\Theta(Q_0) = \dot{Q}_\Theta/\dot{Q}_0. \quad (23)$$

After that substituting (23) into (17), and evaluating the integral for W, we find finally

$$W(Q,t;\,Q_0,t_0)$$

$$= [2\pi\sigma(Q_0,t)]^{-1/2}\exp\{-[Q-Q_\Theta(Q_0,t)]^2/2\sigma(Q_0,t)\} \quad (24)$$

$$\sigma(Q_0,t) = C\Theta[1-\varepsilon^2(Q_0,t)]. \quad (25)$$

In the approximation under consideration the Brownian motion of a non-linear system is thus described by a Gaussian distribution for the transition probability while the dispersion of this distribution depends not only on the time, but also on the initial conditions, according to (23) and (25). The center of the distribution (the average value of the coordinate) is $Q_\Theta(Q_0,t)$.

The average value of the coordinate satisfies Eq. (25) which is in general different from the non-averaged Eq. (7′). It follows from the definition of $F_\Theta(Q)$ [see the third equation of (17)] that this difference is only absent for linear systems ($F_\Theta(Q) \sim Q$), and for nonlinear systems it vanishes only when there is no thermal noise ($\Theta = 0$).

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