

Brownian motion of multidimensional systems in nonpotential velocity-dependent fields of force

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We study the Brownian motion in velocity-dependent fields of force. Our main result is a Smoluchowski equation valid for moderate to high damping constants. We derive that equation by perturbative solution of the Langevin equation and using functional derivative techniques.

A great variety of random processes arising in physical sciences are described by Brownian motion of few relevant degrees of freedom. In many cases the equation that governs the dynamics of such processes is Kramers's equation,¹ which is a special Fokker-Planck equation describing Brownian motion in a (potential) field of force. In the high friction limit, Kramers's equation reduces to a Fokker-Planck equation for the probability density of the position coordinate only. This is the so-called Smoluchowski equation.

There is a wide field of applicability of the Kramers and Smoluchowski equations (that is, of the Brownian motion in a field of force): chemical kinetics,^{1,2} astrophysics,^{3,4} nonlinear optics,^{5,6} electromagnetism,⁷ and solid-state physics and electronics.⁸⁻¹⁰

The Smoluchowski equation, first derived by M. von Smoluchowski in 1915,¹¹ was rederived by Kramers¹ and Chandrasekhar³ from Kramers's equation (i.e., the two-dimensional Fokker-Planck equation in phase space). Later on it was shown that the Smoluchowski equation is the first-order approximation of an inverse friction expansion of Kramers's equation.^{10,12-18} The starting point of all of these derivations is Kramers's (Fokker-Planck) equation and it is generally applied to dynamical systems in coordinate-dependent fields of force. With few exceptions¹⁴ these derivations deal only with one-dimensional potential fields and none of them treats the case of a nonpotential velocity-dependent field.

In this paper we want to address the problem of Brownian motion of multidimensional systems in nonpotential velocity-dependent fields of force. One meets such processes in dealing with self-oscillatory systems,^{7,19} relaxation processes in plasmas,^{7,20} and magnetic systems.^{2,21} They are also of interest in relation to stellar dynamics²² and reaction rates in relativity and astrophysics.²³

Our main result will be a Smoluchowski equation valid for moderate to high damping constant. We will obtain this equation by solving perturbatively the Langevin equation (instead of Kramers's equation) and using the so-called functional derivative method.^{17,24-26}

The starting point of our analysis is the Langevin equation for the position x and velocity v of a Brownian particle initially at (x_0, v_0) in the presence of an external nonpotential field²⁷

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -\beta v + f(x, v) + \xi(t), \end{aligned} \tag{1}$$

where β is the damping, $f(x, v)$ is the acceleration produced by the external field, and $\xi(t)$ is a Gaussian δ -correlated (white) noise with zero mean. We shall assume that the external field $f(x, v)$ is an analytic function in x and v , such that in the high friction limit the damping dominates over the field [i.e., $|f(x, v)| < \alpha|v|$, $0 < \alpha \leq \beta$]. It is easily shown that this assumption allows us to seek a solution to Eq. (1) in the form

$$x(t) = x_0 + \beta^{-1}u(\tau) \equiv \hat{x}(\tau), \tag{2}$$

where $\tau = \beta t$ is a new time scale and $\beta^{-1}|u(\tau, \beta)|$ goes to zero as β tends to infinity.²⁸ Equation (1) is then equivalent to

$$\frac{d^2u}{d\tau^2} + \frac{du}{d\tau} = \beta^{-1} \left[f \left[x_0 + \beta^{-1}u(z), \frac{du}{d\tau} \right] + \eta(\tau) \right], \tag{3}$$

with the initial conditions

$$u(0) = 0, \quad \left. \frac{du}{d\tau} \right|_{\tau=0} = v_0.$$

Here $\eta(\tau) \equiv \xi(\tau/\beta)$ is a Gaussian white noise with zero mean and correlation function

$$\langle \eta(\tau_1)\eta(\tau_2) \rangle = \beta D \delta(\tau_1 - \tau_2). \tag{4}$$

