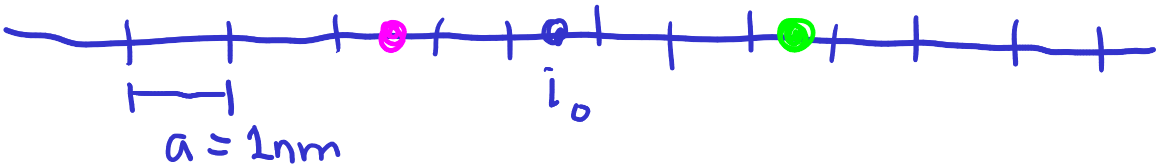
PHYS 320/420 Lecture 3

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

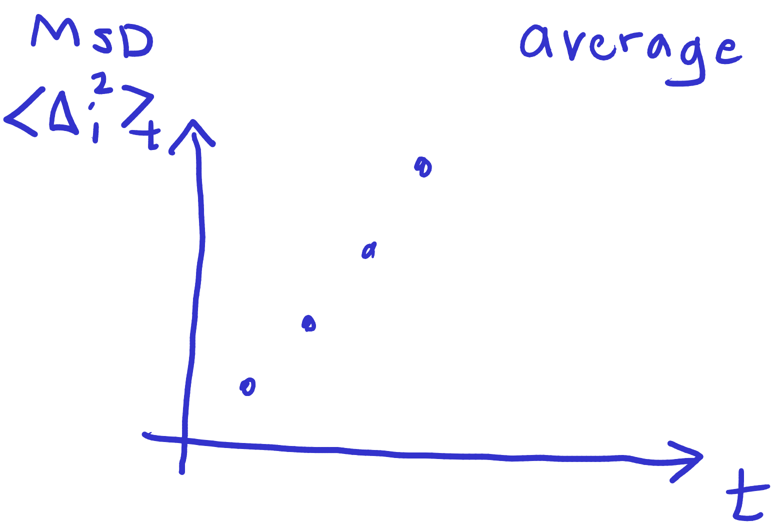
$$\Delta_i = a(i - i_0)$$



$t = 3\,s$

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

average $\Rightarrow \langle \Delta_i^2 \rangle_t = $ m



Simplify dynamics temporarily
to explicitly calculate MSD

$\Rightarrow$ non-random motion in one dir.

$i \to i+1$ w/ prob. 1
$i \to i$ " " 0
$i \to i-1$ " " 0

every trial will lead to same
result (non-random)

avg. $\Rightarrow$ same as one trial result

$t = m\,\delta t$ (m time steps)

$i = i_0 + m$

$$\Delta_i^2 = a^2(i-i_0)^2 = a^2 m^2 = a^2\left(\frac{t}{\delta t}\right)^2$$

$$\langle \Delta_i^2 \rangle_t = \frac{a^2}{\delta t^2}\, t^2 \propto t^2$$

MSD $\propto t^2$ $\Rightarrow$ ballistic motion
(directed,
not random)

MSD $\propto t$ (we will prove this)
$\Rightarrow$ diffusive motion

Where is ballistic regime relevant?

i) very short timescales $\ll 10^{-16}$ s for objects in water

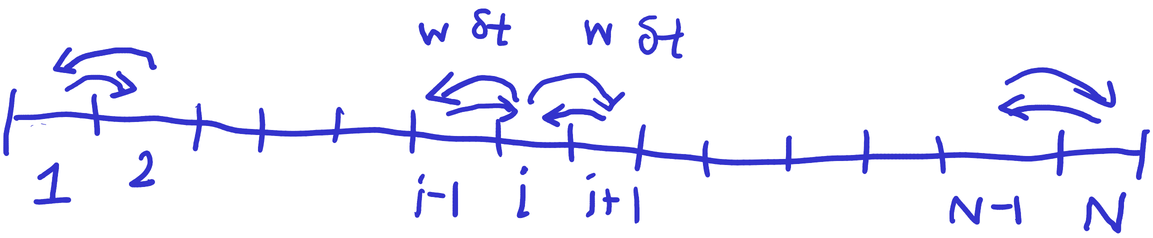
ii) if there is fuel source + "molecular motors"

$\Rightarrow$ dragging cargo in one dir.

How do we prove $MSD \propto t$ in diffusive regime?

$\Rightarrow$ we will have to derive an equation for $p_i(t)$

$\Rightarrow$ <u>master equation</u>



$$p_i(t+\delta t) = p_i(t) - \left[\begin{array}{c}\text{loss in} \\ \text{prob. due} \\ \text{part. leaving} \\ i\end{array}\right] + \left[\begin{array}{c}\text{gain in prob.} \\ \text{due to part.} \\ \text{entering } i\end{array}\right]$$

$$= p_i(t) - \underbrace{2w\,\delta t}_{\substack{\text{prob.} \\ \text{you} \\ \text{left} \\ i \\ \text{in } (t,\,t+\delta t)}} \underbrace{p_i(t)}_{\substack{\text{prob.} \\ \text{of} \\ \text{currently} \\ \text{being in } i}}$$

$$+ \underbrace{w\,\delta t}_{\substack{i-1 \to i \\ \text{jump} \\ \text{prob.}}} p_{i-1}(t) + \underbrace{w\,\delta t}_{\substack{i+1 \to i \\ \text{jump} \\ \text{prob.}}} p_{i+1}(t)$$

$$\Rightarrow \frac{p_i(t+\delta t) - p_i(t)}{\delta t} = -2w\,p_i(t) + w\left(p_{i-1}(t) + p_{i+1}(t)\right)$$

on timescales $t \gg \delta t$, we can approximate time as continuous + treat the left-hand side as a derivative

$$\Rightarrow \quad \frac{dp_i(t)}{dt} = \overbrace{-2w\,p_i(t)}^{\text{loss}} + \overbrace{w\left(p_{i-1}(t) + p_{i+1}(t)\right)}^{\text{gain}}$$

$1 < i < N$

first example of "master equation"

$\Rightarrow$ gain-loss equ. for probability

$\Rightarrow$ conservation eqn. for prob.

note: system of equations for diff. i, all coupled together

$$1 \overset{w\,\delta t}{\rightleftarrows} 2 \qquad \frac{dp_1}{dt} = -w\,p_1(t) + w\,p_2(t)$$

$$N-1 \rightleftarrows N \qquad \frac{dp_N}{dt} = -w\,p_N(t) + w\,p_{N-1}(t)$$

N equations for funcs $p_1(t), \ldots, p_N(t)$

$\Rightarrow$ figure out eqn's for $\langle i \rangle_t$, $\langle i^2 \rangle_t$ without solving master eqn. $\Rightarrow$ solve those to get $\langle \Delta_i^2 \rangle_t$ MSD