Lecture 5 summary

(a) jump process : $A_i(z,t) = B_{ij}(z,t) = 0$

$$\frac{\partial}{\partial t} p(z,t/y,t') = \int dx \left[W(z/x,t) p(x,t/y,t') - \underbrace{W(x/z,t)}_{\text{prob of trans per unit time}} p(z,t/y,t') \right]$$

(b) diffusion process : $A_i(z,t) = W(z/x,t) = 0$

$$\frac{\partial}{\partial t} p(z,t/y,t') = \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial z_i \partial z_j} \left[\underbrace{B_{ij}(z,t)}_{\text{diffusion matrix}} p(z,t/y,t') \right]$$

(c) drift process : $B_{ij}(z,t) = W(z/x,t) = 0$

Liouville equation:

$$\frac{\partial p(z,t/y,t')}{\partial t} = - \sum_i \frac{\partial}{\partial z_i} \left[\underbrace{A_i(z,t)}_{\text{drift vector}} p(z,t/y,t') \right]$$

Combination of (b) and (c)

Fokker – Planck equation

$$\frac{\partial}{\partial t} p(z,t/y,t') = - \sum_i \frac{\partial}{\partial z_i} \left[A_i(z,t) p(z,t/y,t') \right] + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial z_i \partial z_j} \left[B_{ij}(z,t) p(z,t/y,t') \right]$$

2. Classical statistics in non-equilibrium

2.1 Master equation

From (1) one can directly derive Master equation for differential time evolution

(1): we recalled Chap-Kol. equation for Markov proc.

$t'' = t + \Delta t$:

$$p(x,t+\Delta t/x',t') = \int dz\, \delta(x-z) \left[1 - \int dx_2\, W(x_2/z,t) \Delta t \right] p(z,t/x',t') + \int dz\, W(x/z,t) \Delta t\, p(z,t/x',t') =$$

$$= \left[1 - \Delta t \int dx_2\, W(x_2/x,t) \right] p(x,t/x',t') - \Delta t \int dz\, W(x/z,t)\, p(z,t/x',t')$$

$$\Rightarrow \boxed{\frac{\partial}{\partial t} p(x,t/x',t') = \lim_{\Delta t \to 0} \frac{p(x,t+\Delta t/x',t') - p(x,t/x',t')}{\Delta t} = \int dz\, \underbrace{W(x/z,t)}_{x \leftarrow z} p(z,t/x',t') - \int dz\, \underbrace{W(z/x,t)}_{z \leftarrow x} p(x,t/x',t')}$$

Master equation

A discrete random variable $N(t)$:
number of electrons during tunnelling or recombination - generation processes in semiconductors,
number of particles in a chemical reaction.

For the case when the state space consists of integers only, the Master equation takes the form:

$$\boxed{\frac{\partial}{\partial t} p(n,t \mid n',t') = \sum_m \left[W(n \mid m,t)\, p(m,t \mid n',t') - W(m \mid n,t)\, p(n,t \mid n',t') \right]}$$

Notation $p_n(t) = p(n,t \mid n',t')$ with I.C. $p_{n'}(t')$

$W_{nm} = W(n \mid m, t)$

$$\boxed{\frac{\partial}{\partial t} p_n(t) = \sum_{\substack{m \\ \neq n}} \left[W_{nm}\, p_m(t) - W_{mn}\, p_n(t) \right]}$$

$n \leftarrow m$ gain $\qquad m \leftarrow n$ loss

NB: 1) $m \neq n$ in the sum

2) $W_{nm} \geq 0$

$\sum_n W_{nm} = 1$ since we either have a transition to another state ($\neq m$) or no transition

$\Rightarrow W_{mm} = 1 - \sum_{\substack{n \\ \neq m}} W_{nm}$

3) quantum physics:

for example, calculation of

$W_{nm} = \frac{2\pi}{\hbar} \left| \langle n | H_1 | m \rangle \right|^2 \delta(E_n - E_m)$

from Fermi's golden rule with perturbation H_1

<u>Example</u>

radioactive decay of $N(t)$ atoms

$W_{nn'} = \gamma n' \delta_{n, n'-1}$

γ is the decay rate ($n' \to n'-1$) or probability per unit time

$$\boxed{\dot{p}_n} = \sum_{n'} \left[\gamma n' \delta_{n,n'-1} p_{n'} - \gamma n \delta_{n',n-1} p_n \right] =$$

$$= \gamma \boxed{\left[(n+1) p_{n+1} - n p_n \right]} \qquad \text{I.C.} \quad p_n(0) = \delta_{n,n_0}$$

