

V.2 Fokker–Planck equation

In this Section, we analyze the Langevin model of Sec. V.1 by adopting a different view of the dynamics of a Brownian particle in an environment. Instead of focusing on the solution $v(t)$ of the Langevin equation for a given initial condition, we rather investigate the dynamics of the *velocity probability density* $f(t, v)$, such that $f(t, v) dv$ is the probability that at time t the Brownian particle velocity lies between v and $v + dv$.

We first argue in Sec. V.2.1 that on time scales larger than the autocorrelation time τ_c of the fluctuating force, the velocity is a Markov process. The density $f(t, v)$ thus obeys the usual consistency equation involving the transition probability, which is recast in Sec. V.2.2 in the form of a partial differential equation of first order in t , yet involving an infinite number of successive derivatives with respect to v . Truncating this equation at second order yields the Fokker–Planck equation (Sec. V.2.3), whose solutions we examine in Sec. V.2.4. Eventually, we repeat the same analysis in the case of the position of the Brownian particle and its probability density (Sec. V.2.5).

V.2.1 Velocity of a Brownian particle as a Markov process

Assume first that the spectral density of the Langevin force is a white noise, i.e. that its autocorrelation function is proportional to a Dirac distribution, Eq. (V.3d), or equivalently, that the autocorrelation time τ_c vanishes. In that case, we have seen [Eq. (V.26)] that the velocity at a given instant t and the fluctuating force at a later time t' are uncorrelated, $\langle v(t)F_L(t') \rangle = 0$ for $t' > t$. That is, the Langevin force at time t' has no memory of the past of t' .

Now, if the Langevin force is a Gaussian stochastic process, then so is the velocity of the Brownian particle. The covariance $\langle v(t)F_L(t') \rangle = 0$ for $t' > t$ then means that $v(t)$ and $F_L(t')$ are statistically independent for $t' > t$.

If $F_L(t)$ is a Gaussian process, then its Fourier transform $\tilde{F}_L(\omega)$ is a Gaussian random variable. In turn, Eq. (V.30) shows that $\tilde{v}(\omega)$ is also Gaussian—the proportionality factor $1/[M(\gamma - i\omega)]$ is a “deterministic” function of ω . After a last inverse Fourier transform, $v(t)$ is a Gaussian random process, entirely determined by its first two moments.

Since the Langevin equation (V.1) is of first order, with the source $F_L(t)$, the velocity shift between t and $t + \Delta t$ only depends on the velocity at time t and the force in the interval $[t, t + \Delta t]$, yet is totally independent of v and F_L at times prior to t , so that $v(t)$ is a Markov process.

If on the other hand $F_L(t)$ and thus $v(t)$ is not Gaussian, or if τ_c is finite, then the velocity is strictly speaking no longer a Markov process. Restricting oneself to the change on time scales much larger than τ_c —and assuming from now on that $F_L(t)$ and $v(t)$ are Gaussian—, $v(t)$ can be approximated as Markovian. That is, we shall in the remainder of this Chapter consider the evolution of the Brownian particle velocity on a coarse-grained version of time, and “infinitesimal” time steps Δt will actually always be much larger than τ_c , although we shall consider the formal limit $\Delta t \rightarrow 0$.

Remark: From the physical point of view, the coarse-graining of time actually corresponds to the experimental case, in which observations are not performed continuously—in the mathematical sense—, but rather at successive instants, between which the Brownian particle has actually undergone many collisions with its environment.

Since the velocity $v(t)$ of the Brownian particle is assumed to be a Markov process, it is entirely described by its probability density, which will be denoted by $f(t, v)$ instead of the notation $p_1(t, v)$ used in Appendix C.2.5, and by the transition probability $p_{1|1}(t_2, v_2 | t_1, v_1)$. These obey the consistency condition (C.24), which for the evolution between times t and $t + \Delta t$ reads

$$f(t + \Delta t, v) = \int p_{1|1}(t + \Delta t, v | t, v') f(t, v') dv', \quad (\text{V.41a})$$

where $\Delta t \gg \tau_c$.

