IV.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.

IV.2.3 a 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 (IV.1) between t and $t + \Delta t$, one finds

$$v(t + \Delta t) = v(t) - \gamma \int_t^{t+\Delta t} v(t') \, \mathrm{d}t' + \frac{1}{M} \int_t^{t+\Delta t} F_{\mathrm{L}}(t') \, \mathrm{d}t'. \tag{IV.48}$$

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

[bg] A. Fokker, 1887–1972 [bh] M. Planck, 1858–1947

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

$$\mathscr{M}_1(t,t+\Delta t,v) = -\gamma\int_t^{t+\Delta t}\big\langle v(t')\,\big|\,v(t)=v\big\rangle\,\mathrm{d}t' + \frac{1}{M}\int_t^{t+\Delta t}\big\langle F_{\mathrm{L}}(t')\,\big|\,v(t)=v\big\rangle\,\mathrm{d}t',$$

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 $F_{\mathrm{L}}(t')$ and $v(t)$ when $t'>t$, see Eq. (IV.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

$$\mathscr{M}_1(t,t+\Delta t,v) = -\gamma v\Delta t + \mathcal{O}\big((\gamma\Delta t)^2\big). \tag{IV.49a}$$

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

$$\mathscr{M}_1(t,t+\Delta t,v) \underset{\Delta t\ll\tau_{\mathrm{r}}}{\simeq} \mathcal{M}_1(t,v)\Delta t + o(\gamma\Delta t) \quad\text{with}\quad \mathcal{M}_1(t,v)\equiv -\gamma v, \tag{IV.49b}$$

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

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

$$\begin{aligned}\big[v(t+\Delta t)-v(t)\big]^2 = \gamma^2\left[\int_t^{t+\Delta t} v(t')\,\mathrm{d}t'\right]^2 &- \frac{2\gamma}{M}\int_t^{t+\Delta t}\int_t^{t+\Delta t} v(t')F_{\mathrm{L}}(t'')\,\mathrm{d}t'\,\mathrm{d}t'' \\ &+ \frac{1}{M^2}\int_t^{t+\Delta t}\int_t^{t+\Delta t} F_{\mathrm{L}}(t')F_{\mathrm{L}}(t'')\,\mathrm{d}t'\,\mathrm{d}t''.\end{aligned}$$

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 $\Delta t \gg \tau_{\mathrm{c}}$, we can use approximation (IV.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 $2D_vM^2\delta(t''-t')$ [Eq. (IV.3d)], which gives

$$\mathscr{M}_2(t,t+\Delta t,v) = 2D_v\Delta t + \mathcal{O}\big((\Delta t)^2\big), \tag{IV.50a}$$

that is, a second jump moment

$$\mathscr{M}_2(t,t+\Delta t,v) \underset{\Delta t\ll\tau_{\mathrm{r}}}{\simeq} \mathcal{M}_2(t,v)\Delta t + o(\Delta t) \quad\text{with}\quad \mathcal{M}_2(t,v)\equiv 2D_v. \tag{IV.50b}$$

Here again Eq. (IV.44) holds.

IV.2.3 b Fokker–Planck equation

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

$$\boxed{\frac{\partial f(t,v)}{\partial t} = \gamma\frac{\partial}{\partial v}\big[vf(t,v)\big] + D_v\frac{\partial^2 f(t,v)}{\partial v^2}.} \tag{IV.51}$$

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

Remarks:

∗ Interestingly, the jump moments $\mathscr{M}_1$, $\mathscr{M}_2$ 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.[(64)] The transition probability is thus entirely determined by its first two moments, which are precisely the jump moments $\mathscr{M}_1$, $\mathscr{M}_2$, and we may write

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

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

∗ 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.

IV.2.4 Solution of the Fokker–Planck equation

The Fokker–Planck equation (IV.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 § IV.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

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

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

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

for the probability density.

IV.2.4 a Stationary solution

One can first investigate the stationary (or steady-state) solutions $f_{\text{st.}}(v)$ to the Fokker–Planck equation. According to Eq. (IV.53b), these solutions make the probability current (IV.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 $\mathcal{J}_v(t,v) = 0$.[(65)] The corresponding stationary solution is then simply

$$f_{\text{st.}}(v) = \sqrt{\frac{\gamma}{2\pi D_v}}\, \mathrm{e}^{-\gamma v^2/2D_v}. \tag{IV.54}$$

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. (IV.12)] shows that the steady-state solution to the Fokker–Planck equation is the Maxwell–Boltzmann distribution. The Brownian particle is thus "thermalized".