$n \leftarrow n+1 \qquad n-1 \leftarrow n$

<u>derivation of a rate equation</u>

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

$$\sum_{n=0}^{\infty} n \dot{p}_n = \gamma \sum_{n=0}^{\infty} \left[n \underbrace{(n+1)}_{\tilde{n}} \underbrace{p_{n+1}}_{\tilde{n}} - n^2 p_n \right] = \qquad \Big| \; n+1 = \tilde{n}$$

$$= \gamma \left[\sum_{\tilde{n}=\cancel{1}\,0}^{\infty} (\tilde{n}-1)\tilde{n}\, p_{\tilde{n}} - \sum_{n=0}^{\infty} n^2 p_n \right] =$$

since $\tilde{n} = 0$ gives no contribution

$$= -\gamma \sum_{n=0}^{\infty} n\, p_n$$

$$\frac{d}{dt} \langle N(t) \rangle = -\gamma \langle N \rangle \Rightarrow \langle N(t) \rangle = n_0 e^{-\gamma t}$$

valid only for linear processes!

Birth – death processes:

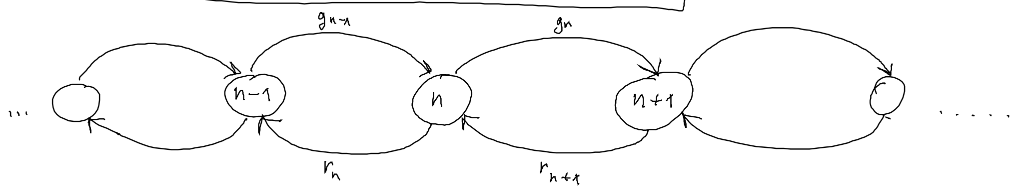
Examples: population, chem. reaction, absorbtion / emission of photons, generation / recombination of electrons in semiconductors.

$$W_{nn'} = \underbrace{r_{n'}\, \delta_{n,n'-1}}_{\substack{n' \to n'-1 \\ \text{(recombination)} \\ r_{n'}}} + \underbrace{g_{n'}\, \delta_{n,n'+1}}_{\substack{n' \to n'+1 \\ \text{(generation)} \\ g_{n'}}}$$

These are transition probabilities per unit time $\Rightarrow$ depend on n'!

Master equation

$$\boxed{\dot{p}_n = r_{n+1}\, p_{n+1} + g_{n-1}\, p_{n-1} - (r_n + g_n)\, p_n}$$



Boundary effects $(n=0)$: $\dot{p}_0 = r_1 p_1 - g_0 r_0$

Birth – death population example

The one dimensional prototype of all birth-death systems consists of a population of individuals X in which the number that can occur is called x, which is a non-negative integer. Conditional probability $P(x,t / x', t')$ and its master equation. The concept of birth and death is usually that only a finite number of X are created (born) or destroyed (die) in a given event. The simplest case is when the X are born or die one at at a time, with a time independent probability so that the transition probabilities $W(x/x',t)$ can be written

$$\boxed{W(x/x',t) = t^+(x')\, \delta_{x,x'+1} + t^-(x')\, \delta_{x,x'-1}}$$

$x \longrightarrow x+1$: $t^+(x)$ = transition probability per unit time

$x \rightarrow x-1$: $t^-(x)$ = — // —

Master equation

$$\boxed{\begin{aligned}\partial_t P(x,t/x't') = {} & t^+(x-1)\, P(x-1,t/x',t') + t^-(x+1)\, P(x+1,t/x',t') \\ & - [t^+(x) + t^-(x)]\, P(x,t/x',t').\end{aligned}}$$

Classification

(i) r_n, g_n = const (do not depend on n) <u>random walk</u>

(ii) r_n, g_n linear in n (e.g., random process)

(iii) r_n, g_n nonlinear in n (e.g., Auger effect, bimolecular recombination)

Special case of (i): $g_n = q$, $r_n = 0$, $p_n(0) = \delta_{n,0}$ $\longrightarrow$ <u>Poisson process</u>

<u>Master equation</u>: $\boxed{\dot{p}_n = q\,(p_{n-1} - p_n) \quad (n \neq 0)}$, Solution: $p_n(t) = \frac{(qt)^n}{n!} e^{-qt}$

$\langle n \rangle = qt$