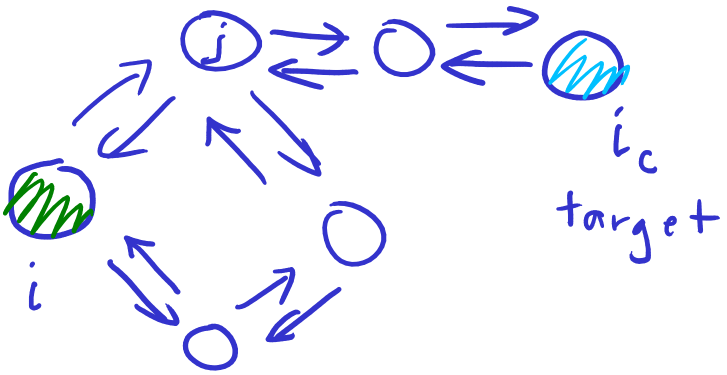
PHYS 320/420 Lecture 9

$$\tau_i^{esc} = \frac{1}{|\Omega_{ii}|}$$ = avg. time to leave state i

$$\Pi_{ji} = \frac{\Omega_{ji}}{|\Omega_{ii}|}$$ = prob. to go to state j immediately leaving i



τ_i = avg. time to get from i to i_c for the 1st time

$$\tau_{i_c} = 0$$

$i \neq i_c$:

$$\tau_i = \tau_i^{esc} + \sum_{j \neq i} \Pi_{ji} \tau_j$$

$$|\Omega_{ii}| = -\Omega_{ii}$$

$$\tau_i = \frac{1}{-\Omega_{ii}} + \sum_{j \neq i} \frac{\Omega_{ji}}{(-\Omega_{ii})} \tau_j$$

$$\Omega_{ii} = -\sum_{j \neq i} \Omega_{ji} \leq 0$$

multiply by Ω_{ii} + rearrange:

$$\Omega_{ii} \tau_i + \sum_{j \neq i} \Omega_{ji} \tau_j = -1$$

$$\boxed{\sum_{j=1}^{N} \Omega_{ji} \tau_j = -1}$$

this equ is valid for all $i \neq i_c$ ($N-1$ equations)

unknowns: $\tau_1, \tau_2, \ldots\ldots$ (N unknowns)

last eqn: $\boxed{\tau_{i_c} = 0}$ $\Rightarrow$ sys of equations where you can solve for τ_i

example:

$$1 \underset{k_u}{\overset{k_s}{\rightleftharpoons}} 2 \xrightarrow{k_b} \underset{\text{target}}{3} \qquad i_c = 3$$

goal: figure out τ_1 = avg. time from $1 \rightarrow 3$

$$\Omega = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & & & \\ 2 & & \left(\begin{array}{c|c|c} -k_s & k_u & 0 \\ \hline k_s & -k_u - k_b & 0 \\ \hline 0 & k_b & 0 \end{array}\right) & \\ 3 & & & \end{array}$$

$$\Omega = \begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \left(\begin{array}{c|c|c} -k_s & k_u & 0 \\ \hline k_s & -k_u - k_b & 0 \\ \hline 0 & k_b & 0 \end{array}\right) \end{array}$$

$\tau_{i_c} = 0 \quad \Longrightarrow \quad \tau_3 = 0$

$$\sum_j \Omega_{ji} \tau_j = -1 \quad : \quad i=1: \; -k_s \tau_1 + k_s \tau_2 = -1$$

$i = 1, 2$

$i=2$: $k_u \tau_1 - (k_u + k_b) \tau_2 + k_b \tau_3 = -1$

$\Rightarrow$ solve sys of eqn's for T_1, T_2, T_3

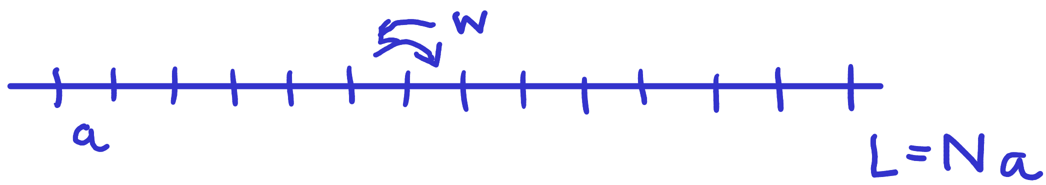
$$\Rightarrow \quad T_1 = \frac{k_s + k_u + k_b}{k_s k_b}$$

if $i_c = 2 \Rightarrow T_1 = T_1^{esc} = \frac{1}{k_s}$ for this problem

Returning to spatial diffusion

$\rightarrow$ continuum approximation

<u>Recall</u>



$a \to 0, \; N \to \infty$

$D = wa^2$ constant

$L =$ constant

$$p_j(t) \longrightarrow p(x,t)$$

$$\sum_j \Omega_{ij} p_j = \frac{dp_i}{dt} \Rightarrow D \frac{\partial^2 p}{\partial x^2} = \frac{\partial p}{\partial t}$$