Physically, the collisions with the much lighter constituents of the environment lead on short time scales—i.e. for Δt much smaller than the relaxation time $\tau_r = \gamma^{-1}$ —only to small shifts of the velocity v of the Brownian particle. That is, the modulus of $w = v - v'$ is much smaller than v . In order to later exploit this property, let us rewrite Eq. (V.41a) as

$$f(t + \Delta t, v) = \int p_{1|1}(t + \Delta t, v | t, v - w) f(t, v - w) dw, \quad (\text{V.41b})$$

where we now integrate over the change in velocity.

V.2.2 Kramers–Moyal expansion

We shall now assume that the transition probability $p_{1|1}(t + \Delta t, v | t, v')$ and the probability density $f(t, v')$ are continuous functions of t and Δt , and that their product is analytic in the velocity variables, which will allow us to derive a partial differential equation obeyed by f . Note that the calculations in this subsection hold more generally for any Markovian stochastic process with the necessary regularity properties; the specific case of the velocity in the Langevin model will be studied in further detail in the next subsection.

Under the above assumptions, the integrand in the evolution equation (V.41b) can be expanded in Taylor series as

$$\begin{aligned} p_{1|1}(t + \Delta t, v | t, v - w) f(t, v - w) &= p_{1|1}(t + \Delta t, v + w - w | t, v - w) f(t, v - w) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} w^n \frac{d^n}{dv^n} [p_{1|1}(t + \Delta t, v + w | t, v) f(t, v)]. \end{aligned}$$

Introducing for $n \in \mathbb{N}$ the *jump moments*

$$\mathcal{M}_n(t, t + \Delta t, v) \equiv \int w^n p_{1|1}(t + \Delta t, v + w | t, v) dw = \int (v' - v)^n p_{1|1}(t + \Delta t, v' | t, v) dv', \quad (\text{V.42})$$

and exchanging the order of integration over w and partial differentiation with respect to v , the evolution equation (V.41) can be rewritten as

$$f(t + \Delta t, v) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial v^n} [\mathcal{M}_n(t, t + \Delta t, v) f(t, v)]. \quad (\text{V.43})$$

Definition (V.42) shows that $\mathcal{M}_0(t, t + \Delta t, v) = 1$ for arbitrary t and Δt —which actually only states that the integral over all possible final states of the transition probability of a Markov process is 1.

For $n \geq 1$, the “initial condition” $p_{1|1}(t, v' | t, v) = \delta(v' - v)$ and the assumed continuity in Δt mean that $\mathcal{M}_n(t, t + \Delta t, v)$ tends to 0 in the limit $\Delta t \rightarrow 0$. Assume now—this will be shown explicitly in the next subsection in the cases $n = 1$ and 2 for the jump moments of the velocity of a Brownian particle—that the jump moments with $n \geq 1$ are to leading order linear in Δt at small Δt :

$$\mathcal{M}_n(t, t + \Delta t, v) \underset{\Delta t \rightarrow 0}{\sim} \mathcal{M}_n(t, v) \Delta t + o(\Delta t), \quad (\text{V.44})$$

where $o(\Delta t)/\Delta t$ tends towards 0 when $\Delta t \rightarrow 0$. Subtracting then from both sides of Eq. (V.43) the term with $n = 0$, dividing by Δt , and finally taking the formal limit $\Delta t \rightarrow 0$ leads to⁽⁵⁴⁾

$$\frac{\partial f(t, v)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial v^n} [\mathcal{M}_n(t, v) f(t, v)]. \quad (\text{V.45})$$

⁽⁵⁴⁾ As in the study of the Boltzmann kinetic equation (Chapter IV), we take the mathematical limit of infinitesimal small Δt , notwithstanding the fact that physically it should be larger than τ_c .

This equation is the so-called *Kramers^(az)–Moyal^(ba) expansion*, which may be written for any Markovian stochastic process fulfilling the regularity hypotheses we have made.