We define the "scaled velocity" of the process as

$$\hat{v}(\tau) \equiv \frac{du(\tau)}{d\tau} = \frac{dx(t)}{dt} = v(t). \tag{5}$$

For each realization of the noise $\eta(\tau)$ we have a trajectory in the phase space which is a solution of Eq. (3). We write this solution in the form [cf. Eqs. (2) and (5)]

$$\begin{aligned} \hat{x}(\tau) &\equiv \hat{x}(\tau; x_0, v_0; [\eta]), \\ \hat{v}(\tau) &\equiv \hat{v}(\tau; x_0, v_0; [\eta]) = \beta \frac{d\hat{x}}{d\tau}, \end{aligned} \tag{6}$$

where the symbol $[\eta]$ stands for functional dependence on noise. The reduced density of trajectories in the configuration space

$$\rho(x; \tau | x_0, v_0; [\eta]) = \delta(x - x(\tau)) \tag{7}$$

obeys the continuity equation

$$\frac{\partial}{\partial \tau} \delta(x - \hat{x}(\tau)) + \beta^{-1} \frac{\partial}{\partial x} [\hat{v}(\tau) \delta(x - \hat{x}(\tau))] = 0 .$$

Averaging over all realizations of the noise and integrating over all possible initial velocities, with a given proba-

bility density $\rho(v_0)$, we get the probability density function

$$\rho(x, \tau | x_0) = \int dv_0 \rho(v_0) \langle \rho(x, \tau | x_0, v_0; [\eta]) \rangle ,$$

which obeys the equation

$$\frac{\partial}{\partial \tau} \rho(x, \tau | x_0) = -\beta^{-1} \int dv_0 \rho(v_0) \frac{\partial}{\partial x} \langle \hat{v}(\tau) \rho(x, \tau | x_0, v_0; [\eta]) \rangle . \quad (8)$$

Since the scaled velocity $\hat{v}(\tau)$ depends functionally on $\eta(\tau)$, our next step will be to evaluate the average on the right-hand side of Eq. (8). Due to the linearity of the noise term in Eq. (3), we may define the ‘‘stochastic velocity’’ as

$$\hat{v}_s(\tau; [\eta]) \equiv \hat{v}(\tau; [\eta]) - \hat{v}_d(\tau) , \quad (9)$$

where $\hat{v}(\tau, [\eta])$ is the derivative of the solution of Eq. (3) and $v_d(\tau)$ is the derivative of the solution of Eq. (3) when $\eta(\tau) = 0$ (i.e., the deterministic velocity). Thus

$$\langle \hat{v}(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle = \langle \hat{v}_d(\tau) \rho(x, \tau | x_0, v_0; [\eta]) \rangle + \langle \hat{v}_s(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle . \quad (10)$$

In order to evaluate the last term of Eq. (10) we shall use the Dubkov-Malakov formula:²⁹

$$\begin{aligned} \langle \hat{v}_s(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle &= \langle \hat{v}_s(\tau; [\eta]) \rangle \langle \rho(x, \tau | x_0, v_0; [\eta]) \rangle \\ &+ \sum_{n=1}^{n=\infty} \frac{\beta^n D^n}{n!} \int_0^\tau d\tau_1 \cdots \int_0^\tau d\tau_n \left\langle \frac{\delta^n v_s(\tau; [\eta])}{\delta \eta(\tau_1) \cdots \delta \eta(\tau_n)} \right\rangle \left\langle \frac{\delta^n \rho(x, \tau | x_0, v_0; [\eta])}{\delta \eta(\tau_1) \cdots \delta \eta(\tau_n)} \right\rangle , \end{aligned} \quad (11)$$

where the symbol $\delta/\delta\eta(\tau)$ means functional derivative. Now the high friction assumption allows a perturbative solution to Eq. (3) by a series expansion in the small parameter β^{-1} :

