Supplemental note for Week 5 Part 1

ver. 20170417-01

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1 Langevin Eq. $\rightarrow$ Fokker-Planck Eq.

Let us start with the Langevin equation for a Brownian particle

$$m\frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) + \mathbf{F}(t), \tag{F2}$$

where the random force satisfies

$$\langle \mathbf{F}(t) \rangle = \mathbf{0} \tag{F3}$$

$$\langle \mathbf{F}(t)\mathbf{F}(0) \rangle = 2k_BT\zeta\mathbf{I}\delta(t). \tag{F4}$$

To derive a useful partial differential equation for the probability distribution functions, we redefine the Langevin equation in the following 1-dimensional form, assuming that the particle is subject to a conservative force $F_p(R(t), t) = -\frac{\partial U}{\partial R}$ due to a potential $U(R(t), t)$,

$$m\frac{dV(t)}{dt} = -\zeta V(t) + F(t) + F_p(R(t), t), \tag{1}$$

where $R(t)$ represents the position of the Brownian particle at time t.
Hereafter, we neglect the inertial term $m\frac{dV}{dt} \simeq 0$, since we are mainly interested in the long-time behavior $t \gg \frac{\zeta}{m}$ of the Brownian particle. We thus obtain the overdamped Langevin equation,

$$0 = -\zeta V(t) + F(t) + F_p(R(t), t) \tag{2}$$

$$V(t) = \frac{dR(t)}{dt} = \frac{F_p(R(t), t)}{\zeta} + \frac{F(t)}{\zeta}. \tag{3}$$

Let us now rewrite this equation (3) in the following more general form (making the substitution $R(t) \longrightarrow r(t)$)

$$\frac{dr(t)}{dt} = f(r(t), t) + g\eta(t), \tag{4}$$

where f is an arbitrary function of $r(t)$ and t, g is a constant, and $\eta(t)$ is a Gaussian white noise random variable with

$$\langle \eta(t) \rangle = 0 \tag{5}$$

$$\langle \eta(t)\eta(t') \rangle = \delta(t - t'). \tag{6}$$

Integration of Eq.(4) from $t = t_i$ to $t_{i+1} = t_i + \Delta t$, yields

$$r(t_{i+1}) - r(t_i) = \int_{t_i}^{t_{i+1}} f(r(t), t)dt + g\int_{t_i}^{t_{i+1}} \eta(t)dt \tag{7}$$

$$\simeq f(r(t_i), t_i)\Delta t + g\sqrt{\Delta t}\tilde{\eta}(t_i), \tag{8}$$

with

$$\begin{aligned}\langle\tilde{\eta}(t)\rangle &= 0 \qquad (9)\\ \langle\tilde{\eta}(t_i)\tilde{\eta}(t_j)\rangle &= \delta_{ij} \qquad (10)\end{aligned}$$

(see Eq.(F11) and the supplemental note for Week 4 Part 1).
We now consider a general function $p\left[r(t)\right]$ of $r(t)$ and make a Taylor expansion of it in terms of Δt, keeping only the terms equal to and lower than the first-order in Δt

$$\begin{aligned}p\left[r(t_{i+1})\right] &= p\left[r(t_i) + f(r(t_i),t_i)\Delta t + g\sqrt{\Delta t}\tilde{\eta}(t_i)\right] \qquad (11)\\ &\simeq p\left[r(t_i)\right] + \dot{p}\left[r(t_i)\right]\left(f(r(t_i),t_i)\Delta t + g\sqrt{\Delta t}\tilde{\eta}(t_i)\right)\\ &\quad + \frac{\ddot{p}\left[r(t_i)\right]}{2}\left(f(r(t_i),t_i)\Delta t + g\sqrt{\Delta t}\tilde{\eta}(t_i)\right)^2 + \cdots \qquad (12)\\ &\simeq p\left[r(t_i)\right] + \dot{p}\left[r(t_i)\right]g\tilde{\eta}(t_i)\Delta t^{0.5} + \dot{p}\left[r(t_i)\right]f(r(t_i),t_i)\Delta t\\ &\quad + \frac{\ddot{p}\left[r(t_i)\right]}{2}g^2\tilde{\eta}^2(t_i)\Delta t + \mathcal{O}(\Delta t^{1.5}), \qquad (13)\end{aligned}$$

where $\dot{p}\left[r(t_i)\right] \equiv \left.\frac{dp}{dr}\right|_{r=r(t_i)}$ and $\ddot{p}\left[r(t_i)\right] \equiv \left.\frac{d^2p}{dr^2}\right|_{r=r(t_i)}$.
Moving $p\left[r(t_i)\right]$ to the left-hand-side, dividing by Δt, and taking a statistical average, we obtain

