PHYS 320/420 : Lecture 2

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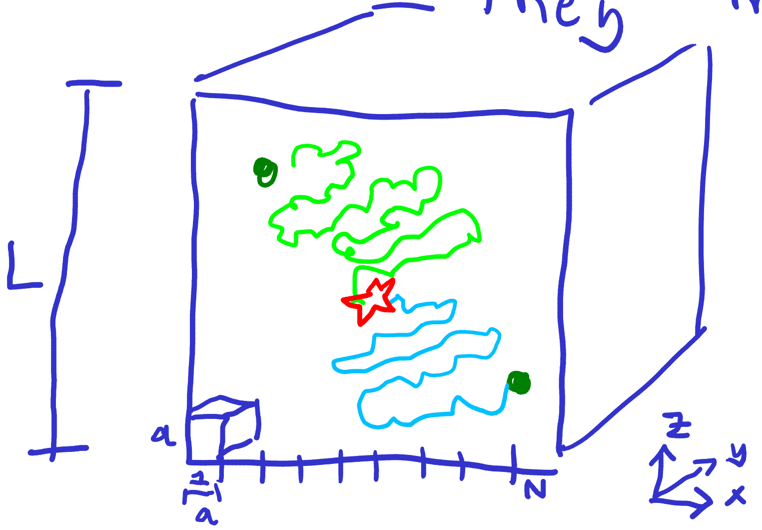
molecules diffusing in a volume ⇝ collide + react: "chemistry" ⇝ networks of chemical reactions

⇝ add fuel (energy source) ⇝ living systems (organisms) ⇝ populations + evolution

link b/t levels: mathematics of stochastic (random) processes

Start: crowded "soup" of the cell

Question: two molecules diffusing inside, how long before they meet?



volume $V = L^3$

dynamics are complex + random

assume above some timescale $t > \underbrace{\delta t}$

"micro time scale"

randomization occurs b/c of many interactions of particle w/ surroundings

many physical aspects (temp., viscosity, density, boundaries) may influence this randomization

divide up volume into little boxes of size a

1) state of particle $\vec{n} = (i, j, k)$ = label of box where the particle resides

$$i = 1, \ldots, N = \frac{L}{a}$$
$$j = 1, \ldots, N$$
$$k = 1, \ldots, N$$

physical position : $\vec{r} = a\vec{n}$

2) define dynamics: focus on 1D description

at time t particle is at i

where is it at time $t + \delta t$?

		probability
$i \to i+1$	:	$w\,\delta t$
$i \to i-1$	:	$w\,\delta t$
$i \to i$	:	$1-2w\,\delta t$

symmetry

sum to 1

large steps are unlikely b/c δt is small enough

whole dynamics described by one param:

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

$$= \text{transition rate}$$

$$\Rightarrow \text{units: } [\text{time}]^{-1}$$

$w \downarrow$ depends on all physical characteristics

(if constant in time $\Rightarrow$ w constant)

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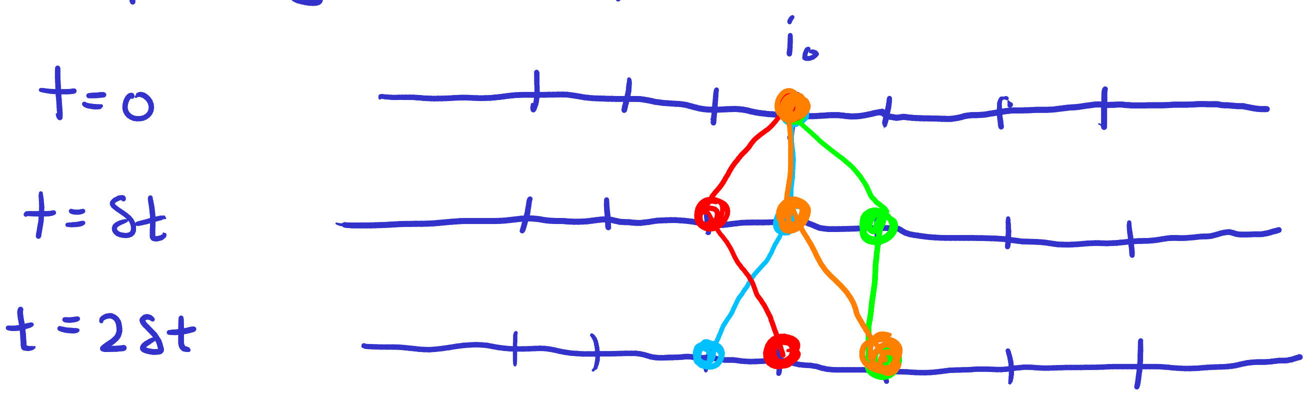
imagine running many experiments all starting w/ one molecule (for simplicity) at pos. i_0 at $t=0$



$p_i(t)$ = prob. of having pos. i at time t

$$= \frac{\text{\# exper. w/ molec. at } i \text{ at time } t}{\text{total \# exper} = N_{\text{trials}}}$$

$\uparrow$ large #

$t=0$ $\qquad$ $t=\delta t$ $\qquad$ $t=2\delta t$

$p_i(0)$ $\qquad$ $p_i(\delta t)$ $\qquad$ $p_i(2\delta t)$

average pos: $\qquad \langle i \rangle_t = \sum_{i=1}^{N} i\, p_i(t)$

average of any func. of i $\qquad \langle f(i) \rangle_t = \sum_{i=1}^{N} f(i)\, p_i(t)$

$f(i) = i^2$ $\qquad \langle i^2 \rangle_t = \sum_{i=1}^{N} i^2 p_i(t)$

2nd moment of p

$\langle f(i) \rangle_t$

$\uparrow$ subscript denotes dep. on t

$\langle i^n \rangle_t$ = nth moment of p

focus on one quantity: displacement

$f(i) \equiv \Delta_i = a(i - i_0)$ = how far has part. moved from i_0?

mean squared displacement (MSD)

$$\equiv \langle \Delta_i^2 \rangle_t$$

How to calculate? Two questions:

1) How does $p_i(t)$ evolve in time?

2) How to calculate $\langle \Delta_i^2 \rangle_t$ average?

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

$$= \left[\sum_i i^2 p_i(t) - 2 i_0 \sum_i i\, p_i(t) + i_0^2 \sum_i p_i(t) \right] a^2$$

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

$\Rightarrow$ How to calculate dynamics of moments?