In many situations, the first two jump moments yield a suitable description, and one truncates the expansion at second order, neglecting the terms with $n \geq 3$. This approximation yields the *Fokker^(bb)–Planck^(bc) equation*

$$\frac{\partial f(t, v)}{\partial t} = -\frac{\partial}{\partial v} [\mathcal{M}_1(t, v) f(t, v)] + \frac{1}{2} \frac{\partial^2}{\partial v^2} [\mathcal{M}_2(t, v) f(t, v)]. \quad (\text{V.46})$$

The first resp. second term on the right hand side is referred to as *drift* resp. *diffusive* term, and accordingly $\mathcal{M}_1(t, v)$ resp. $\mathcal{M}_2(t, v)$ as drift resp. diffusion coefficient.

Remarks:

- * To give an interpretation of the jump moments, let us introduce the notation

$$\langle g(v(t)) | v(t_0) = v_0 \rangle_v \equiv \int g(v) p_{1|1}(t, v | t_0, v_0) dv,$$

which denotes the average value at time t of the function $g(v)$ of the stochastic process $v(t)$, under the condition that at some earlier instant t_0 the latter takes the value v_0 . Comparing with definition (V.42), the jump moment can be rewritten as

$$\mathcal{M}_n(t, t + \Delta t, v) = \langle [v(t + \Delta t) - v]^n | v(t) = v \rangle_v. \quad (\text{V.47})$$

That is, $\mathcal{M}_n(t, t + \Delta t, v)$ represents the n -th moment of the probability distribution for the change in velocity between t and $t + \Delta t$, starting from velocity v at time t .

Hereafter, we shall use the fact that such moments can actually be computed in two equivalent ways: either, as in the above two equations, by using the conditional probability $p_{1|1}(t + \Delta t, v' | t, v)$ and integrating over v' ; or by following explicitly trajectories in velocity space that start with the fixed velocity v at time t , and computing the average velocity at a later time as in Sec. V.1.2, from which the average velocity shift easily follows.

- * If the Markov process under consideration is stationary, the jump moments are independent of time. As we shall see below, the reciprocal does not hold.

- * The Kramers–Moyal expansion (V.45) is sometimes referred to as *generalized Fokker–Planck equation*.

V.2.3 Fokker–Planck equation for the Langevin model

We now apply the formalism developed in the previous subsection to the specific case of the Langevin model.

V.2.3a Jump moments for the Langevin model

Let us compute the first two jump moments of the velocity in the Langevin model. Integrating the Langevin equation (V.1) between t and $t + \Delta t$, one finds

$$v(t + \Delta t) = v(t) - \gamma \int_t^{t+\Delta t} v(t') dt' + \frac{1}{M} \int_t^{t+\Delta t} F_L(t') dt'. \quad (\text{V.48})$$

Considering now that $v(t)$ is fixed and equal to v , and subtracting it from both sides of the equations, one obtains the velocity change between t and $t + \Delta t$ for a given realization of the Langevin force. Averaging over the possible realizations of the latter, one finds the average velocity shift between t

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and $t + \Delta t$ under the condition that $v(t) = v$, i.e. according to Eq. (V.47) precisely the first jump moment

$$\mathcal{M}_1(t, t + \Delta t, v) = -\gamma \int_t^{t+\Delta t} \langle v(t') | v(t) = v \rangle dt' + \frac{1}{M} \int_t^{t+\Delta t} \langle F_L(t') | v(t) = v \rangle dt',$$

where the fact that the averages over realizations of the Langevin force are conditional ones has explicitly been specified. Thanks to the absence of correlation between $F_L(t')$ and $v(t)$ when $t' > t$, see Eq. (V.26), the condition on $v(t)$ actually plays no role in the expectation value of the Langevin force, which vanishes. In turn, a Taylor expansion of the integrand of the first integral yields

$$\mathcal{M}_1(t, t + \Delta t, v) = -\gamma v \Delta t + \mathcal{O}((\gamma \Delta t)^2). \quad (\text{V.49a})$$

For time steps $\Delta t \ll \tau_r$, the term of order $(\gamma \Delta t)^2$ is much smaller than the linear term and we may write

$$\mathcal{M}_1(t, t + \Delta t, v) \underset{\Delta t \ll \tau_r}{\simeq} \mathcal{M}_1(t, v) \Delta t + o(\gamma \Delta t) \quad \text{with} \quad \mathcal{M}_1(t, v) \equiv -\gamma v, \quad (\text{V.49b})$$

so that Eq. (V.44) holds here.