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

(65) 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 (IV.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 $p_{Y,1}(y)\ldots$ 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 (IV.51) would have no stationary solution.

IV.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 (IV.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

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

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

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

  in agreement with expressions (IV.5) and (IV.8), with $t_0 = 0$, found in the case $t - t_0 \gg \tau_\mathrm{c}$.

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

In agreement with the consistency condition (C.24), the fundamental solution (IV.55) equals the transition probability $p_{1|1}(t,v\,|\,t_0=0,v_0)$. At small $t \ll \tau_\mathrm{r}$—which is then rewritten as Δt—, one actually recovers Eq. (IV.52). More generally, one recognizes in $p_{1|1}(t,v\,|\,0,v_0)$ given by Eq. (IV.55) the transition probability (C.31b) of the Ornstein–Uhlenbeck process [49].

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 $t \gg \tau_\mathrm{r}$, in which case the terms $\mathrm{e}^{-\gamma t}$ and $\mathrm{e}^{-2\gamma t}$ in Eq. (IV.55) vanish.

IV.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 (IV.1) is of second order. As a consequence, the displacement $x(t+\Delta t) - x(t)$ in a small time step depends not only on $x(t)$ and $F_\mathrm{L}(t')$ for $t' \geq t$ only, but also 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 $\Delta t \gg \tau_\mathrm{r}$, 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 (IV.20a) valid in the viscous limit (cf. § IV.1.3 c)

$$\eta_v \frac{\mathrm{d}x(t)}{\mathrm{d}t} = F_\mathrm{L}(t).$$

Additionally, the condition $\Delta t \gg \tau_\mathrm{r}$ automatically leads to $\Delta t \gg \tau_\mathrm{c}$, so that the autocorrelation time of the Langevin force can be neglected:

$$\langle F_\mathrm{L}(t) F_\mathrm{L}(t+\tau)\rangle = 2D\eta_v^2\,\delta(\tau)$$

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

Repeating the derivation of § IV.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

$$\frac{\partial f(t,x)}{\partial t} = D\frac{\partial^2 f(t,x)}{\partial x^2}. \tag{IV.56}$$

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

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

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

Again, the fundamental solution (IV.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).

IV.3 Generalized Langevin dynamics

In Sec. IV.1, we have seen that the Langevin equation (IV.1), with an instantaneous friction term $-M\gamma v(t)$, leads at large times, when the Brownian particle is in equilibrium with the surrounding fluid, to the velocity [cf. Eq. (IV.25)]

$$v(t) = \frac{1}{M}\int_{-\infty}^{t} F_{\mathrm{L}}(t')\,\mathrm{e}^{-\gamma(t-t')}\,\mathrm{d}t' = \int_{-\infty}^{\infty} \chi(t-t')\,F_{\mathrm{L}}(t')\,\mathrm{d}t' \quad \text{with} \quad \chi(\tau) \equiv \frac{1}{M}\,\mathrm{e}^{-\gamma\tau}\Theta(\tau),$$

where $\Theta(\tau)$ denotes the Heaviside function. $\chi(\tau)$ is the *response function*, whose Fourier transform is precisely the admittance $Y(\omega)$, Eq. (IV.39b).

The velocity thus responds instantaneously to the Langevin force and is independent of its own past values, which is physically unrealistic. A more realistic model consists in introducing a time-non-local friction term, which leads to a generalized Langevin equation (§ IV.3.1), whose spectral properties we analyse in § IV.3.2. This generalized form of the Langevin equation is actually that which naturally emerges from a more microscopic description, in particular for the dynamics of a free classical particle interacting with an infinite bath of degrees of freedom in thermal equilibrium (§ IV.3.3).

IV.3.1 Generalized Langevin equation

To account for retardation effects in the motion of the Brownian particle, one can replace Eq. (IV.1) by the linear integro-differential equation

$$M\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -M\int_{-\infty}^{t} \gamma(t-t')\,v(t')\,\mathrm{d}t' + F_{\mathrm{L}}(t) \quad \text{with} \quad v(t) = \frac{\mathrm{d}x(t)}{\mathrm{d}t}, \tag{IV.61a}$$

called *generalized Langevin equation*, with a memory kernel $\gamma(\tau)$ for the friction force, where τ denotes the retardation $t-t'$. While only values for $\tau \geq 0$ play a role in this equation, yet it is convenient to view γ as an even function of $\tau \in \mathbb{R}$, whose integral over $\mathbb{R}$ equals a number denoted as 2γ, and to recast Eq. (IV.61a) as

$$M\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -M\int_{-\infty}^{\infty} \gamma(t-t')\,\Theta(t-t')v(t')\,\mathrm{d}t' + F_{\mathrm{L}}(t). \tag{IV.61b}$$

As before, the Langevin force $F_{\mathrm{L}}(t)$ is a stationary stochastic process with vanishing average. Since retardation effects are taken into account in the evolution of the velocity, they should for

consistency also be present in the fluctuating force, whose autocorrelation time τ_c will thus be non-zero.

