

Recap from last lecture:

continuum position: $x = i a$

$$P_i(t) \rightarrow p(x, t)$$

master equation:

$$(1) \quad 1 \leq i \leq N: \quad \frac{dp_i}{dt} = -2w p_i + w(p_{i+1} + p_{i-1})$$

$$(2) \quad i=1: \quad \frac{dp_1}{dt} = -w p_1 + w p_2$$

$$(3) \quad i=N: \quad \frac{dp_N}{dt} = -w p_N + w p_{N-1}$$

$$P_i(t) \rightarrow p(x, t)$$

$$P_{i+1}(t) \rightarrow p(x+a, t) \approx p(x, t) + a \frac{\partial p}{\partial x} + \frac{1}{2} a^2 \frac{\partial^2 p}{\partial x^2}$$

$$P_{i-1}(t) \rightarrow p(x-a, t) \approx p(x, t) - a \frac{\partial p}{\partial x} + \frac{1}{2} a^2 \frac{\partial^2 p}{\partial x^2} + \dots$$

$$\text{equ. (1)} \Rightarrow \frac{\partial p}{\partial t}(x, t) = \underbrace{w a^2}_{D} \frac{\partial^2 p}{\partial x^2}(x, t)$$

$$\Rightarrow \boxed{\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}} \quad \text{diffusion equation}$$

equ. (2)

$$P_1(t) \rightarrow p(a, t)$$

$$\therefore \frac{\partial p}{\partial t}(a, t) = w a \frac{\partial p}{\partial x}(a, t) + \frac{1}{2} \underbrace{w a^2}_{D} \frac{\partial^2 p}{\partial x^2}(a, t)$$

$$x = i a \quad i=1$$

$$a \frac{\partial p}{\partial t} = \underbrace{w a^2}_{D} \frac{\partial p}{\partial x} + \frac{1}{2} a D \frac{\partial^2 p}{\partial x^2}$$

$$a \rightarrow 0:$$

$$0 = D \frac{\partial p}{\partial x}(0, t)$$

\Rightarrow

$$\frac{\partial p}{\partial x}(0, t) = 0$$

boundary condition
at $x=0$

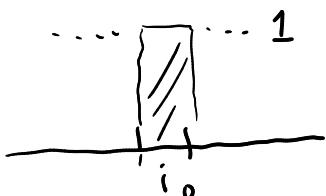
eqn. (3) \Rightarrow

$$\frac{\partial p}{\partial x}(L, t) = 0$$

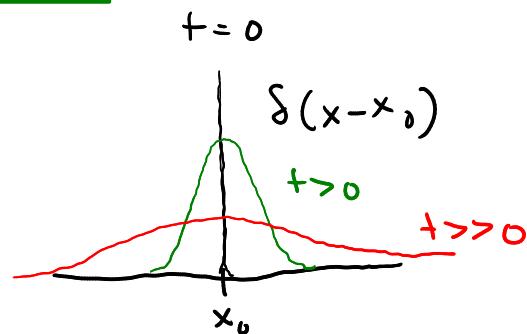
" " "
at $x=L$

 $t=0$

discrete:



\Rightarrow
continuum



$$\sum_i p_i(0) = 1 \Rightarrow \int_0^L dx \delta(x - x_0) = 1$$

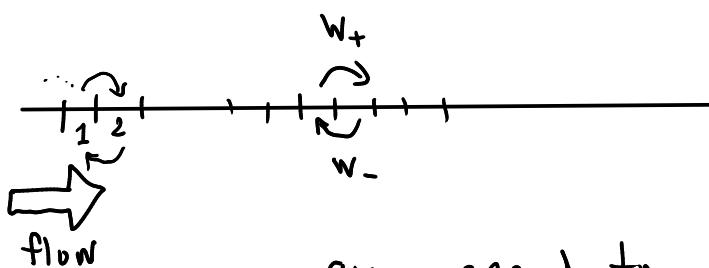
$$t \rightarrow \infty: p(x, t) \rightarrow \frac{1}{L} \quad \text{since} \quad \int_0^L dx p(x, t) = 1$$

for short times, the following is a solution to

diffusion:

$$p(x, t) \approx \frac{1}{\sqrt{4\pi D t}} e^{-\frac{(x-x_0)^2}{4Dt}}$$

Gaussian centered at x_0
w/ width $\propto \sqrt{Dt}$



$$w_+ > w_-$$

because of
a biasing
flow

avg. speed to right:

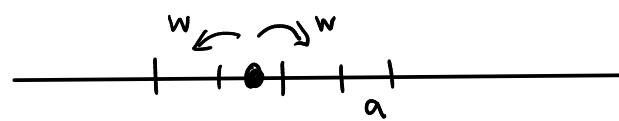
$$v = a(w_+ - w_-) > 0$$

analogous steps:

$$\frac{\partial p}{\partial t} = -v \frac{\partial p}{\partial x} + D \frac{\partial^2 p}{\partial x^2}$$

Fokker-
Planck
equation

Summary:



$$D = w a^2$$

discrete: $\Omega = \begin{pmatrix} -w & w & 0 & 0 \\ w & -2w & w & 0 \\ & \ddots & \ddots & \ddots \end{pmatrix}$