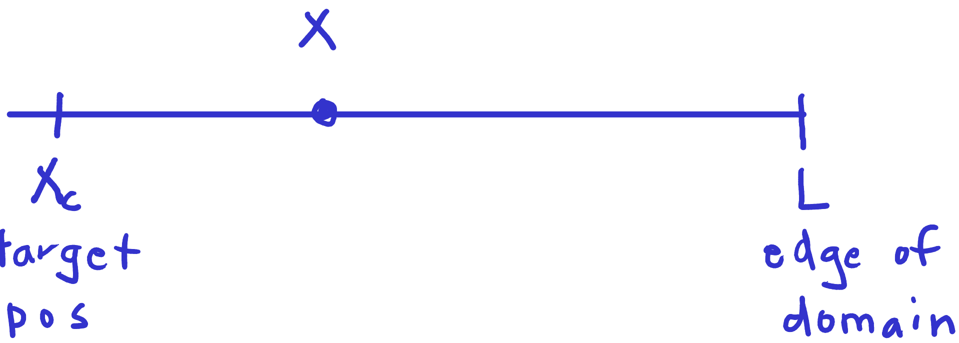
boundaries (where can't jump past) : $\Rightarrow \left.\frac{\partial p}{\partial x}\right|_{x=0,L} = 0$

for MFPT equ: (1D diff.) $\tau_i \longrightarrow \tau(x)$

$$\sum_j{}' \Omega_{ji} \tau_j = -1 \Rightarrow \boxed{D \frac{\partial^2 \tau}{\partial x^2} = -1}$$

$$\boxed{\left.\frac{\partial \tau}{\partial x}\right|_{x=L} = 0 \quad \text{(boundary)}}$$

How long on avg. to hit x_c?



$$\tau(x_c) = 0 \qquad \left.\frac{\partial \tau}{\partial x}\right|_{x=L} = 0$$

$$D \frac{\partial^2 \tau}{\partial x^2} = -1$$

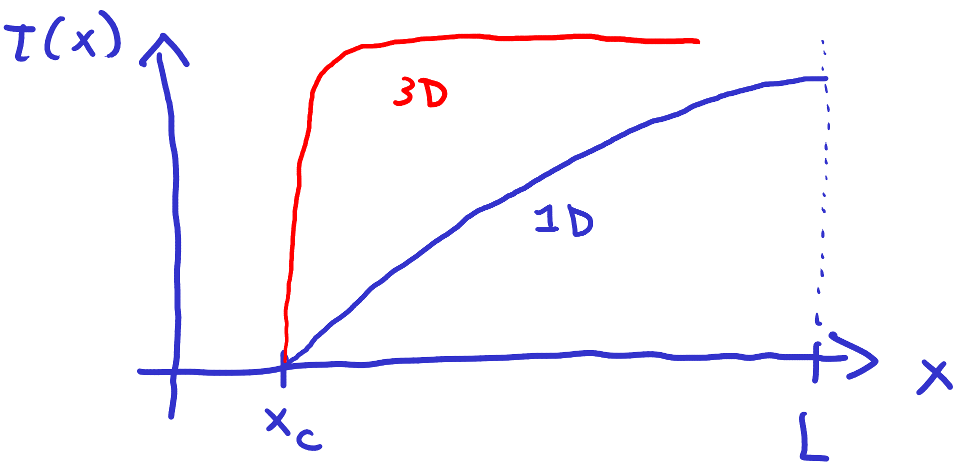
$$\frac{\partial \tau}{\partial x} = -\frac{x}{D} + c_1$$

$$\tau = -\frac{x^2}{2D} + c_1 x + c_2$$

$$\left.\frac{d\tau}{dx}\right|_{x=L} = -\frac{L}{D} + c_1 = 0 \Rightarrow c_1 = \frac{L}{D}$$

$$\tau(x_c) = 0 \Rightarrow c_2 = \frac{x_c^2}{2D} - \frac{Lx_c}{D}$$

$$\Rightarrow \tau(x) = \frac{(x-x_c)(2L-x-x_c)}{2D}$$



as $L \to \infty$, for $x \ll L$:

$$\tau(x) \approx \frac{(x-x_c)L}{D}$$