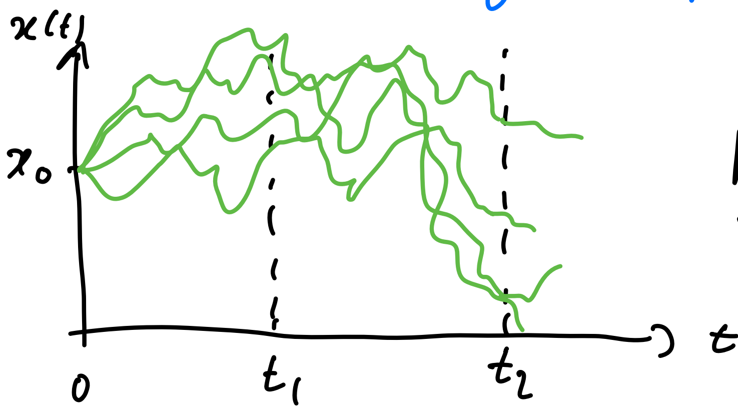
Chapter 3: The Fokker-Planck equation

Reference: Risken, "The Fokker-Planck equation", Springer

Take $x(t)$ such that $x(0)=x_0$ & $\dot{x}(t) = F(x(t)) + \xi(t)$ (1), where ξ is a GWN s.t. $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\,\xi(t') \rangle = 2D\,\delta(t-t')$

Consider several realizations of $x(t)$



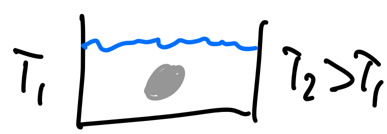
We denote by $P(x(t)=\bar{x}, t \mid x_0, 0)$ the probability that the process $x(t)$ reaches the position $\bar{x}$ at time t, given that it was at x_0 at time 0.

More concisely, we write $P(\bar{x}, t \mid x_0, 0)$ and stress that $\bar{x}$ & x_0 are numbers while $x(t)$ is a stochastic process.

Clearly $P(\bar{x}, t_1 \mid x_0, 0) \neq P(\bar{x}, t_2 \mid x_0, 0) \Rightarrow$ Q: how does $P(\bar{x}, t \mid x_0, 0)$ evolves in time?

1) The Fokker Planck Equation

In Eq (1), the statistics of $\xi(t)$ do not depend on $x(t)$. This is called an additive noise. Instead we can consider a case where, say, the temperature is inhomogeneous



Then $T(x)$ & the Langevin equation is of the type

$$\dot{x} = F(x) + \sqrt{2D(x)}\,\xi(t) \quad (2)$$

with $\langle \xi \rangle = 0$ & $\langle \xi(t)\, \xi(t') \rangle = \delta(t-t')$

This is called a multiplicative noise. Itō formula can be extended to this case, which requires the time discretization of Eq (2) to be

$$x(t+dt) = x(t) + F(x(t))\,dt + \sqrt{2D(x(t))}\int_t^{t+dt} \xi(s)\,ds$$

Let us derive the evolution of $P(x,t|x_0,0)$ in this more general case

dummy integration variable

number

Trick: $P(x,t|x_0,0) = \int dy\, P(y,t|x_0,0)\,\delta(x-y) = \langle \delta(x-y(t)) \rangle$

number

stochastic process

$\langle O(y) \rangle = \int dy\, P(y,t|x_0,0)\, O(y)$ is an average over the realization of the process $y(t)$.

Then we find

$$\frac{dP(x,t|x_0,0)}{dt} = \left\langle \frac{d}{dt}\delta(x-y(t)) \right\rangle_y$$

$$\overset{\text{Itō}}{=} \left\langle \left[\partial_y \delta(x-y)\right] \dot{y} + \frac{1}{2}\, 2D(y)\, \partial_y^2 \delta(x-y) \right\rangle_y$$

where $\partial_y f \equiv \frac{\partial f}{\partial y}$

$$= \langle F(y)\partial_y \delta(x-y) \rangle + \underbrace{\left\langle \xi(t)\sqrt{2D(y(t))}\,\partial_y \delta(x-y(t)) \right\rangle}_{\overset{\text{Itō}}{=}\ \underbrace{\langle \xi(t) \rangle}_{=0} \langle \sqrt{2D(y)}\,\partial_y \delta(x-y) \rangle} + \langle D(y)\partial_y^2 \delta(x-y) \rangle$$

