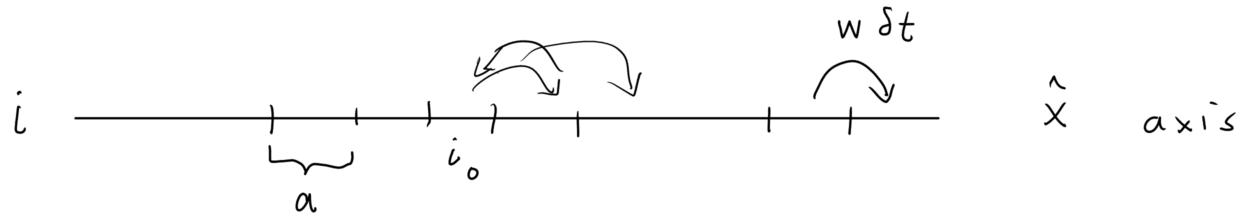
MSD: $\Delta_i = a(i-i_0)$



$$\langle \Delta_i^2 \rangle_t = 2Dt$$

$\hookrightarrow$ diffusion const.

$$\langle \Delta_i^2 \rangle_t = \sum_i p_i(t)\,\Delta_i^2$$

$D = w a^2$, where $w \sim \frac{1}{\text{time}}$ and $a^2 \sim \text{length}^2$

$$D \sim \frac{\text{length}^2}{\text{time}}$$

easily generalize to multiple dim:

box labels

3D box location: $\vec{r} = a(i, j, k)$

initial loc: $\vec{r}_0 = a(i_0, j_0, k_0)$

1D displacements:

$$\Delta_i = a(i - i_0)$$
$$\Delta_j = a(j - j_0)$$
$$\Delta_k = a(k - k_0)$$

3D MSD:

$$\langle (\vec{r} - \vec{r}_0)^2 \rangle_t$$
$$= \langle a^2(i-i_0)^2 + a^2(j-j_0)^2 + a^2(k-k_0)^2 \rangle_t$$
$$= \underbrace{\langle \Delta_i^2 \rangle_t}_{2Dt} + \underbrace{\langle \Delta_j^2 \rangle_t}_{2Dt} + \underbrace{\langle \Delta_k^2 \rangle_t}_{2Dt}$$
$$= 6Dt$$

2D MSD: $\langle (\vec{r}-\vec{r}_0)^2 \rangle_t = 4Dt$

$$MSD \sim L^2 = 6Dt \Rightarrow t = \frac{L^2}{6D}$$

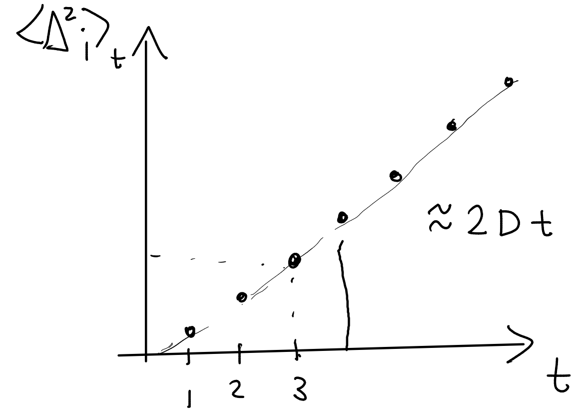
$L \sim$ rough distance covered by diffusing particle

compare this to "ballistic" motion:

$$L = \underset{\substack{\uparrow \\ \text{const. vel}}}{v}\, t \Rightarrow t = \frac{L}{v}$$

calculate MSD experimentally (numerically):

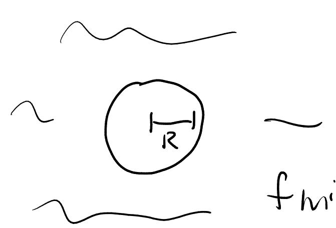
trial	$i-i_0$	$a^2(i-i_0)^2$
1	3	9 nm^2
2	-2	4 nm^2
3	-1	1 nm^2
⋮	⋮	



choose: $t = 3\,s$
$a = 1$ nm

avg: $\langle \Delta_i^2 \rangle_{t=3s}$

to estimate D, nice result from fluid dynamics:



fluid viscosity η
temp. T

Stokes law:

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

$R = 1$ nm

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

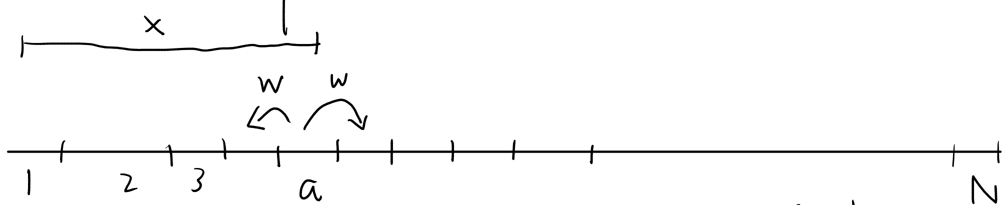
$T = 298$ K

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

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

(order of magnitude)

How to solve for prob's $p_i(t)$ from master equ?



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

$a \to 0$

$w \to$ increases

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

define continuum position: $x = ia$

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

total length of box $L = Na$

$a \to 0$: $N = \frac{L}{a}$ large

master equ:

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

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

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

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

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

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

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

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

diffusion equation