Equations (V.47) and (V.48) also give the higher jump moments, in particular the second one, which follows from

$$\begin{aligned} [v(t + \Delta t) - v(t)]^2 &= \gamma^2 \left[\int_t^{t+\Delta t} v(t') dt' \right]^2 - \frac{2\gamma}{M} \int_t^{t+\Delta t} \int_t^{t+\Delta t} v(t') F_L(t'') dt' dt'' \\ &\quad + \frac{1}{M^2} \int_t^{t+\Delta t} \int_t^{t+\Delta t} F_L(t') F_L(t'') dt' dt''. \end{aligned}$$

Fixing the initial value $v(t)$ to v and averaging over an ensemble of realizations of the environment amounts to performing the conditional averaging with $p_{1|1}(\cdot | t, v)$. In that average, the first term on the right-hand side is of order $(\gamma \Delta t)^2$. Since $\Delta t \gg \tau_c$, we can use approximation (V.26) for the integrand of the second term, which again leads to a quadratic term in $\gamma \Delta t$. Eventually, the integrand of the third term can be approximated by $2D_v M^2 \delta(t'' - t')$ [Eq. (V.3d)], which gives

$$\mathcal{M}_2(t, t + \Delta t, v) = 2D_v \Delta t + \mathcal{O}((\Delta t)^2), \quad (\text{V.50a})$$

that is, a second jump moment

$$\mathcal{M}_2(t, t + \Delta t, v) \underset{\Delta t \ll \tau_r}{\simeq} \mathcal{M}_2(t, v) \Delta t + o(\Delta t) \quad \text{with} \quad \mathcal{M}_2(t, v) \equiv 2D_v. \quad (\text{V.50b})$$

Here again Eq. (V.44) holds.

V.2.3b Fokker–Planck equation

Inserting the jump moments (V.49b) and (V.50b) in the general relation (V.46), one obtains the Fokker–Planck equation for the Langevin model

$$\frac{\partial f(t, v)}{\partial t} = \gamma \frac{\partial}{\partial v} [v f(t, v)] + D_v \frac{\partial^2 f(t, v)}{\partial v^2}. \quad (\text{V.51})$$

We thus recover the interpretation of D_v as a diffusion coefficient in velocity space.

Remarks:

* Interestingly, the jump moments \mathcal{M}_1 , \mathcal{M}_2 for the velocity of the Langevin model are not explicitly time-dependent but only depend on Δt , even though the velocity is not a stationary process as long as equilibrium has not been reached.

* If the Langevin force is a Gaussian stochastic process, so is the velocity, and the transition probability $p_{1|1}(t + \Delta t, v' | t, v)$ is also Gaussian.⁽⁵⁵⁾ The transition probability is thus entirely determined by its first two moments, which are precisely the jump moments \mathcal{M}_1 , \mathcal{M}_2 , and we may write

$$p_{1|1}(t + \Delta t, v' | t, v) = \frac{1}{\sqrt{4\pi D_v \Delta t}} \exp\left\{-\frac{[v' - (1 - \gamma \Delta t)v]^2}{4D_v \Delta t}\right\} \quad \text{for } \tau_c \ll \Delta t \ll \tau_r, \quad (\text{V.52})$$

where we have used the fact that \mathcal{M}_2 is also the variance, since it is much larger than \mathcal{M}_1^2 .

* If the Langevin force and the velocity are not Gaussian processes, then one may still argue that the transition probability, as function of the velocity shift $v' - v$ at fixed v , is given by a Gaussian distribution when $\Delta t \gg \tau_c$. In such a time interval, many statistically independent collisions between the Brownian particle and its environment take place, which lead to as many statistically independent tiny velocity shifts: according to the central limit theorem, the resulting total velocity shift over Δt , which is the sum of these tiny shifts, is Gaussian distributed.