Using that $\langle O(x) \rangle = \int dx\, O(x) P(x)$, we get

$$\frac{d}{dt}P(x,t|x_0,0) = \int dy\, P(y,t|x_0,0)\left[F(y)\,\partial_y \delta(x-y) + D(y)\,\partial_y^2 \delta(x-y)\right]$$

$$\overset{IBP}{=} \int dy\, \delta(x-y) \left\{ -\frac{\partial}{\partial y}\left[F(y) P(y,t|x_0,0)\right] + \frac{\partial^2}{\partial y^2}\left[D(y) P(y,t|x_0,0)\right] \right\} \qquad (3)$$

$+$ boundary terms

Boundary terms:

Case 1: periodic boundary condition $[\ldots]_{\text{boundary } 1}^{\text{boundary } 2} = 0$

Case 2: closed box, $x \in [x_1, x_2]$, then $P(x < x_1 | x_0, 0) = P(x > x_2 | x_0, 0) = 0$

$$\Rightarrow [\ldots]_{\text{boundary } 1}^{\text{boundary } 2} = 0$$

Case 3: Infinite system. $\int dx\, P(x,t|x_0,0) = 1 \Rightarrow P(x \to \pm\infty, t | x_0, 0) = 0$

$$\Rightarrow [\ldots]_{\text{boundary } 1}^{\text{boundary } 2} = 0$$

$\Rightarrow$ In all standard cases, the boundary terms vanish.

Then, in (3), $\int dy\, \delta(x-y) H(y) = H(x)$ so that

$$\boxed{\frac{d}{dt} P(x,t|x_0,0) = \frac{\partial}{\partial x}\left[-F(x) + \frac{\partial}{\partial x} D(x) \right] P(x,t|x_0,0)} \qquad (4)$$

where $\frac{\partial}{\partial x}$ is an operator that acts on everything to its right.

This is the celebrated Fokker-Planck equation.

⚠ Be careful with the position of $D(x)$ that does <u>not</u> commute with $\frac{\partial}{\partial x}$.

Mathematical a parte

Let us follow a slightly more mathematical route to the FPE.

Let $f: \mathbb{R} \to \mathbb{R}$ be a C^2 function. By definition $\langle f(x(t))\rangle = \int dx\, f(x)\, P(x,t|x_0,0)$

Thus
$$\boxed{\frac{d}{dt}\langle f(x(t))\rangle = \int dx\, f(x)\, \frac{\partial P(x,t|x_0,0)}{\partial t}} \quad ①$$

Itō formula also tells us that $\frac{d}{dt} f(x(t)) = f'(x(t))\,\dot{x} + D f''(x(t))$

Taking the average,

$$\frac{d}{dt}\langle f(x(t))\rangle = \langle f'(x(t))\cdot F(x(t))\rangle + \underbrace{\langle f'(x(t))\,\xi(t)\rangle}_{\text{Itō } \langle f'\rangle\langle \xi(t)\rangle = 0} + D\langle f''(x(t))\rangle$$

$$= \int dx \left[\frac{\partial f}{\partial x}\cdot F(x)\, P(x,t|x_0,0) + D\frac{\partial^2 f}{\partial x^2} P(x,t|x_0,0)\right]$$

$$\underset{\text{IBP}}{=} \underbrace{\cancel{\Big[f(x)F(x)\,P(x,t|x_0,0) + D f'(x)\,P(x,t|x_0,0)\Big]_{\text{boundary }1}^{\text{boundary }2}}}_{=0 \text{ as before}}$$

$$- \int dx \left\{ f(x)\frac{\partial}{\partial x}\left[F(x)P(x,t|x_0,0)\right] + \frac{\partial f}{\partial x}\cdot\frac{\partial}{\partial x}\left[D\,P(x,t|x_0,0)\right]\right\}$$

$$= \int dx\, f(x) \left\{ \frac{\partial^2}{\partial x^2}\left[D\,P(x,t|x_0,0)\right] - \frac{\partial}{\partial x}\left[F(x)\,P(x,t|x_0,0)\right]\right\}$$

① & ② hold for any function f so that

$$\boxed{\frac{\partial P(x,t|x_0,0)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} D - F(x)\right] P(x,t|x_0,0)}$$

Intuition:

① $F=0$; $\dot{x}=\sqrt{2D}\,\eta \iff$ random walk $\Rightarrow \frac{dP}{dt} = D\Delta P$ which is the diffusion eq°.

