§6 Boundary conditions for the Fokker-Planck equation

- We need to consider the different types of boundary conditions for the FPE, with a view towards applications. We'll mostly use the 1D case for examples, but all boundary conditions have higher-dimensional analogues also.

- **1. Natural boundary conditions**

- This is the condition we have used in most of our examples so far: $P(x,t) \to 0$ as $x \to \infty$ or $x \to -\infty$, with the decay to zero being sufficiently fast to ensure the normalization integral is

$$\int_{-\infty}^{\infty} P(x,t)dx = 1.$$

In the 1D case this requires $P(x,t) \to 0$ faster than $|x|^{-1}$ as $|x| \to \infty$.

- The natural BC typically is applied when the range of the random variable $x(t)$ is infinite or semi-infinite.

- We saw an example of natural BCs in two dimensions also: for the nonlinear oscillator example we had $P_\infty \to 0$ as $r \to \infty$.

- **2. Reflecting boundary conditions**

- For e.g. Brownian particles near a wall, the wall provides an impenetrable barrier.

- We write the FPE for $P(x,t)$ in the form

$$\frac{\partial P}{\partial t} + \frac{\partial S}{\partial x} = 0,$$

where $S(x,t)$ is the "probability flux (or current)" [Risken p. 84] given for

$$\dot{x} = f(x) + g(x)\eta(t)$$

as

$$S(x,t) = f(x)P(x,t) - \kappa g(x)\frac{\partial}{\partial x}\left[g(x)P(x,t)\right].$$

- The name for S can explained by considering the rate of change of probability (or concentration of Brownian particles) between two fixed positions $x = A$ and $x = B$:

$$\frac{d}{dt}\int_A^B P(x,t)dx = \int_A^B \frac{\partial P}{\partial t}dx = -\int_A^B \frac{\partial S}{\partial x}dx = S(A,t) - S(B,t).$$

- This is interpreted as:
rate of change of probability of being in $[A,B]$ = (flow into $[A,B]$ through $x = A$)-(flow out of $[A,B]$ through $x = B$).

- Thus $S(x,t)$ represents the flow or flux of particles (or current) through the point x at time t.
- Now suppose there is an impenetrable wall at some position $x = a$.
- Since particles cannot penetrate the wall the flux at $x = a$ must be zero:

$$\Rightarrow S(a,t) = 0$$

for all t.

- This provides the boundary condition at $x = a$:

$$f(a)P(a,t) - \kappa\, g(x)\frac{\partial}{\partial x}\left[g(x)P(x,t)\right]\Big|_{x=a} = 0.$$

- This simplifies in many common cases.
- E.g. Brownian motion with $f \equiv 0$ and $g \equiv 1$. We have seen the use of natural boundaries when the particles can move freely in the infinite interval $x \in (-\infty, \infty)$. Suppose there is an impenetrable wall at $x = a$, so the particles are constrained to move in the semi-infinite interval $x \in (-\infty, a]$.
- The FPE is

$$\frac{\partial P}{\partial t} = \kappa \frac{\partial^2 P}{\partial x^2}$$

with initial condition $P(x,0) = \delta(x)$ as before.

- The boundary conditions are:

$$P(x,t) \to 0 \text{ as } x \to -\infty$$

(natural BC) and a no-flux BC at $x = a$:

$$\kappa\, \frac{\partial P}{\partial x}\Big|_{x=a} = 0,$$

or simply

$$\frac{\partial P}{\partial x}\Big|_{x=a} = 0.$$

- The probability flux can be defined for higher-dimensional problems also [Risken p.84], e.g. for the convection-diffusion problem

$$\dot{x} = v(x) + \eta(t)$$

with

$$\langle \eta_i(t)\eta_j(t')\rangle = 2\kappa\delta_{ij}\delta(t-t'),$$

we found the FPE

$$\frac{\partial P}{\partial t} = -\nabla\cdot(vP) + \kappa\nabla^2 P.$$

- The FPE may be written in terms of the probability flux vector S as

$$\frac{\partial P}{\partial t} + \nabla S = 0$$

and

$$S(x,t) = v(x)P(x,t) - \kappa\nabla P(x,t).$$

- Consider a 2D example, with a wall at $y = a$.
- Writing $\hat{n}$ as the (outward) unit normal vector at the wall, the no-flux condition is

$$\begin{aligned} \hat{n}\cdot S &= 0 \\ \Rightarrow \left[v\cdot\hat{n}\,P - \kappa\,\hat{n}\cdot\nabla P\right]_{y=a} &= 0. \end{aligned}$$

