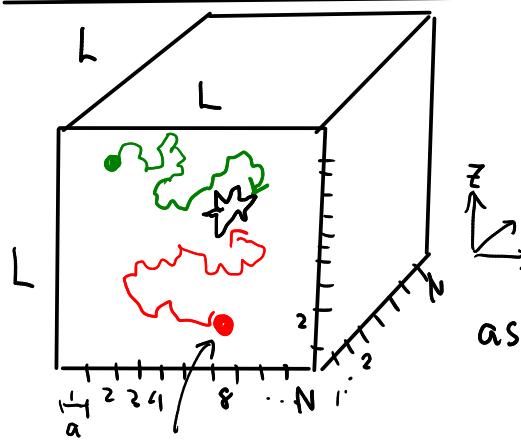


molecules
diffusing in a volume \rightsquigarrow collide + react: \rightsquigarrow "chemistry"
 \rightsquigarrow networks of chem. reactions

\rightsquigarrow add fuel \rightsquigarrow living Systems \rightsquigarrow populations + evolution



Question: how long on average before these two molecules meet?

assumption: in the time scale δt
 between "snapshots" enough collisions w/ environment have occurred
 \Rightarrow random motion of two molecules

influences: temperature, density, viscosity

focus on one molecule:

1) state $\vec{n} = (i, j, k)$ = label of the box in volume

$$i = 1, \dots, N = \frac{L}{a}$$

$$j = \dots$$

$$k = \dots$$

2) look at dynamics (focus on 1D: label i along \hat{x} direction)

time + position i \Rightarrow $t + \delta t$ the position is ?

assume δt is small enough that i can only change by at most ± 1

$i \rightarrow i+1 :$

probability

$$w \delta t$$

$i \rightarrow i-1 :$

$$w \delta t$$

$i \rightarrow i :$

$$1 - 2w \delta t$$

sum to 1

$$w = \frac{\text{probability}}{\text{time}}$$

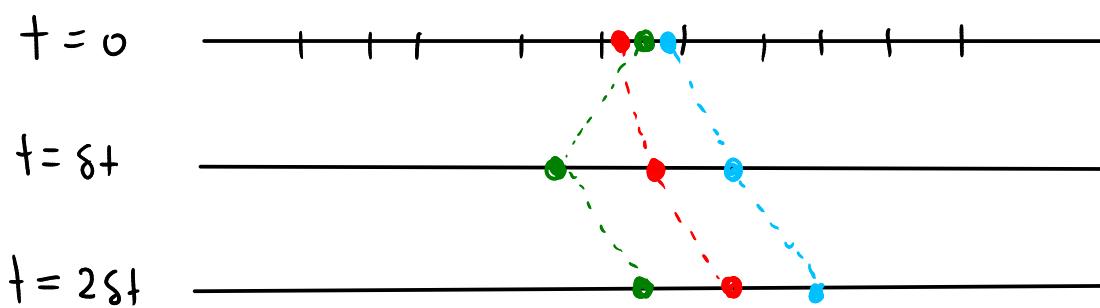
= prob. rate

= transition rate

(value of w

depends on temp., etc.)

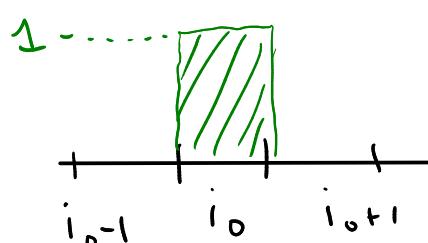
imagine running many "experiments" all starting w/ molecule at position i_0 at $t=0$



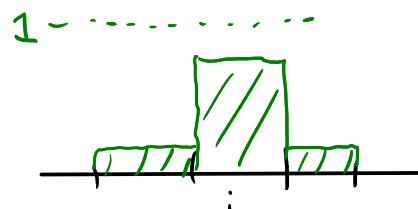
$$\begin{aligned} P_i(t) &= \text{prob. of observing pos. } i \text{ at time } t \\ &= \frac{\# \text{ exper. trajectories w/ molec. at } i \text{ at } t}{\text{total } \# \text{ experiments}} \end{aligned}$$

$P_i(t)$

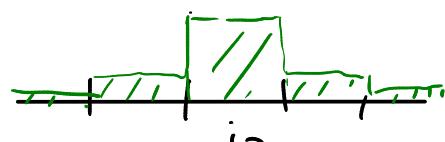
$t=0$



\nearrow
 $\rightarrow \infty$



$t = \delta t$



$t = 2\delta t$

characterize distribution $p_i(t)$ by looking at certain properties:

$$\text{avg. position } \langle i \rangle_t = \sum_{i=1}^N i p_i(t) = \text{"moment"}$$

depends
on time

$$\text{avg. of func. } f(i) \quad \langle f(i) \rangle_t = \sum_{i=1}^N f(i) p_i(t)$$

$$f(i) = i^n \quad \langle i^n \rangle_t = \text{n th "moment" of distribution}$$

$$\langle i^2 \rangle_t = \text{2nd moment, etc.}$$

focus on $f(i) = \Delta_i = a(i - i_0) = \text{dist. moved from } i_0$

$$\langle \Delta_i \rangle_t = 0 \quad \text{by symmetry}$$

$\langle \Delta_i^2 \rangle_t = \text{mean squared displacement (MSD)}$

↳ \Rightarrow how to calculate?

↳ should increase with time

$$\langle \Delta_i^2 \rangle_t = \sum_{i=1}^N a^2 (i - i_0)^2 p_i(t)$$

$$= a^2 \left[\underbrace{\sum_{i=1}^N i^2 p_i(t)}_{\langle i^2 \rangle_t} - 2 i_0 \underbrace{\sum_{i=1}^N i p_i(t)}_{\langle i \rangle_t} + i_0^2 \underbrace{\sum_{i=1}^N p_i(t)}_1 \right]$$

$$= a^2 \left[\langle i^2 \rangle_t - 2 i_0 \langle i \rangle_t + i_0^2 \right]$$

need an equation for $p_i(t)$ as a function of time