② $D=0$; $\dot{x} = F(x) \iff$ advection & $\frac{dP}{dt} = -\partial_x (F.P)$

The Fokker-Planck is the combination of diffusion due to the noise & advection of probability due to the force

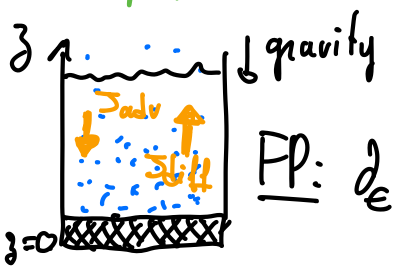
Conservation of probability & probability current

$\int_{-\infty}^{+\infty} P(x)\,dx = 1$ is a global conservation law for $P(x)$

(1) $\iff \partial_t P = -\partial_x [J(x)]$ with $J(x) = +F(x)P - D\partial_x P$ is a local conservation law for the probability density and $J(x)$ is called a probability current.

Example:

$\dot{z} = -\mu\,\delta m g + \sqrt{2\mu kT}\,\eta$ where δm is the difference between the colloid mass & the mass of the same volume of fluid.



FP: $\partial_t P = \frac{\partial}{\partial z}\left[\mu\,\delta m g P + \mu kT\,\partial_z P\right]$; $J = \underbrace{-\mu\,\delta m g P}_{J_{adv.}} \underbrace{-\mu kT\,\partial_z P}_{J_{diff.}}$

Start with $P(z,0)$ and wait until the system reaches a steady state in which it does not evolve statistically: $\partial_t P(z,t) = 0 \Rightarrow \mu\,\delta m g P + \mu kT\,\partial_z P = C^{te}$

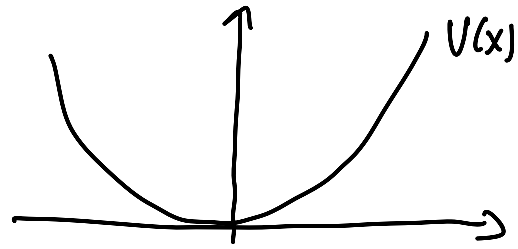
Since $P=0$ for $z<0$, $C^{te}=0$ & $\partial_z P = -\frac{\delta m g}{kT} P \Rightarrow P(z) = P_0 e^{-\frac{\delta m g z}{kT}}$

This exponential "atmosphere" is called a Perrin profile & was measured experimentally by Jean Perrin (Nobel prize in 1926)

More generally: $\dot{x} = -\mu V'(x) + \sqrt{2kT}\,\eta(t)$, where $V(x)$ is a confining potential

The Fokker Planck equation reads

$$\partial_t P = \frac{\partial}{\partial x}\left[\mu kT \frac{\partial P}{\partial x} + \mu V'(x) P\right]$$



so that $P(x) = \frac{1}{Z} e^{-\frac{V(x)}{kT}}$ is a steady-state solution of the system.

This is the Boltzmann weight & the colloid reaches thermal equilibrium. The solvent acts like a thermostat: an equilibrated fluid drives an inert particle into an equilibrated stationary state.

Object in equilibrated bath $\xrightarrow{\text{coarse graining}}$ Langevin equation $\xrightarrow{\text{stationary state}}$ Canonical measure

Comment: For $P(x)$ to be normalizable, we need $\int dx\, e^{-\beta V(x)} < +\infty$

$\Rightarrow$ $V(x)$ has to diverge fast enough.

If $V(x) \underset{x\to\pm\infty}{\sim} \varepsilon \log|x|$, $e^{-\beta V(x)} \underset{x\to\pm\infty}{\sim} \frac{1}{|x|^{\beta\varepsilon}}$ not integrable for $\varepsilon\beta \leq 1$ $\Leftrightarrow$ $kT \geq \varepsilon$

$\Rightarrow$ at high temperature, the system does not equilibrate.

The potentials that diverge <u>faster</u> than logarithmically are called confining potentials.