- For fluid flows, the velocity vector $v(x)$ has no component perpendicular to the wall, so $v\cdot\hat{n} = 0$ at $y = a$.
- Thus the no-flux BC is

$$\hat{n}\cdot\nabla P = 0$$

at the wall; in other words the normal derivative of P is zero at the wall. In our example with the wall at $y = a$, this yields

$$\left.\frac{\partial P}{\partial y}\right|_{y=a} = 0.$$

- **3. Absorbing boundary conditions**
- An absorbing wall at $x = a$ means that particles are removed from the interval $(-\infty, a]$ as soon as they first hit $x = a$.
- This can occur for physical reasons (e.g. a chemical reaction at the wall causes molecules to be absorbed or changed to a different chemical species), or for mathematical reasons (we will impose absorbing BCs when looking at first passage time problems).
- The appropriate BC for an absorbing wall at $x = a$ is

$$P(a,t) = 0,$$

i.e. zero probability of finding particles at the wall, since they are immediately absorbed.

- **Example:** A microelectrode recessed into a surface. Concentration of ions in bulk is c_b. Consider the electrode to be at $z = 0$, with the flat surface at $z = L$.

- The Langevin equation for the freely diffusing ions (take 1D approx for a long, narrow recess) with vertical position $z(t)$ is

$$\frac{dz}{dt} = \eta(t)$$

with $\langle \eta(t)\eta(t') \rangle = 2\kappa\delta(t - t')$.

- The FPE for the PDF $P(z, t)$ (or concentration $c(z, t) \equiv P(z, t)$) is

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial z^2},$$

with absorbing BC at $z = 0$:

$$c(0, t) = 0.$$

- The other boundary condition is

$$c(L, t) = c_b,$$

assuming the concentration at the mouth of the recess is equal to the bulk concentration.

- Our goal is to find the steady-state current at the electrode in terms of c_b and L.

- The electrode current is proportional to the probability flux at $z = 0$, i.e.,

$$I = \beta \left. \frac{\partial c}{\partial z} \right|_{z=0}$$

for appropriate constant β (since current is proportional to rate of change of charge = flux of ions onto electrode).

- In steady state, $c = c_\infty(z)$ and

$$\frac{d^2 c_\infty}{dz^2} = 0.$$

- Solution:

$$c_\infty(z) = Az + B$$

for constants A and B.

- Applying boundary conditions gives $B = 0$ and $A = \frac{c_b}{L}$, so

$$c_\infty(z) = \frac{c_b}{L} z.$$

- Then
$$\frac{dc_\infty}{dz} = \frac{c_b}{L}$$
and so
$$I = \beta \frac{c_b}{L}$$
gives the electrode current dependence on c_b and L.

- **4. Periodic boundary conditions**

- If the random variable is naturally periodic, e.g., an angular variable with $\theta \in [0, 2\pi]$ then periodic boundary conditions must be imposed on the FPE [Risken p.103]:
$$\begin{aligned} P(\theta + 2\pi, t) &= P(\theta, t) \\ S(\theta + 2\pi, t) &= S(\theta, t) \end{aligned}$$

- Example: the phase angle for a nonlinear oscillator, with strong amplitude control (so $r \equiv 1$).

- Motion is restricted to the limit cycle, with deterministic rotation frequency Ω, plus noise effects:
$$\dot{\theta} = \Omega + \text{noise terms.}$$

- Then PDF $P(\theta, t)$ is defined only for $\theta \in [0, 2\pi]$ with
$$P(0, t) = P(2\pi, t)$$
and
$$S(0, t) = S(2\pi, t).$$