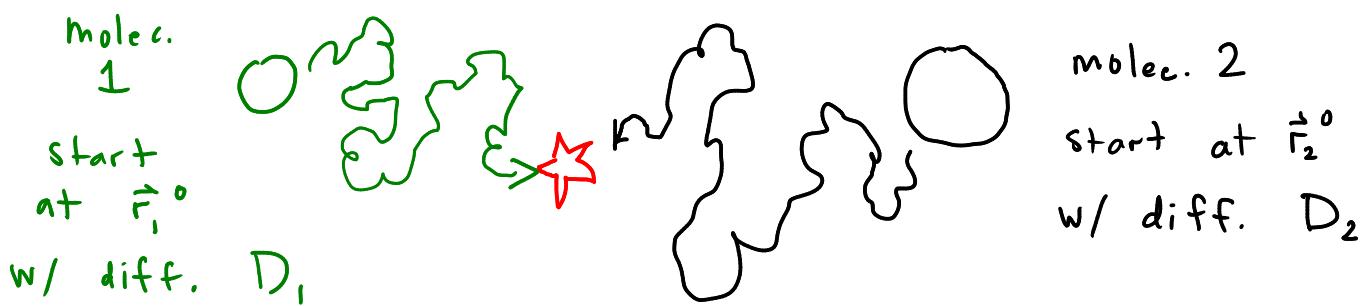
$$\text{MSD } \langle \Delta_i^2 \rangle_t = 2Dt$$

master equi: $\frac{dp_i}{dt} = \sum_j \Omega_{ij} p_j$



continuum: $\frac{\partial p}{\partial t} = D \frac{\partial^2}{\partial x^2} P$

Next question: on average, how long before two diffusing particles meet?



$$\langle (\vec{r}_1 - \vec{r}_1^0)^2 \rangle_t = 6 D_1 t$$

$$\langle (\vec{r}_2 - \vec{r}_2^0)^2 \rangle_t = 6 D_2 t$$

$$\vec{r}_1 = a(i_1, j_1, k_1)$$

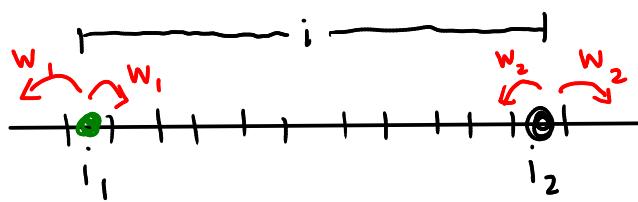
$$D_1 = w_1 a^2$$

$$\vec{r}_2 = a(i_2, j_2, k_2)$$

$$D_2 = w_2 a^2$$

$$\vec{r} = \vec{r}_2 - \vec{r}_1 = a(\underbrace{i_2 - i_1}_i, \underbrace{j_2 - j_1}_j, \underbrace{k_2 - k_1}_k)$$

dynamics: what happens to i in one time step?



$$i \rightarrow i+1: \quad \begin{matrix} \text{prob} \\ w_1 \delta t + w_2 \delta t \end{matrix}$$

1 left 1 staying
2 staying 2 right

only consider single particle motions in time step δt , b/c anything else $\propto \delta t^2$ or higher

$$i \rightarrow i-1: \quad \begin{matrix} w_1 \delta t + w_2 \delta t \\ 1 \text{ right } \quad 1 \text{ staying } \\ 2 \text{ staying } \quad 2 \text{ left } \end{matrix}$$

$$i \rightarrow i+2: \quad \begin{matrix} w_1 w_2 \delta t^2 + \dots \\ \propto \delta t^2 \text{ (ignore) } \end{matrix}$$

$$i \rightarrow i: \quad 1 - 2(w_1 + w_2) \delta t$$

Same dynamics as earlier w/ one particle:

$$\text{substitution: } w = w_1 + w_2$$

diffusion of two particle separation

looks like one particle motion w/

$$D = w a^2 = (w_1 + w_2) a^2 = D_1 + D_2$$

restate problem:

radius R_1



\vec{r}_0 separation

$\sim \sim \sim \sim$

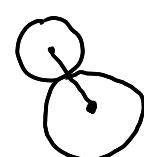
\vec{r}_0 diffusion

$$r_0 = |\vec{r}_0|$$



dynamics

$$w/ D = D_1 + D_2$$



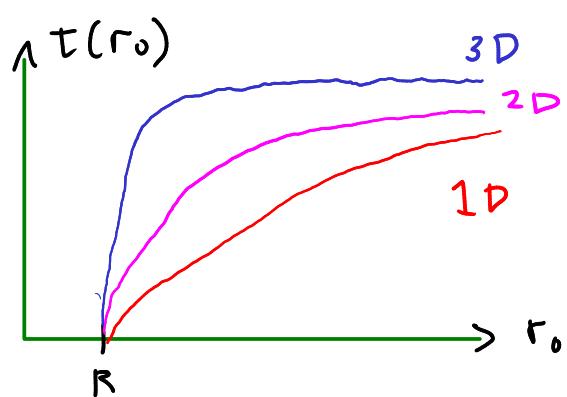
at contact

$$r = R_1 + R_2$$

$$\equiv R$$

goal: calculate avg. time to contact
starting at r_0 : capture time $T(r_0)$

Show:



$$\tau(R) = 0$$