$$\begin{aligned}\left\langle\frac{p\left[r(t_{i+1})\right] - p\left[r(t_i)\right]}{\Delta t}\right\rangle &= \left\langle\dot{p}\left[r(t_i)\right]g\tilde{\eta}(t_i)\Delta t^{-0.5}\right\rangle + \left\langle\dot{p}\left[r(t_i)\right]f(r(t_i),t_i)\right\rangle\\ &\quad + \left\langle\frac{\ddot{p}\left[r(t_i)\right]}{2}g^2\tilde{\eta}^2(t_i)\right\rangle \qquad (14)\\ &= \left\langle\dot{p}\left[r(t_i)\right]\right\rangle g\left\langle\tilde{\eta}(t_i)\right\rangle\Delta t^{-0.5} + \left\langle\dot{p}\left[r(t_i)\right]f(r(t_i),t_i)\right\rangle\\ &\quad + \left\langle\frac{\ddot{p}\left[r(t_i)\right]}{2}g^2\right\rangle\left\langle\tilde{\eta}^2(t_i)\right\rangle \qquad (15)\end{aligned}$$

Substituting $\langle\tilde{\eta}(t_i)\rangle = 0$ and $\langle\tilde{\eta}^2(t_i)\rangle = 1$, and then taking the limit of $\Delta t \to 0$, one finally obtains

$$\left\langle\frac{dp(r(t))}{dt}\right\rangle = \langle\dot{p}(r(t)f(r(t),t)\rangle + \left\langle\frac{\ddot{p}(r(t))}{2}g^2\right\rangle \qquad (16)$$

Using the definition of a statistical average in terms of the probability distribution function $P(r,t)$, we have

$$\langle p(r(t))\rangle = \int P(r,t)p(r)dr. \qquad (17)$$

The corresponding expressions for each of the terms appearing in Eq.(16) are

$$\begin{aligned}\left\langle\frac{dp(r(t))}{dt}\right\rangle &= \frac{\partial}{\partial t}\int P(r,t)p(r)dr \qquad (18)\\ \langle\dot{p}(r(t)f(r(t),t)\rangle &= \int P(r,t)\dot{p}(r)f(r,t)dr \qquad (19)\\ \left\langle\frac{\ddot{p}(r(t))}{2}g^2\right\rangle &= \int P(r,t)\frac{\ddot{p}(r)}{2}g^2dr. \qquad (20)\end{aligned}$$

In the case that $p(r(t)) = \delta(r(t) - R)$, the above averages can be calculated as follows,

$$\left\langle \frac{dp(r(t))}{dt} \right\rangle = \frac{\partial}{\partial t} \int P(r,t)\delta(r-R)dr = \frac{\partial}{\partial t} P(R,t) \tag{21}$$

$$\langle \dot{p}(r(t)f(r(t),t)\rangle = \int P(r,t)\frac{d}{dr}\delta(r-R)f(r,t)dr \tag{22}$$

$$= -\int \frac{d}{dr}\left(P(r,t)f(r,t)\right)\delta(r-R)dr \tag{23}$$

$$= -\frac{\partial}{\partial R}\left(P(R,t)f(R,t)\right) \tag{24}$$

$$\left\langle \frac{\ddot{p}(r(t))}{2} g^2 \right\rangle = \int P(r,t)\frac{g^2}{2}\frac{d^2}{dr^2}\delta(r-R)dr \tag{25}$$

$$= \int \delta(r-R)\frac{d^2}{dr^2}P(r,t)\frac{g^2}{2}dr \tag{26}$$

$$= \frac{g^2}{2}\frac{\partial}{\partial R^2}P(R,t). \tag{27}$$

Finally, substituting the above expression into Eq.(16) yields the Fokker-Planck equation shown below

$$\frac{\partial}{\partial t}P(R,t) = -\frac{\partial}{\partial R}\left(P(R,t)f(R,t)\right) + \frac{g^2}{2}\frac{\partial}{\partial R^2}P(R,t). \tag{28}$$

We can recover the original Langevin equation by changing variables as follows

$$R = R_\alpha \tag{29}$$

$$f(R,t) = 0 \tag{30}$$

$$g^2 = \frac{2k_BT}{\zeta} = 2D, \tag{31}$$

then, the Fokker-Planck equation takes the usual form of a diffusion equation

$$\frac{\partial}{\partial t}P(R_\alpha,t) = D\frac{\partial}{\partial R_\alpha^2}P(R_\alpha,t). \tag{32}$$

Solving this with an initial condition $P(R_\alpha,t) = \delta(R_\alpha)$, yields

$$P(R_\alpha,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{R_\alpha^2}{4Dt}\right] \tag{33}$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{R_\alpha^2}{2\sigma^2}\right] \tag{34}$$

with $\sigma^2 = \frac{2k_BTt}{\zeta} = 2Dt$. This is equivalent to Eq.(G1)-(G3).