Lecture 7 summary

Stationary solution of master equation p_n^*

$$\boxed{p_n^* = p_0^* \prod_{n'=1}^{n} \frac{g_{n'-1}}{r_{n'}}}$$

Rate equations for $\langle N(t) \rangle = \sum_{n=0}^{\infty} n \, p_n(t)$

$$\langle \dot{N}(t) \rangle = \langle g_n \rangle - \langle r_n \rangle$$

$\langle \dot{N} \rangle = -\gamma \langle N \rangle$ linear decay

(see example of radioactive decay of $N(t)$ atoms, lecture 6)

Example: chemical reaction $X \underset{k_2}{\overset{k_1}{\rightleftarrows}} A$

- master equation

  $\dot{p}_n = \dots$

- generating function

  $\partial_t G(s,t) = \dots$

  $G(s,t) = \dots$

- moment equations

$$\frac{d}{dt} \underbrace{\langle N(t)^k \rangle_f}_{\text{factorial moment}} = k \left[k_2 a \langle N(t)^{k-1} \rangle_f - k_1 \langle N(t)^k \rangle_f \right]$$

2.2 Fokker-Planck equation (FPE)

Here we will discuss the theory of continuous Markov processes from the point of view of FPE, which gives the time evolution of the probability density function for the system.

In one dimension $\rightarrow$ 1D random variable $X(t)$

$$\frac{\partial}{\partial t} f(x,t) = -\frac{\partial}{\partial x} \left[\underbrace{A(x,t)}_{\text{drift}} f(x,t) \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[\overbrace{B(x,t)}^{\text{diffusion}} f(x,t) \right]$$

We have previously shown (see lecture 5) that FPE is valid for conditional probability

$$f(x,t) = p(x,t \mid x_0, t_0)$$

for any initial x_0, t_0, and initial condition

(*) $p(x, t_0 / x_0, t_0) = \delta(x - x_0)$

However, using definition of one time probability

$$p(x,t) = \int dx_0 \, p(x,t; x_0, t_0) =$$

$$= \int dx_0 \, p(x,t / x_0, t_0) \, p(x_0, t_0),$$

we see that it is also valid for $p(x,t)$ with I.C. $p(x,t)\big|_{t=t_0} = p(x, t_0)$, which is generally less singular than (*).

<u>Boundary conditions</u>

FPE is a second order parabolic PDE, and for solutions we need I.C. and boundary conditions (B.C.) at the end of the interval inside which x is constrained. These B.C. take on a variety of forms.

It is simple to derive the B.C. in general, than to restrict consideration to the one variable situation.

<u>n - dimensional boundary conditions</u>

We consider the forward FPE

| $\vec{A}$ / $\underline{A}$ vector

$$\partial_t \, p(\vec{x}, t) = - \sum_i \frac{\partial}{\partial x_i} A_i(\vec{x}, t) p(\vec{x}, t) + \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} B_{ij}(\vec{x}, t) \, p(\vec{x}, t)$$

We note that this can be written

$$\frac{\partial}{\partial t} p(\vec{x}, t) + \sum_i \frac{\partial}{\partial x_i} J_i(\vec{x}, t) = 0 \quad (**)$$

where we define the <u>probability current</u>

$$J_i(\vec{x}, t) = A_i(\vec{x}, t) p(\vec{x}, t) - \frac{1}{2} \sum_j \frac{\partial}{\partial x_j} \left[B_{ij}(\vec{x}, t) \, p(\vec{x}, t) \right]$$

Equation (**) has the form of a local conservation equation, and can be written in an integral form as follows. Consider some region R with a boundary S and define:

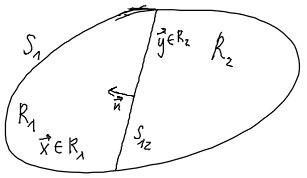
$$P(R, t) = \int_R d\vec{x} \, p(\vec{x}, t)$$

then (**) is equivalent to

$$\frac{\partial}{\partial t} P(R, t) = - \int_S dS \, \vec{n} \cdot \vec{J}(\vec{x}, t) \qquad (***)$$

where $\vec{n}$ is the outward pointing normal to S.

Thus (* * *) indicates that the total loss of probability is given by the surface integral of $\vec{J}$ over boundary of R. We can show as well that the current $\vec{J}$ does have the stronger property, that a surface integral over any surface S gives the net flow of probability across that surface.



