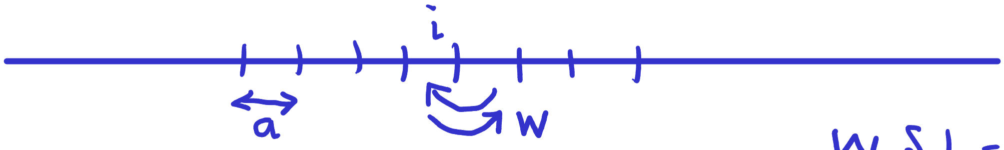
PHYS 320/420 Lecture 6

MSD $\langle \Delta_i^2 \rangle_t = 2Dt$ $\qquad D = wa^2$



$w\,\delta t$ = prob. to jump to next box

D should be indep. of choice of a

$$\Rightarrow \quad w = \frac{D}{a^2} \quad \Rightarrow \quad w \text{ increases as } a \text{ decreases}$$

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

to allow some solutions:

$N \to$ large, $L = Na$ constant (length of our cell)

$a \to$ small

$w = \dfrac{D}{a^2}$ increases

define position $x = ia \to$ continuous variable

$$p_i(t) \longrightarrow p(x,t)$$

RHS $\to$ derivatives of p (not obvious!)

orig. master equations:

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

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

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

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

$$p_{i+1}(t) \rightarrow p(x+a, t) = p(x,t) + a\frac{\partial p}{\partial x} + \frac{1}{2}a^2\frac{\partial^2 p}{\partial x^2} + \cdots$$

$$p_{i-1}(t) \rightarrow p(x-a, t) = p(x,t) - a\frac{\partial p}{\partial x} + \frac{1}{2}a^2\frac{\partial^2 p}{\partial x^2} + \cdots$$

(1): $$\frac{\partial p(x,t)}{\partial t} = \cancel{-2w\,p(x,t)} + \cancel{2w\,p(x,t)} + \underbrace{wa^2}_{D}\frac{\partial^2}{\partial x^2}p(x,t)$$

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

$$(2) \Rightarrow \quad \frac{\partial p}{\partial t}(a,t) = \cancel{-w\,p(a,t)}$$

$i=1$

$x=a$

$$+\cancel{w\,p(a,t)} + wa\frac{\partial p}{\partial x}(a,t)$$

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

multiply both sides by a:

$$a\frac{\partial p}{\partial t} = \overbrace{wa^2}^{D}\frac{\partial p}{\partial x} + \frac{1}{2}aD\frac{\partial^2 p}{\partial x^2}$$

lim a → small:

bound. cond.

$$0 = D\frac{\partial p}{\partial x}(0,t) \Rightarrow \boxed{\left.\frac{\partial p}{\partial x}\right|_{x=0} = 0}$$

(3) Same argument:

$i=N$

$x=Na \equiv L$

$$\boxed{\left.\frac{\partial p}{\partial x}\right|_{x=L} = 0}$$

What do the solutions look like?

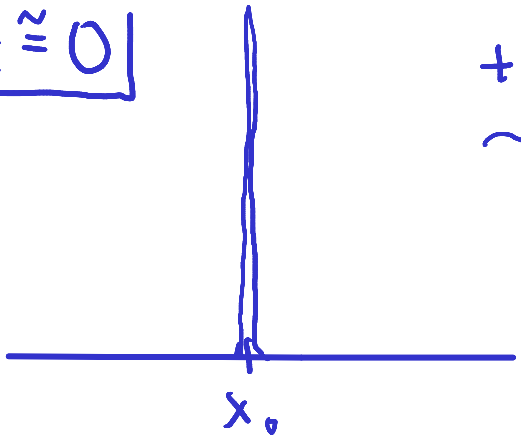
ignore boundaries (i.e. large cell)

focus on diff. equation + not bound. cond.

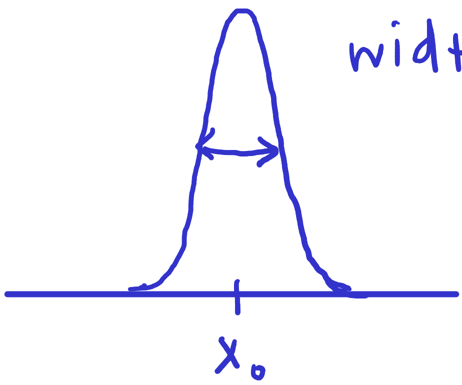
$$p(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{(x-x_0)^2}{4Dt}}$$

where initial cond: all systems start at x_0

$\boxed{t \cong 0}$

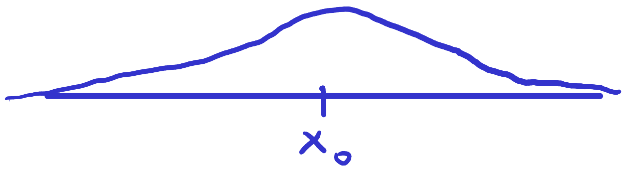


t increases

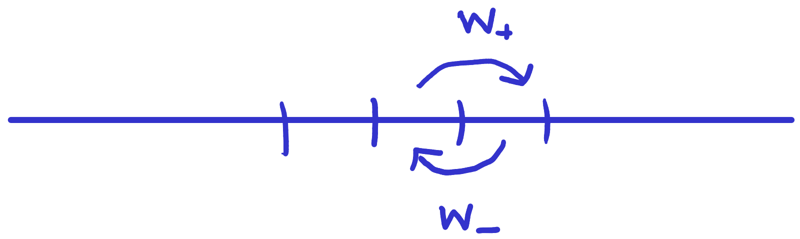


width $\sim \sqrt{MSD} \propto \sqrt{Dt}$

t inc.



What happens if there is some overall flow to the right?



$w_+ > w_-$

overall fluid speed: $v = a(w_+ - w_-)$ $\Rightarrow$ constant

vel. of fluid

diff. Ω matrix $= \begin{pmatrix} -w_+ & w_- & \\ w_+ & -(w_+ + w_-) & w_- \\ & w_+ & \ddots \end{pmatrix}$

analogous steps: continuum approx

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

Fokker-Planck equ.

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