$$\begin{aligned} u(\tau) &= v_0(1 - e^{-\tau}) + \beta^{-1} \int_0^\tau ds_1 e^{-s_1} \int_0^{s_1} ds_2 e^{s_2} [f(s_2) + \eta(s_2)] \\ &+ \beta^{-2} \int_0^\tau ds_1 e^{-s_1} \int_0^{s_1} ds_2 \left[(e^{s_2} - 1) A(s_2) v_0 + B(s_2) \int_0^{s_2} ds e^s [f(s) + \eta(s)] \right] \\ &+ \beta^{-3} \int_0^\tau ds_1 e^{-s_1} \int_0^{s_1} ds_2 e^{s_2} \left\{ \frac{1}{2} v_0^2 A'(s_2) (1 - e^{-s_2}) \right. \\ &\quad + \frac{1}{2} e^{-2s_2} B'(s_2) \int_0^{s_2} ds_3 e^{s_3} \int_0^{s_2} ds e^s [f(s_3) + \eta(s_3)] [f(s) + \eta(s)] \\ &\quad + v_0 C(s_2) (1 - e^{-s_2}) e^{-s_2} \int_0^{s_2} ds e^s [f(s) + \eta(s)] \\ &\quad + A(s_2) \int_0^{s_2} ds_3 e^{-s_3} \int_0^{s_3} ds e^s [f(s) + \eta(s)] \\ &\quad \left. + B(s_2) e^{-s_2} \int_0^{s_2} ds \left[(e^s - 1) A(s) v_0 + B(s) \int_0^s dr e^r [f(r) + \eta(r)] \right] \right\} + O(\beta^{-4}) , \end{aligned} \quad (12)$$

where

$$f(\tau) \equiv f(x_0, v_0 e^{-\tau}), \quad A(\tau) \equiv A(x_0, v_0 e^{-\tau}) \equiv \left. \frac{\partial f(y, z)}{\partial y} \right|_{(x_0, v_0 e^{-\tau})} , \quad (13a)$$

and, similarly,

$$B(y, z) \equiv \frac{\partial f(y, z)}{\partial z}, \quad A' \equiv \frac{\partial^2 f(y, z)}{\partial y^2} , \quad (13b)$$

$$B'(y, z) \equiv \frac{\partial^2 f(y, z)}{\partial z^2}, \quad C(y, z) \equiv \frac{\partial^2 f(y, z)}{\partial y \partial z} . \quad (13c)$$

In Appendix A we show that

$$\langle \hat{v}_s(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle = \langle \hat{v}_s(\tau; [\eta]) \rangle \langle \delta(x - \hat{x}(\tau)) \rangle - \frac{1}{2} D \beta^{-2} (1 - e^{-\tau})^2 \left\langle \frac{\partial \delta(x - \hat{x}(\tau))}{\partial x} \right\rangle + O(\beta^{-3}) \quad (14)$$

and

$$\langle \hat{v}_s(\tau; [\eta]) \rangle = \frac{1}{4} D \beta^{-2} e^{-\tau} \int_0^\tau ds (e^s - e^{-s}) B'(s) + O(\beta^{-3}). \quad (15)$$

In the asymptotic limit $\tau \gg 1$, we have

$$\langle v_s(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle = \frac{1}{4} D \beta^{-2} B'(x_0, 0) \langle \delta(x - \hat{x}(\tau)) \rangle - \frac{1}{2} D \beta^{-2} \frac{\partial}{\partial x} \langle \delta(x - \hat{x}(\tau)) \rangle + O(\beta^{-3}, e^{-\tau}). \quad (16)$$

Since $\hat{x}(\tau) = x_0 + O(\beta^{-1}, e^{-\tau})$ [cf. Eqs. (2) and (12)] then, up to the same order of approximation as in Eq. (16), we may write

$$\langle \hat{v}_s(\tau; [\eta]) \rho(x, \tau | x_0, v_0; [\eta]) \rangle = \frac{1}{4} D \beta^{-2} B'(x, 0) \langle \delta(x - \hat{x}(\tau)) \rangle - \frac{1}{2} D \beta^{-2} \frac{\delta}{\delta x} \langle \delta(x - \hat{x}(\tau)) \rangle + O(\beta^{-3}, e^{-\tau}). \quad (17)$$

