

Lecture 5 summary

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

$$\frac{\partial}{\partial t} p(z, t | y, t') = \int dx [W(x/z, t) p(x, t | y, t') - W(x/z, t) p(z, t | y, t')]$$

↑  
prob of trans per unit time

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

$$\frac{\partial}{\partial t} p(z, t | y, t') = \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial z_i \partial z_j} [B_{ij}(z, t) p(z, t | y, t')]$$

↑  
diffusion matrix

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

Liouville equation.

$$\frac{\partial}{\partial t} p(z, t | y, t') = - \sum_i \frac{\partial}{\partial z_i} [A_i(z, t) p(z, t | y, t')]$$

↑  
drift vector

Combination of (b) and (c)

Fokker-Planck equation

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

## 2. Classical statistics in non-equilibrium

### 2.1 Master equation

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

we recalled  
Chap-Kol. equation  
for Markov proc.

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

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

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

$$\Rightarrow \frac{\partial}{\partial t} p(x, t | x', t') = \lim_{\Delta t \rightarrow 0} \frac{p(x, t + \Delta t | x', t') - p(x, t | x', t')}{\Delta t} = \int_{x < z} dz W(x/z, t) p(z, t | x', t') - \int_{z < x} dz W(z/x, t) p(x, t | x', t')$$

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:

$$\frac{\partial}{\partial t} p(n, t | n', t') = \sum_m [W(n/m, t) p(m, t | n', t') - W(m/n, t) p(n, t | n', t')]$$

Notation  $p_n(t) = p(n, t | n', t')$  with i.c.  $p_{n'}(t')$

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

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

$n \leftarrow m$   
gain

$m \leftarrow n$   
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

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

3) quantum physics:

for example, calculation of

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

from Fermi's golden rule with perturbation  $H_1$

### Example

radioactive decay of  $N(t)$  atoms

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

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

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

$$= \gamma [ (n+1) p_{n+1} - n p_n ] \quad \text{i.c. } p_n(0) = \delta_{n, n_0}$$

$n \leftarrow n+1 \quad n-1 \leftarrow n$

derivation of a rate equation

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

$$\begin{aligned} \sum_{n=0}^{\infty} n \dot{p}_n &= \gamma \sum_{n=0}^{\infty} \left[ n \frac{(n+1)}{\tilde{n}} p_{n+1} - n^2 p_n \right] = & \left| n+1 = \tilde{n} \right. \\ &= \gamma \left[ \sum_{\tilde{n}=1}^{\infty} (\tilde{n}-1) \tilde{n} p_{\tilde{n}} - \sum_{n=0}^{\infty} n^2 p_n \right] = \\ & \quad \text{since } \tilde{n}=0 \text{ gives no contribution} \end{aligned}$$

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

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

valid only for linear processes!

### Birth-death processes:

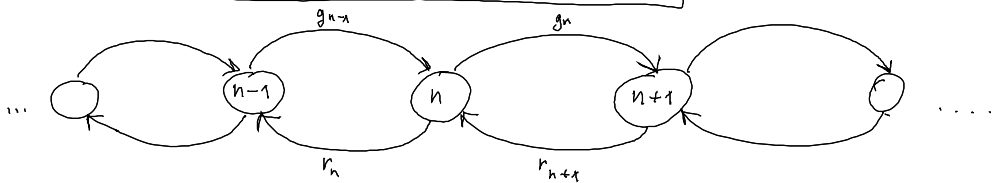
Examples: population, chem. reaction, absorption/emission of photons, generation/recombination of electrons in semiconductors.

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

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

### Master equation

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



Boundary effects ( $n=0$ ):  $\dot{p}_0 = r_1 p_1 - g_0 p_0$

### 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 a time, with a time independent probability so that the transition probabilities  $W(x/x', t)$  can be written

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

$x \rightarrow x+1: t^+(x) = \text{transition probability per unit time}$   
 $x \rightarrow x-1: t^-(x) = \text{--- // ---}$

Master equation

$$\partial_t P(x, t | x', t') = t^+(x-1) P(x-1, t | x', t') + t^-(x+1) P(x+1, t | x', t') - [t^+(x) + t^-(x)] P(x, t | x', t').$$

Classification

- (i)  $r_n, g_n = \text{const}$  (do not depend on  $n$ ) random walk
- (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):  $g_n = q, r_n = 0, p_n(0) = \delta_{n,0} \rightarrow$  Poisson process

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