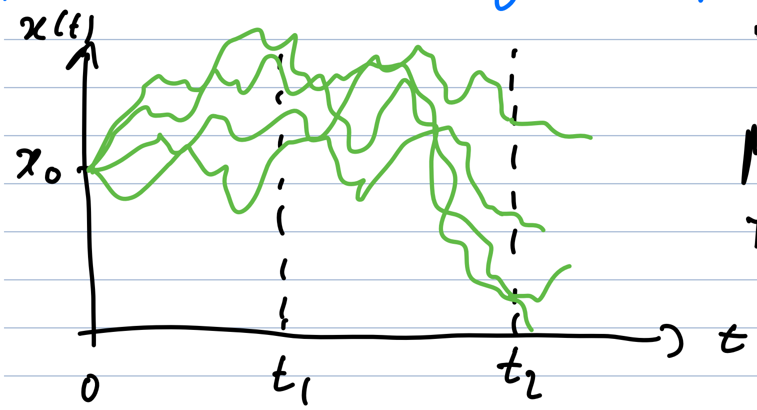
# Chapter 3: The Fokker-Planck equation



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 $\xi$ is a GWN s.t. $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\, \xi(t') \rangle = 2D\,\delta(t-t')$

Consider several realizations of $x(t)$



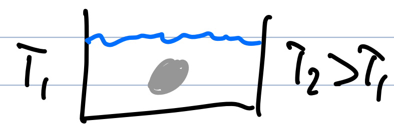

We denote by $P(x(t)=\bar{x}, t \,|\, x_0, 0)$ the probability that the process $x(t)$ reaches the position $\bar{x}$ at time $t$, given that it was at $x_0$ at time 0.

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

Clearly $P(\bar{x}, t_1 | x_0, 0) \neq P(\bar{x}, t_2 | x_0, 0) \Rightarrow$ Q: how does $P(\bar{x}, t | x_0, 0)$ 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

Trick: $\underset{\text{number}}{P(x},t|x_0,0) = \int dy\, P(y,t|x_0,0)\, \delta(x-y) = \langle \delta(\overset{\text{number}}{x} - \underset{\text{stochastic process}}{y(t)}) \rangle_{y(t)}$

average over the realization of the process $y(t)$.

Then we find

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

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

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

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

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

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

$+$ boundary terms (3)

Boundary terms:

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

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

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

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

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

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

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

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

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

This is the celebrated Fokker-Planck equation.

⚠ Be careful with the position of $D(y)$ that does not commute with $\frac{\partial}{\partial y}$.

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

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

Taking the average,

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

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

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

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

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

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

② $D=0$ ; $\dot{x} = F(x) \Leftrightarrow$ 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

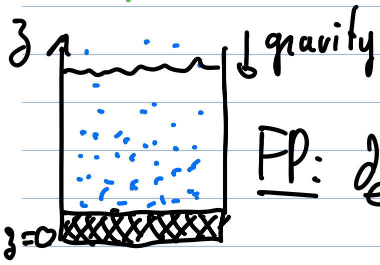
## Conservation of probability:

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

(1) $\Leftrightarrow \partial_t P = -\partial_x [J(x)]$ 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 $\delta m$ is the difference between the colloid mass & the mass of the same volume of fluid.




FP: $\partial_t P = \frac{\partial}{\partial z}\left[\mu\,\delta m g P + \mu kT\,\partial_z P\right]$

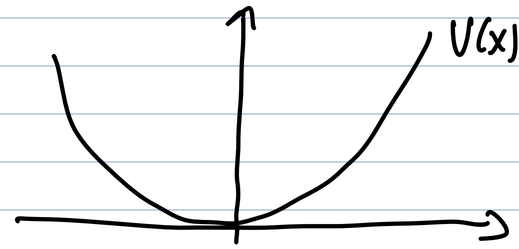
Start with $P(z,0)$ and wait until the system reaches a steady state in which it does not evolve statistically: $\partial_t P(z,t) = 0 \Rightarrow \mu\,\delta m g P + \mu kT\,\partial_z P = C^{te}$

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




$$\partial_t P = \frac{\partial}{\partial x}\left[\mu k T \frac{\partial P}{\partial x} + \mu V'(x) P\right]$$

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

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

The potentials that diverge faster than logarithmically are called confining potentials.

## 4.2) The N-dimensional Fokker-Planck equation



Let's consider $\dot{x}_i = F_i(x_1, \dots, x_N) + \eta_i$ where $\eta_i$ are GWN s.t. $\langle \eta_i \rangle = 0$

and $\langle \eta_i(t)\, \eta_k(s) \rangle = B_{ik}\, \delta(t-s)$

numbers

$$P(x_1, \dots, x_N; t) = \Big\langle \prod_i \delta(x_i - y_i) \Big\rangle_{\vec{y}}$$

stochastic processes

$$\frac{\partial P}{\partial t} = \underbrace{\sum_k \Big\langle \frac{\partial}{\partial y_k} \Big( \prod_i \delta(x_i - y_i) \Big) \dot{y}_k \Big\rangle_{\vec{y}}}_{\text{Itô } \left\langle \frac{\partial}{\partial y_k} \left( \prod_i \delta(x_i - y_i) \right) F_k \right\rangle_{\vec{y}}} + \sum_{j,k} \Big\langle \frac{B_{jk}}{2} \frac{\partial^2}{\partial y_j \partial y_k} \prod_i \delta(x_i - y_i) \Big\rangle_{\vec{y}}$$