On the other hand, it is shown in Appendix B that

$$\langle v_d(\tau) \delta(x - \hat{x}(\tau)) \rangle = \beta^{-1} [f(x, 0) + \beta^{-1} B(x, 0) f(x, 0)] \langle \delta(x - \hat{x}(\tau)) \rangle + O(\beta^{-3}, e^{-\tau}). \quad (18)$$

The substitution of Eqs. (18), (17), and (10) into Eq. (8) results in a Fokker-Planck equation for the probability density $p(x, \tau | x_0)$, that, expressed in the original time scale $t = \beta^{-1} \tau$, reads

$$\begin{aligned} \frac{\partial}{\partial t} p(x, \tau | x_0) = & - \frac{\partial}{\partial x} \{ [\beta^{-1} f(x, 0) + \beta^{-2} B(x, 0) f(x, 0) + \frac{1}{4} D \beta^{-2} B'(x, 0)] p(x, \tau | x_0) \} \\ & + \frac{1}{2} D \beta^{-2} \frac{\partial^2}{\partial x^2} p(x, \tau | x_0) + O(\beta^{-3}, e^{-\beta t}). \end{aligned} \quad (19)$$

Following an analogous reasoning we can derive the Smoluchowski equation for a three-dimensional Brownian particle with position $\mathbf{x} = (x^1, x^2, x^3)$ and velocity $\mathbf{v} = (v^1, v^2, v^3)$ in a nonpotential field $\mathbf{f}(\mathbf{x}, \mathbf{v})$. The final result is

$$\begin{aligned} \frac{\partial}{\partial t} p(\mathbf{x}, t | \mathbf{x}_0) = & - \frac{\partial}{\partial x^k} \{ [\beta^{-1} f^k(\mathbf{x}, 0) + \beta^{-2} B_l^k(\mathbf{x}, 0) f^l(\mathbf{x}, 0) + \frac{1}{4} D \beta^{-2} \delta^{lm} B_{lm}^k(\mathbf{x}, 0)] p(\mathbf{x}, t | \mathbf{x}_0) \} \\ & + \frac{1}{2} D \beta^{-2} \delta^{kl} \frac{\partial^2}{\partial x^k \partial x^l} p(\mathbf{x}, t | \mathbf{x}_0) + O(\beta^{-3}, e^{-\beta t}) \end{aligned} \quad (20)$$

(summation over repeated indices is understood). Where δ^{kl} is the Kronecker symbol and

$$B_l^k(\mathbf{x}, \mathbf{v}) \equiv \frac{\partial f^k(\mathbf{x}, \mathbf{v})}{\partial v^l}, \quad B_{lm}^k(\mathbf{x}, \mathbf{v}) \equiv \frac{\partial^2 f^k(\mathbf{x}, \mathbf{v})}{\partial v^l \partial v^m}. \quad (21)$$

Equation (19) [Eq. (20)] is the Smoluchowski equation for Brownian motion of systems in nonpotential velocity-dependent fields of force. For velocity-independent fields we have

$$B(x, 0) = B'(x, 0) = 0$$

and Eq. (19) [Eq. (20)] reduces to previous results.^{1-3,10-18} Up to order β^{-2} , Eq. (19) [Eq. (20)] still remains a Fokker-Planck equation. Nevertheless, the inclusion of higher-order terms breaks down this structure since higher-order derivatives of $p(x, t | x_0)$ appear linked to these terms. A peculiarity of Eq. (19) [Eq. (20)] is that the diffusion coefficient D also occurs in the drift term.