The net flow of probability can be computed by noting that we are dealing with a process with continuous sample paths, so that in a sufficiently short time Δt, the prob. of crossing S_{12} from R_2 to R_1 is the joint probability of being in R_2 at time t and R_1 at time $t+\Delta t$:

$$\int_{R_1} d\vec{x} \int_{R_2} d\vec{y}\, p(\vec{x}, t+\Delta t; \vec{y}, t)$$

The net flow of prob-ty from R_2 to R_1 is obtained by substracting from this the prob-ty of crossing in the reverse direction, and dividing by Δt:

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{R_1} d\vec{x} \int_{R_2} d\vec{y} \left[\underbrace{p(\vec{x}, t+\Delta t; \vec{y}, t) - p(\vec{y}, t+\Delta t; \vec{x}, t)}_{R_1 \leftarrow R_2} \right] =$$

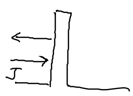
$$= \int_{S_{12}} dS\, \vec{n} \cdot \vec{J}(\vec{x}, t)$$

$\vec{n}$ points from R_2 to R_1.

<u>Boundary conditions</u>

(a) Reflecting barrier

The particle cannot leave R, hence there is zero net flow of prob. across S, the boundary of R.



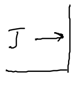
$$\vec{n} \cdot \vec{J}(\vec{x}, t) = 0 \quad \text{for } X \in S, \; \vec{n} = \text{normal to } S.$$

Since the particle cannot cross S, it must be reflected there, $\Rightarrow$ reflecting barrier

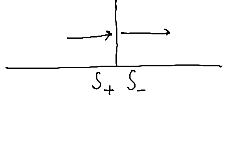
(b) Absorbing barrier

particle reaches $S \Rightarrow$ it is removed from the system, thus the barrier absorbs $\Rightarrow$ the prob-ty of being on the boundary is zero:

$$p(\vec{x}, t) = 0 \quad \text{for } \vec{x} \in S$$



(c) Boundary conditions at a discontinuity (medium 1 and medium 2 separated by S)



$$\vec{n} \cdot \vec{J}(\vec{x})\Big|_{S_+} = \vec{n} \cdot \vec{J}(\vec{x})\Big|_{S_-}$$

$$p(\vec{x})\Big|_{S_+} = p(\vec{x})\Big|_{S_-}$$

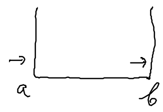
S_+, S_- mean the limits of the quantities from the left and right hand sides of the surface.

The definition of the prob. current indicates that the derivatives of $p(\vec{x})$ are not necessarily continuous at S.

(d) periodic boundary conditions

$[a, b]$ the two end points are identified with each other

We impose boundary conditions derived from those for a discontinuity:



$$\text{I}: \lim_{x \to b_-} p(x,t) = \lim_{x \to a_+} p(x,t)$$

$$\text{II}: \lim_{x \to b_-} J(x,t) = \lim_{x \to a_+} J(x,t)$$

Most frequently, periodic B.C. are imposed when the functions $A(x,t)$ and $B(x,t)$ are periodic on the same interval:

$A(b,t) = A(a,t)$

$B(b,t) = B(a,t)$

(e) Natural boundary

$A(a,t) = 0$

The particle, once it reaches $x=a$, will remain there.
It can be, however, demonstrated it cannot ever reach this point.
This is a boundary from which we can neither absorb nor at which we can introduce any particles.

Stationary solutions for homogeneous FPE.

hom. process: drift and diffusion coefficients are time independent.

$$\frac{d}{dx}\left[A(x)\, p^*(x)\right] - \frac{1}{2}\frac{d^2}{dx^2}\left[B(x), p^*(x)\right] = 0$$

and in terms of current

$$\frac{d}{dt} J(x) = 0$$

$\Rightarrow$ solution $J(x) = \text{const}$

Suppose the process takes place on an interval (a, b).
Then we must have:

$$J(a) = J(x) = J(b) \equiv J \quad ☺$$

and if one of the boundary cond. is reflecting, this means that both are reflecting and $J=0$.

If the B.C. are not reflecting ☺ requires them to be periodic.

(i) Zero current – potential solution

$J=0$, we rewrite ☺ as

$$A(x)\,p^*(x) - \frac{1}{2}\frac{d}{dx}\left[B(x)\,p^*(x)\right] = 0$$

the solution

$$p^*(x) = \frac{\mathcal{N}}{B(x)} \exp\left[2\int_a^x dx' \frac{A(x')}{B(x')}\right]$$

$\mathcal{N}$ - normalization constant $\displaystyle\int_a^b dx\, p^*(x) = 1$

Such a solution is known as potential solution because the stationary solution is obtained by a single integration.