V.2.4 Solution of the Fokker–Planck equation

The Fokker–Planck equation (V.51) is a linear partial differential equation with non-constant coefficients relating the time derivative of the velocity density to its first two “spatial” derivatives—or, equivalently, an equation with constant coefficients involving time derivative, the first two spatial derivatives, and the function itself. Accordingly, it has the form of a generalized diffusion equation in velocity space, with a diffusion coefficient D_v —we recover the interpretation of that coefficient found in Sec. V.1.2—, and a “drift term” $\gamma \partial[vf(t, v)]/\partial v$ —so that γ is referred to as *drift coefficient*.

Defining a probability current (in velocity space) as

$$\mathcal{J}_v(t, v) \equiv -\gamma v f(t, v) - D_v \frac{\partial f(t, v)}{\partial v}, \quad (\text{V.53a})$$

the Fokker–Planck equation can be recast in the form of a continuity equation

$$\frac{\partial f(t, v)}{\partial t} + \frac{\partial \mathcal{J}_v(t, v)}{\partial v} = 0 \quad (\text{V.53b})$$

for the probability density.

V.2.4a Stationary solution

One can first investigate the stationary (or steady-state) solutions $f_{\text{st.}}(v)$ to the Fokker–Planck equation. According to Eq. (V.53b), these solutions make the probability current (V.53a) constant. To be normalizable, a solution $f_{\text{st.}}(v)$ should decrease faster than $1/|v|$ when $|v|$ tends to ∞ . The only possibility is when $\mathcal{J}_v(t, v) = 0$.⁽⁵⁶⁾ The corresponding stationary solution is then simply

$$f_{\text{st.}}(v) = \sqrt{\frac{\gamma}{2\pi D_v}} e^{-\gamma v^2/2D_v}. \quad (\text{V.54})$$

If the environment of the Brownian particle is in thermal equilibrium at temperature T , then the fluctuation–dissipation relation $D_v/\gamma = k_B T/M$ [Eq. (V.12)] shows that the steady-state solution to the Fokker–Planck equation is the Maxwell–Boltzmann distribution. The Brownian particle is thus “thermalized”.

⁽⁵⁵⁾ According to Bayes’ theorem (C.13), it equals the ratio of two Gaussian distributions.

⁽⁵⁶⁾ For a generic stochastic process $Y(t)$, whose realizations take their values in a bounded real interval $[a, b]$, the existence and number of stationary solutions of the corresponding Fokker–Planck equation (V.46) depend on the choice of boundary conditions imposed at a and b : vanishing $\mathcal{J}_Y \equiv \mathcal{M}_1 p_{Y,1} - \frac{1}{2} \partial(\mathcal{M}_2 p_{Y,1})/\partial y$ for $y = a$ and $y = b$ —i.e. so-called *reflecting boundary conditions*—, vanishing $p_{Y,1}(y) \dots$. The stationary solutions also depend on the dimension of the stochastic process—in two or more dimensions, non-vanishing probability currents exist without involving a flow of probability towards infinitely large values.

Remark: If the drift coefficient γ were negative, the Fokker–Planck equation (V.51) would have no stationary solution.

V.2.4 b Fundamental solution

As next step, one can search for the fundamental solutions—also called Green’s functions—of the Fokker–Planck equation, namely the solutions to equation (V.51) obeying the initial condition $f(0, v) = \delta(v - v_0)$ for an arbitrary $v_0 \in \mathbb{R}$.

One can show that this fundamental solution is given by

$$f(t, v) = \sqrt{\frac{\gamma}{2\pi D_v(1 - e^{-2\gamma t})}} \exp\left[-\frac{\gamma}{2D_v} \frac{(v - v_0 e^{-\gamma t})^2}{1 - e^{-2\gamma t}}\right] \quad \text{for } t > 0. \quad (\text{V.55})$$

- At a given instant $t > 0$, this distribution is Gaussian, with average value and variance

$$\langle v(t) \rangle = v_0 e^{-\gamma t}, \quad \sigma_v(t)^2 = \frac{D_v}{\gamma} (1 - e^{-2\gamma t}),$$

in agreement with expressions (V.5) and (V.8), with $t_0 = 0$, found in the case $t - t_0 \gg \tau_c$.