$$= \int \Big( \prod_i dy_i \Big) \Big\{ \sum_k \frac{\partial}{\partial y_k} \Big[ \prod_i \delta(x_i - y_i) \Big] F_k P + \sum_{j,k} \frac{\partial^2}{\partial y_j \partial y_k} \Big[ \prod_i \delta(x_i - y_i) \Big] \frac{B_{jk}}{2} P \Big\}$$

$$\overset{\text{IBP}}{=} \int \prod_i dy_i \cdot \Big[ \prod_i \delta(x_i - y_i) \Big] \Big\{ \sum_k - \frac{\partial}{\partial y_k} \big[ F_k P \big] + \sum_{j,k} \frac{\partial^2}{\partial y_j \partial y_k} \Big[ \frac{B_{jk}}{2} P \Big] \Big\}$$

leading to the Fokker planck equation

$$\frac{\partial P(x_1, \dots, x_N, t)}{\partial t} = \sum_k \frac{\partial}{\partial x_k} \Big[ - F_k - \sum_j \frac{\partial}{\partial x_j} \frac{B_{jk}}{2} \Big] P(x_1, \dots, x_N, t)$$

### Conservation of probability:

This can again be written as

$$\partial_t P = - \sum_k \frac{\partial}{\partial x_k} \cdot J_k = - \vec{\nabla} \cdot \vec{J}$$

, where the probability current is given by

$$J_k = \underbrace{F_k P}_{\text{advection}} - \underbrace{\sum_j \frac{\partial}{\partial x_j} \frac{B_{jk}}{2} P}_{\text{diffusion}}$$

$B_{jk}$ tells us how noise along $\hat{j}$ leads to a diffusive current along $\hat{k}$.

## Application: Underdamped Langevin equation & the Kramers equation

$\dot{q} = p$ ; $\dot{p} = -\gamma p - V'(q) + \sqrt{2\gamma kT}\,\eta(t)$ with $\langle \eta(t) \rangle = 0$ $(m=1)$

and $\langle \eta(t)\eta(s) \rangle = \delta(t-t')$. As before, we can understand this equation as experiencing noise on both $q$ & $p$, but with $B_{qq} = B_{qp} = B_{pq} = 0$ & $B_{pp} = 2\gamma kT$. Then the equation for $P(q,p,t)$ reads

$$\boxed{\partial_t P(\vec{q},\vec{p},t) = -\frac{\partial}{\partial q}(pP) + \frac{\partial}{\partial p}\left[(\gamma p + V'(q))P\right] + \gamma kT \frac{\partial^2}{\partial p^2} P}$$

This is called the Kramers equation.

## Steady state solution in the presence of a confining potential

$H = \frac{p^2}{2} + V(q)$

Let's show that the steady-state solution is $Z^{-1}e^{-\beta H}$.

$$-\frac{\partial}{\partial q}\left(p e^{-\beta H}\right) + \frac{\partial}{\partial p}\left(\cancel{\gamma p e^{-\beta H}} + V'(q) e^{-\beta H} + \cancel{\gamma kT \overbrace{\left(-\beta p e^{-\beta H}\right)}^{\frac{\partial}{\partial p} e^{-\beta H}}}\right)$$

$$= -p\left[-\beta V'(q) e^{-\beta H}\right] + V'(q)\left[-\beta p e^{-\beta H}\right] = 0$$

Again, the steady state corresponds to the Boltzmann weight.

**Comment:** The steady state is independent from $\gamma$, which is a purely *kinetic* parameter and plays no role in the *thermodynamics* of equilibrium systems. It, however, controls the relaxation rate of the system towards steady-state.

Comment: The same result holds for a space-dependent viscosity $\gamma(\vec{q})$, but not for $T(\vec{q})$, which leads to a nonequilibrium steady state.

## Recap so far:

Stochastic dynamics: $\dot{\vec{r}} = -\mu \vec{\nabla} V + \sqrt{2\mu k T}\, \vec{\eta}$

- → clear physical picture of the dynamics
- → simulations
- → stochastic calculus → evolution of observables
  → correlation functions

Fokker-Planck equation: $\partial_t P = -\vec{\nabla} \cdot [-\mu \vec{\nabla} V P - \mu k T \vec{\nabla} P]$

- → hard to simulate
- → statistical information/intuition through $P(\vec{r})$
  e.g. Show that $P_s(\vec{r}) \propto e^{-\beta H}$
- → Now: very powerful operator calculus

## 4.3) The Fokker-Planck operator

$$\partial_t P = \frac{\partial}{\partial x}\left[kT \frac{\partial}{\partial x} - F(x)\right] P(x,t) \quad (1) \iff \partial_t P = -H_{FP} P \quad \text{where}$$

$$H_{FP} = -\frac{\partial}{\partial x}\left[kT \frac{\partial}{\partial x} - F(x)\right]$$ which acts on the Hilbert space of functions $\mathcal{H}(P)$ that depends on the dimensions & boundary conditions of the problem.