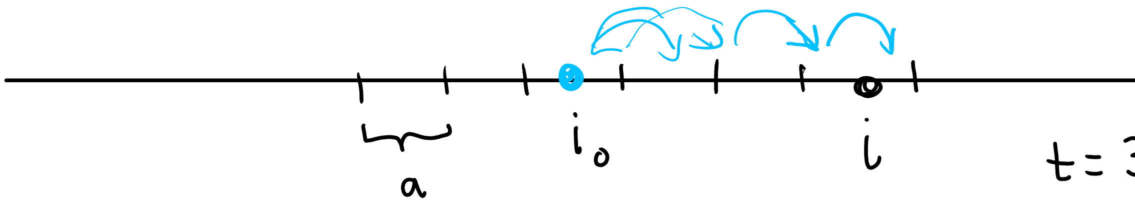
MSD: $\langle \Delta_i^2 \rangle_t = 2Dt = \sum_i p_i(t)\Delta_i^2$

$$\Delta_i = a(i - i_0)$$

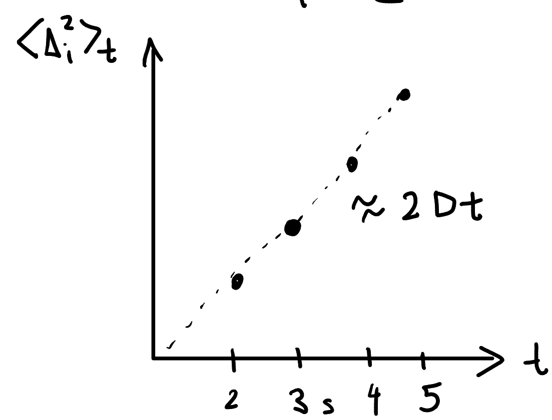


$t = 3$ s

$a = 1$ nm

trial	$i-i_0$	$a^2(i-i_0)^2$
1	3	9 nm^2
2	−2	4 nm^2
3	−1	1 nm^2
	⋮	⋮

average $\Rightarrow \langle \Delta_i^2 \rangle_{t=3s}$



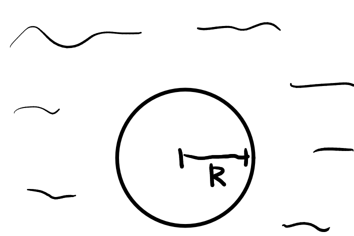
rough timescale to diffuse a distance L in 1D:

$$MSD \sim L^2 = 2Dt \Rightarrow t \sim \frac{L^2}{2D}$$

$D = wa^2$

trans. rate to left/right

box length



fluid viscosity η

temp. T

Stokes law: $D = \frac{k_B T}{6\pi\eta R}$

$R = 1$ nm

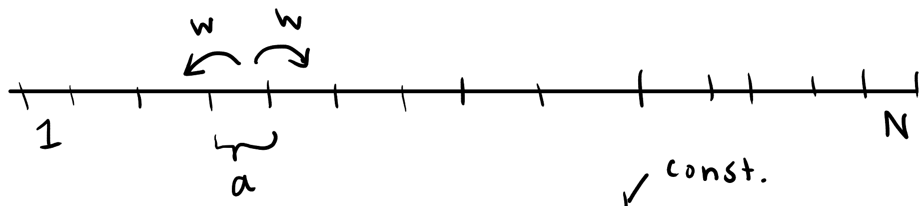
$D = 245$ $\mu m^2/s$

$k_B = 1.38 \times 10^{-23}$ J/K

$T = 298$ K (room temp.)

$\eta \approx 0.89 \times 10^{-3}$ Pa·s (water)

How to solve for probs. $p_i(t)$ from master equ? continuum limit: $a \to 0$



$$D = w a^2 \Rightarrow w = \frac{D}{a^2}$$ ← const.

$a \to 0$
$w \to$ increases

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

define continuum position: $x = i a$

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

total length of box $L = Na$

$a \to$ small $\quad N = \frac{L}{a} \to$ large

$w = \frac{D}{a^2} \to$ large

master equ:

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

(2) $\quad i = 1: \quad \frac{dp_1}{dt} = -wp_1 + wp_2$

(3) $\quad i = N: \quad \frac{dp_N}{dt} = -wp_N + wp_{N-1}$

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

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

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

Plug into eq. (1): $\frac{\partial p(x,t)}{\partial t} = \underbrace{wa^2}_{D} \frac{\partial^2}{\partial x^2} p(x,t)$

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

eq. (2): $\frac{\partial p}{\partial t}(a,t) = wa \frac{\partial p}{\partial x}(a,t) + \frac{1}{2} wa^2 \frac{\partial^2}{\partial x^2} p(a,t)$

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

$x = ia \quad i=1$

$$\cancel{a \frac{\partial p}{\partial t}}^{\,0} = \underbrace{wa^2}_{D} \frac{\partial p}{\partial x} + \cancel{\frac{1}{2} \underbrace{wa^3}_{Da} \frac{\partial^2}{\partial x^2} p}^{\,0}$$

$a \to 0$: $\quad 0 = D \frac{\partial p}{\partial x}(0,t)$ boundary condition

eq. (2): $\boxed{\frac{\partial p}{\partial x}(0,t) = 0}$

eq. (3): $\boxed{\frac{\partial p}{\partial x}(L,t) = 0}$

boundary condition