This fact is a consequence of the nonlinear character of Eq. (1) which results in nonlinear noise terms in its perturbative solution [cf. Eqs. (12) and (15)]. We should note that other possible approaches (e.g., the adiabatic approximation^{5,7,18}) fail to produce that term. The reason for it lies in the fact that the asymptotic limit $\beta t \gg 1$ and the operation of averaging $\langle \rangle$ may not commute due to the character of the generalized function of the white noise $\xi(t)$.³⁰

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APPENDIX A: DERIVATION OF EQS. (14) AND (15)

From Eqs. (5), (9), and (12) we have

$$\begin{aligned} \hat{v}_s(\tau; [\eta]) = & \beta^{-1} e^{-\tau} \int_0^\tau ds e^s \eta(s) + \beta^{-2} e^{-\tau} \int_0^\tau ds_1 B(s_1) \int_0^{s_1} ds_2 e^{s_2} \eta(s_2) \\ & + \beta^{-3} e^{-\tau} \int_0^\tau ds_1 e^{s_1} \left[\frac{1}{2} e^{-2s_1} B'(s_1) \int_0^{s_1} ds_2 e^{s_2} \int_0^{s_2} ds_3 e^{s_3} \eta(s_2) \eta(s_3) \right. \\ & \quad + v_0 C(s_1) (1 - e^{-s_1}) e^{-s_1} \int_0^{s_1} ds_2 e^{s_2} \eta(s_2) + A(s_1) \int_0^{s_1} ds_3 e^{s_3} \eta(s_3) \\ & \quad \left. + B(s_1) e^{-s_1} \int_0^{s_1} ds_2 B(s_2) \int_0^{s_2} ds_3 e^{s_3} \eta(s_3) \right] + O(\beta^{-4}). \end{aligned} \quad (A1)$$

Averaging and taking into account that $\eta(\tau)$ is a zero-centered noise we get

$$\langle \hat{v}_s(\tau, [\eta]) \rangle = \frac{1}{2} \beta^{-3} e^{-\tau} \int_0^\tau ds_1 e^{-s_1} B'(s_1) \int_0^{s_1} ds_2 e^{-s_2} \int_0^{s_1} ds_2' e^{-s_2'} \langle \eta(s_2) \eta(s_2') \rangle + O(\beta^{-4}),$$

and now the substitution of Eq. (4) immediately leads to Eq. (15). On the other hand, the functional derivative of Eq. (A1) yields

$$\frac{\delta \hat{v}_s(\tau, [\eta])}{\delta \eta(\tau_1)} = \beta^{-1} e^{-(\tau-\tau_1)} + \beta^{-2} e^{-(\tau-\tau_1)} \int_{\tau_1}^\tau ds B(s) + O(\beta^{-3}) \quad (\text{A2})$$

and

$$\frac{\delta^n v_s(\tau, [\eta])}{\delta \eta(\tau_1) \cdots \delta \eta(\tau_n)} = O(\beta^{-3}) \quad (n = 2, 3, 4, \dots). \quad (\text{A3})$$

Now from Eq. (12) we have

$$\frac{\delta u(\tau)}{\delta \eta(\tau_1)} = \beta^{-1} (1 - e^{-(\tau-\tau_1)}) + \beta^{-2} \int_{\tau_1}^\tau ds_1 e^{-(s_1-\tau_1)} \int_{\tau_1}^{s_1} ds_2 B(s_2) + O(\beta^{-3})$$

and

$$\frac{\delta^n u(\tau, [\eta])}{\delta \eta(\tau_1) \cdots \delta \eta(\tau_n)} = O(\beta^{-3}) \quad (n = 2, 3, 4, \dots). \quad (\text{A3}')$$

Therefore [cf. Eqs. (2) and (7)]

$$\frac{\delta \rho(x, \tau | x_0, v_0; [\eta])}{\delta \eta(\tau_1)} = -\beta^{-1} \frac{\delta u(\tau)}{\delta \eta(\tau_1)} \frac{\partial \delta(x - \hat{x}(\tau))}{\partial x} = \beta^{-2} (1 - e^{-(\tau-\tau_1)}) \frac{\partial \delta(x - \hat{x}(\tau))}{\partial x} + O(\beta^{-3}) \quad (\text{A4})$$

and

$$\frac{\delta^n \rho(x, \tau | x_0, v_0; [\eta])}{\delta \eta(\tau_1) \cdots \delta \eta(\tau_n)} = O(\beta^{-3}) \quad (n = 2, 3, 4, \dots). \quad (\text{A5})$$

Substitution of Eqs. (A2)–(A5) into Eq. (11) finally yields Eq. (14).

