

## IV.2 Fokker–Planck equation

In this Section, we analyze the Langevin model of Sec. IV.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 § IV.2.1 that on time scales larger than the autocorrelation time  $\tau_c$  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 § IV.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 (§ IV.2.3), whose solutions we examine in § IV.2.4. Eventually, we repeat the same analysis in the case of the position of the Brownian particle and its probability density (§ IV.2.5).

### IV.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. (IV.3d), or equivalently, that the autocorrelation time  $\tau_c$  vanishes. In that case, we have seen [Eq. (IV.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. (IV.30) shows that  $\tilde{v}(\omega)$  is also Gaussian—the proportionality factor  $1/[M(\gamma - i\omega)]$  is a “deterministic” function of  $\omega$ . After a last inverse Fourier transform,  $v(t)$  is a Gaussian random process, entirely determined by its first two moments.

Since the Langevin equation (IV.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  $\tau_c$  is finite, then the velocity is strictly speaking no longer a Markov process. Restricting oneself to the change on time scales much larger than  $\tau_c$ —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  $\Delta t$  will actually always be much larger than  $\tau_c$ , 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

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

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  $\Delta t$  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. (IV.41a) as

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

where we now integrate over the change in velocity.

### IV.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  $\Delta t$ , 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 (IV.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*

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

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

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

Definition (IV.42) shows that  $\mathcal{M}_0(t, t + \Delta t, v) = 1$  for arbitrary  $t$  and  $\Delta t$ —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  $\Delta t$  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  $\Delta t$  at small  $\Delta t$ :

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

where  $o(\Delta t)/\Delta t$  tends towards 0 when  $\Delta t \rightarrow 0$ . Subtracting then from both sides of Eq. (IV.43) the term with  $n = 0$ , dividing by  $\Delta t$ , and finally taking the formal limit  $\Delta t \rightarrow 0$  leads to<sup>(63)</sup>

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

<sup>(63)</sup>As in the study of the Boltzmann kinetic equation (Chapter ??), we take the mathematical limit of infinitesimal small  $\Delta t$ , notwithstanding the fact that physically it should be larger than  $\tau_c$ .

This equation is the so-called *Kramers–Moyal*<sup>(bf)</sup> *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*<sup>(bg)</sup>–*Planck*<sup>(bh)</sup> *equation*

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

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 (IV.42), the jump moment can be rewritten as

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

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 § IV.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 (IV.45) is sometimes referred to as *generalized Fokker–Planck equation*.