- When t becomes much larger than τ_r , the fundamental solution (V.55) tends to the stationary solution (V.54).

In agreement with the consistency condition (C.24), the fundamental solution (V.55) equals the transition probability $p_{1|1}(t, v | t_0 = 0, v_0)$. At small $t \ll \tau_r$ —which is then rewritten as Δt —, one actually recovers Eq. (V.52). More generally, one recognizes in $p_{1|1}(t, v | 0, v_0)$ given by Eq. (V.55) the transition probability (C.31b) of the Ornstein–Uhlenbeck process [42].

Remark: The Ornstein–Uhlenbeck process is actually defined by both its transition probability and its time-independent single-time probability. The latter condition is not fulfilled by the velocity of a Brownian particle in general—the velocity is not a stationary process—, yet is obeyed in the equilibrium regime $t \gg \tau_r$, in which case the terms $e^{-\gamma t}$ and $e^{-2\gamma t}$ in Eq. (V.55) vanish.

V.2.5 Position of a Brownian particle as a Markov process

We may now repeat the study of the previous subsections for the case of the position $x(t)$ of a free Brownian particle.

The first important point is that the evolution equation for the position deduced from the Langevin equation (V.1) is of second order. As a consequence, the displacement $x(t + \Delta t) - x(t)$ in a small time step does not depend on $x(t)$ and $F_L(t')$ for $t' \geq t$ only, but will also depend on the velocity $v(t)$, which in turn depends on the past of t . That is, the position is in general not a Markov process, even if the Langevin force is a Gaussian process with a vanishing autocorrelation time.

To recover the Markovian character, one has to consider time steps $\Delta t \gg \tau_r$, i.e. a coarser graining than for velocity. Over such a time interval, the velocity of the Brownian undergoes many random changes, and $x(t + \Delta t) - x(t)$ will be independent of the position at previous times.

On such time scales, the acceleration term in the Langevin equation plays no role, and one recovers the first-order equation (V.20a) valid in the viscous limit (cf. § V.1.3 c)

$$\eta_v \frac{dx(t)}{dt} = F_L(t).$$

Additionally, the condition $\Delta t \gg \tau_r$ automatically leads to $\Delta t \gg \tau_c$, so that the autocorrelation time of the Langevin force can be neglected:

$$\langle F_L(t) F_L(t + \tau) \rangle = 2D\eta_v^2 \delta(\tau)$$

[cf. Eq. (V.20b)]. In analogy to the finding in Sec. V.1.4, this leads to $\langle x(t) F_L(t') \rangle = 0$ for $t' > t$, which if $F_L(t)$, and thus $x(t)$, is Gaussian, guarantees their statistical independence.

Repeating the derivation in Sec. V.2.3 with $v(t)$, M , γ and $D_v M^2$ respectively replaced by $x(t)$, η_v , 0 and $D\eta_v^2$, one finds that the jumps moments for the position are $\mathcal{M}_1(t, x) = 0$ and $\mathcal{M}_2(t, x) = 2D$. The Fokker–Planck equation for the evolution of the probability density $f(t, x)$ of the position thus reads

$$\frac{\partial f(t, x)}{\partial t} = D \frac{\partial^2 f(t, x)}{\partial x^2}. \quad (\text{V.56})$$

That is, $f(t, x)$ obeys the ordinary diffusion equation, with the fundamental solution corresponding to the initial condition $f(0, x) = \delta(x - x_0)$ given by

$$f(t, x) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x_0)^2}{4Dt}\right] \quad \text{for } t > 0. \quad (\text{V.57})$$

From this probability density, one recovers the large-time limit of the variance found in Eq. (V.22).

Again, the fundamental solution (V.57) also equals the transition probability of the Markov process $x(t)$. Together with the initial condition $f(t=0, x) = \delta(x - x_0)$, they exactly match the definition of the Wiener process, Eq. (C.26).