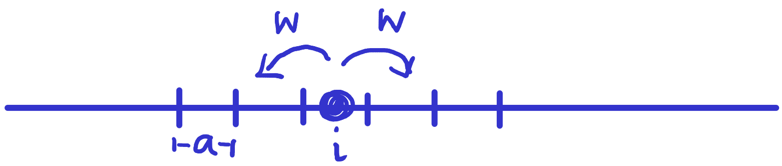
PHYS 320/420 Lecture 7

Summary of results so far:

$D = wa^2$

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



1D random diffusive motion:

$$\Omega = \begin{pmatrix} -w & w & & & \\ w & -2w & w & & \\ & w & -2w & w & \\ & & w & -2w & \\ & & & & \ddots \end{pmatrix}$$

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

continuum version: $$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2}{\partial x^2} p(x,t)$$

$$\left.\frac{\partial p}{\partial x}\right|_{x=0,L} = 0$$

Next question: on average how long before two diffusing particles meet?

molec. 1
diff. const. D_1
starts at $\vec{r}_1^{\,0}$

molec. 2
diff. const. D_2
starts at $\vec{r}_2^{\,0}$

What do we know so far?

$$\langle (\vec{r}_1 - \vec{r}_1^{\,0})^2 \rangle_t = 6 D_1 t$$

$$\langle (\vec{r}_2 - \vec{r}_2^{\,0})^2 \rangle_t = 6 D_2 t$$

but $\vec{r}_1$ + $\vec{r}_2$ can be anything, not necess. close!

$$\frac{\sqrt{MSD}}{t} \sim \frac{\text{dist}}{\text{time}} \sim \frac{1}{\sqrt{t}}$$

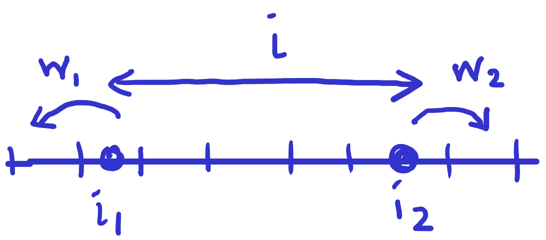
$$\vec{r}_2 = a(i_2, j_2, k_2) \qquad D_1 = w_1 a^2$$

$$\vec{r}_1 = a(i_1, j_1, k_1) \qquad D_2 = w_2 a^2$$

$$\vec{r} = \vec{r}_2 - \vec{r}_1 = a(\underbrace{i_2 - i_1}_{i}, \underbrace{j_2 - j_1}_{j}, \underbrace{k_2 - k_1}_{k})$$

integers: i j k

dynamics? $i \to i+1$ prob: $\underset{(i_2 \to i_2+1)}{w_2 \delta t} + \underset{(i_1 \to i_1 - 1)}{w_1 \delta t}$



$i \to i-1$ prob: $w_1 \delta t + w_2 \delta t$

$i \to i$ prob: $1 - 2(w_1 + w_2)\delta t$

$i \to i+2$ processes involve terms like: $w_1 w_2 \delta t^2$

ignore b/c $\delta t^2 \ll \delta t$

Note: dynamics have same form as one part. case except

$w \to w_1 + w_2$

Separation variable i behaves like 1D diffusion w/ an effective rate of transition: $w = w_1 + w_2$

eff. diff. constant $D = wa^2$

$$= D_1 + D_2$$

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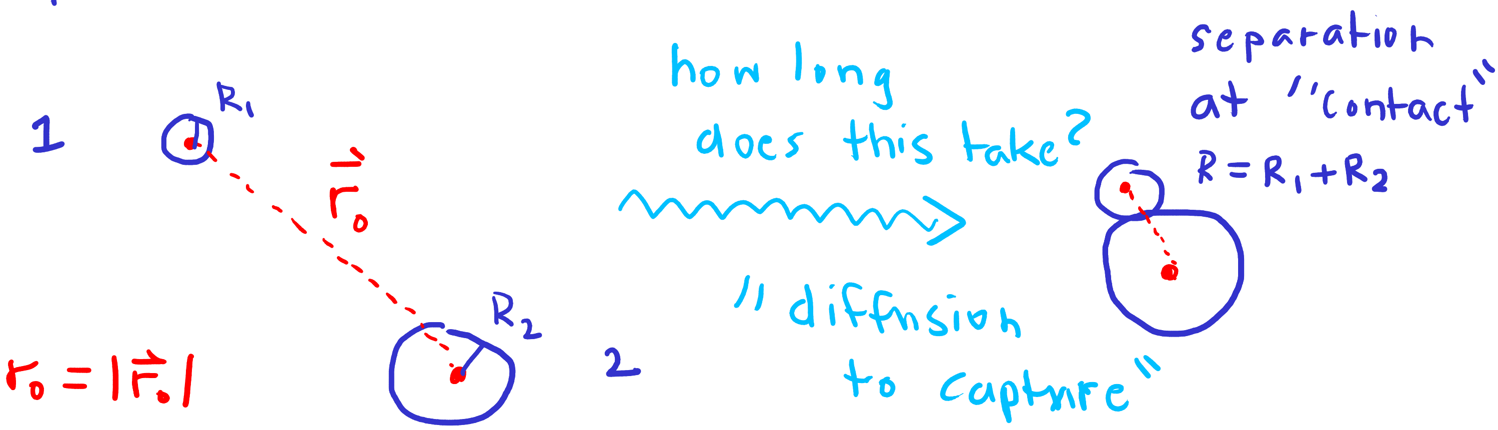
problem can be restated:

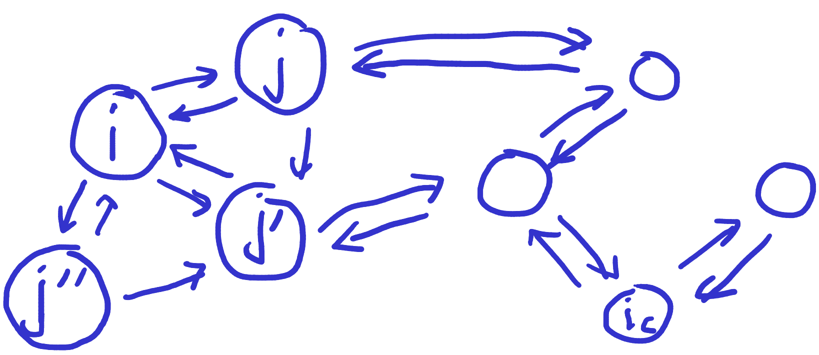


Goal: average capture time

$\tau(r_0)$

↳ starting separation

General formulation: model w/ states i + transition matrix Ω_{ij}



problem: given starting state i, how long on average before reaching target state i_c for first time?

$\Rightarrow$ solve for mean first passage time τ_i = avg. time to get to i_c from i for first time

$$\tau_{i_c} = 0$$

will prove:

$$\sum_i \tau_i \Omega_{ij} = -1 \quad (\text{for all } j \neq i_c)$$