APPENDIX B: DERIVATION OF EQ. (18)

The deterministic velocity $\hat{v}_d(\tau)$ is the τ derivative of Eq. (3) when $\eta(\tau) \equiv 0$, therefore from Eq. (12) we get

$$\hat{v}_d(\tau) = v_0 e^{-\tau} + \beta^{-1} e^{-\tau} \int_0^\tau ds e^s f(s) + \beta^{-2} e^{-\tau} \int_0^\tau ds_1 \left[(e^{s_1} - 1) A(s_1) v_0 + B(s_1) \int_0^{s_1} ds e^s f(s) \right] + O(\beta^{-3}), \quad (\text{B1})$$

where $f(s)$, $A(s_1)$, and $B(s_1)$ are given by Eq. (13). In the asymptotic limit $\tau \gg 1$ Eq. (B1) reads

$$\hat{v}_d(\tau) = \beta^{-1} f(x_0, 0) + \beta^{-2} [A(x_0, 0) v_0 + B(x_0, 0) f(x_0, 0)] + O(\beta^{-3}, e^{-\tau}). \quad (\text{B2})$$

On the other hand, expanding $f(x_0 + \beta^{-1} u(\tau), \hat{v}_d(\tau))$ in power series of β^{-1} we have

$$f(x_0 + \beta^{-1} u(\tau), \hat{v}_d(\tau)) = f(\tau) + \beta^{-1} \left[A(\tau) v_0 (1 - e^{-\tau}) + B(\tau) e^{-\tau} \int_0^\tau ds e^s f(s) \right] + O(\beta^{-2}).$$

When $\tau \gg 1$ this equation reads

$$f(\hat{x}(\tau), \hat{v}_d(\tau)) = f(x_0, 0) + \beta^{-1} [v_0 A(x_0, 0) + f(x_0, 0) B(x_0, 0)] + O(\beta^{-2}, e^{-\tau}). \quad (\text{B3})$$

Comparing Eq. (B2) with Eq. (B3) we see that

$$\hat{v}_d(\tau) = \beta^{-1} f(\hat{x}(\tau), \hat{v}_d(\tau)) + O(\beta^{-2}, e^{-\tau}), \quad (\text{B4})$$

thus

$$\begin{aligned} \langle \hat{v}_d(\tau) \delta(x - x(\tau)) \rangle &= \beta^{-1} \langle f(x, \hat{v}_d(\tau)) \delta(x - \hat{x}(\tau)) \rangle \\ &+ O(\beta^{-2}, e^{-\tau}). \end{aligned} \quad (\text{B5})$$

Now expanding again $f(x, \hat{v}_d(\tau))$ in power series of β^{-1} we have in the asymptotic limit

$$f(x, \hat{v}_d(\tau)) = f(x, 0) + \beta^{-1} B(x, 0) f(x_0, 0) + O(\beta^{-2}, e^{-\tau}). \quad (\text{B6})$$

Finally introducing Eq. (B6) into (B5) and taking into account that $\hat{x}(\tau) = x_0 + O(\beta^{-1}, e^{-\tau})$ we achieve

$$\begin{aligned} & \langle \hat{v}_d(\tau) \delta(x - x(\tau)) \rangle \\ &= \beta^{-1} f(x, 0) \langle \delta(x - x(\tau)) \rangle \\ &+ \beta^{-2} f(x, 0) B(x, 0) \langle \delta(x - \hat{x}(\tau)) \rangle + O(\beta^{-3}, e^{-\tau}), \end{aligned}$$

which is Eq. (18).

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