IV.3.2 Spectral analysis

Since the initial time in the friction term is at $t_0 \to -\infty$, the Brownian particle is at every instant in equilibrium with its environment. Its velocity is thus a stationary stochastic process, to which one can apply the concepts of Appendix C.3. We consider the case of an environment in thermal equilibrium at temperature T.

Generalizing the analysis of § IV.1.6, one easily finds that the stationary response to an external force $F_{\text{ext.}}(t)$ independent of position and velocity reads in Fourier space

$$\langle \tilde{v}(\omega) \rangle = Y(\omega)\, \tilde{F}_{\text{ext.}}(\omega), \tag{IV.62a}$$

with

$$Y(\omega) \equiv \frac{1}{M} \frac{1}{\tilde{\gamma}(\omega) - \mathrm{i}\omega} \tag{IV.62b}$$

the complex admittance, where $\tilde{\gamma}(\omega)$ is given by

$$\tilde{\gamma}(\omega) = \int_0^\infty \gamma(t)\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{d}t = \int \gamma(t)\, \Theta(t)\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{d}t. \tag{IV.62c}$$

Note that $\tilde{\gamma}(\omega{=}0) = \gamma$.

Fourier-transforming the generalized Langevin equation (IV.61a), one finds that the spectral densities of the velocity and the fluctuating force are related by [cf. Eq. (IV.32)]

$$S_v(\omega) = \frac{1}{M^2} \frac{1}{\left|\tilde{\gamma}(\omega) - \mathrm{i}\omega\right|^2} S_F(\omega). \tag{IV.63}$$

Assuming[(68)] that relation (IV.40) between the admittance and the autocorrelation of velocity still holds here, one finds, since the velocity is real-valued, the identity

$$\mathrm{Re}\, Y(\omega) = \frac{1}{2k_B T} \int_{-\infty}^{\infty} \langle v(t)\, v(0) \rangle\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{d}t. \tag{IV.64}$$

Using Eq. (IV.62b), this yields

$$\int \langle v(t)\, v(0) \rangle\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{d}t = 2k_B T\, \mathrm{Re}\, Y(\omega) = \frac{2k_B T}{M} \frac{\mathrm{Re}\, \tilde{\gamma}(\omega)}{\left|\tilde{\gamma}(\omega) - \mathrm{i}\omega\right|^2}.$$

Now, invoking the Wiener–Khinchin theorem, the Fourier transform of the autocorrelation function is exactly the spectral density, i.e.

$$S_v(\omega) = \frac{2k_B T}{M} \frac{\mathrm{Re}\, \tilde{\gamma}(\omega)}{\left|\tilde{\gamma}(\omega) - \mathrm{i}\omega\right|^2}. \tag{IV.65}$$

Comparing with relation (IV.63), there comes

$$S_F(\omega) = 2Mk_B T\, \mathrm{Re}\, \tilde{\gamma}(\omega). \tag{IV.66}$$

From the Wiener–Khinchin theorem, the spectral density of the Langevin force fluctuations is the Fourier transform of the corresponding autocorrelation function, which gives

$$\kappa(\tau) = Mk_B T \gamma(\tau), \tag{IV.67a}$$

[(68)] This will be demonstrated in Sec. III.3.4 in next Chapter.

or equivalently

$$\tilde{\gamma}(\omega) = \frac{1}{Mk_BT}\int_0^\infty \langle F_{\mathrm{L}}(t)\, F_{\mathrm{L}}(t+\tau)\rangle\, \mathrm{e}^{\mathrm{i}\omega\tau}\, \mathrm{d}\tau. \tag{IV.67b}$$

Equation (IV.67a) shows that the memory kernel for the friction term has the same characteristic time scale τ_{c} as the fluctuations of the Langevin force—hence the necessity of considering a finite τ_{c} of the Langevin noise when allowing for retardation effects in the friction term.