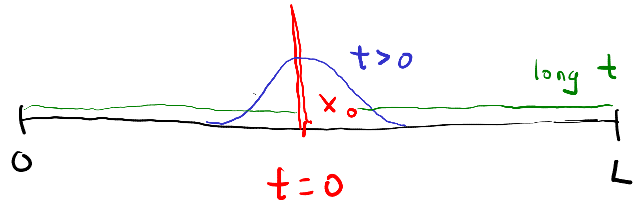
$$\frac{\partial}{\partial t} p(x,t) = D \frac{\partial^2 p}{\partial x^2}(x,t)$$

$$\frac{\partial p}{\partial x}(0,t) = 0$$

$$\frac{\partial p}{\partial x}(L,t) = 0$$



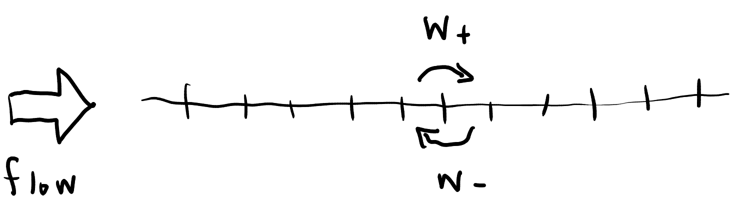
$$p(x,t=0) = \delta(x-x_0)$$

$$t \to \infty: \quad p(x,t) \to \frac{1}{L}$$

$$\int_0^L dx \; p(x,t) = 1$$

for short times, $\displaystyle p(x,t) \approx \frac{1}{\sqrt{4\pi D t}} e^{-\frac{(x-x_0)^2}{4Dt}}$

Gaussian centered at x_0
with width (st. dev.) $\propto \sqrt{Dt}$



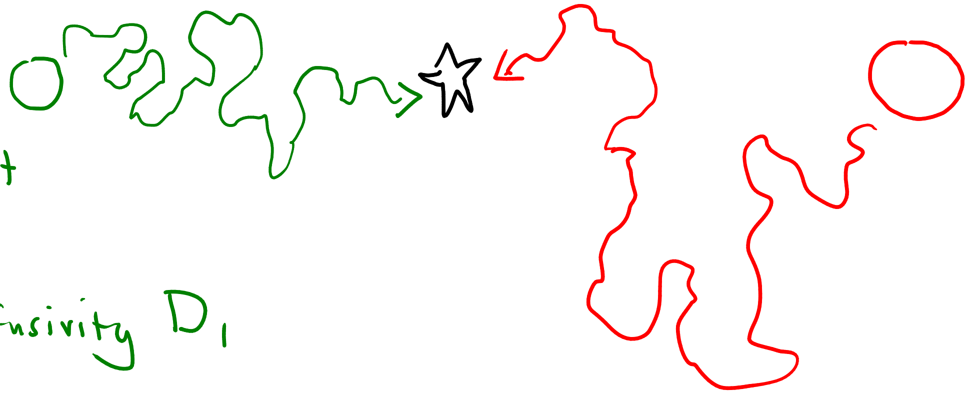
$W_+ > W_-$ because of
flow biasing diffusion

analogous derivation: $\displaystyle \frac{\partial p}{\partial t} = -v \frac{\partial p}{\partial x} + D \frac{\partial^2 p}{\partial x^2}$

simple example of
"Fokker-Planck equ."

$v = a(W_+ - W_-)$ avg. speed to right

Next question: look at two particle case molec. 1 starts at $\vec{r}_1^{\,\circ}$ w/ diffusivity D_1



molec. 2 at $\vec{r}_2^{\,\circ}$ w/ diff. D_2

$$\langle (\vec{r}_1 - \vec{r}_1^{\,\circ})^2 \rangle_t = 6 D_1 t \qquad D_1 = w_1 a^2$$

$$\langle (\vec{r}_2 - \vec{r}_2^{\,\circ})^2 \rangle_t = 6 D_2 t \qquad D_2 = w_2 a^2$$

$$\vec{r}_1 = a(i_1, j_1, k_1)$$

$$\vec{r}_2 = a(i_2, j_2, k_2)$$

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

dynamics: what happens to i in one time step?

case

$i \to i+1$

prob.

$$w_1 \delta t \, (1 - 2 w_2 \delta t) + w_2 \delta t \, (1 - 2 w_1 \delta t)$$

molec. 1 jumps — molec. 2 stays — molec. 2 jumps — molec. 1 stays

+ other possibilites (all terms higher order than δt)

$$\approx \boxed{(w_1 + w_2)\, \delta t} - \cancel{4 w_1 w_2 \delta t^2} + \ldots$$

ignore

$i \to i-1 \qquad (w_1 + w_2)\,\delta t + \ldots$

$i \to i+2 \qquad : \ \propto \delta t^2$ or higher (ignore)

$i \to i \qquad : \ 1 - 2(w_1 + w_2)\,\delta t + \ldots$

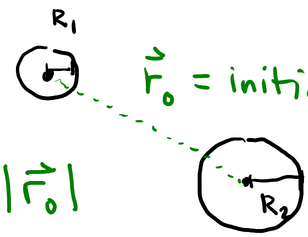
same dynamics as before with $w \equiv w_1 + w_2$

diffusion of separation b/t two particles behave like a single particle w/ $D = w a^2$

$$= w_1 a^2 + w_2 a^2$$

$$= D_1 + D_2$$

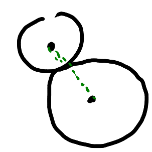
restate problem:



$\vec{r}_0$ = initial separation

$r_0 = |\vec{r}_0|$

diffusion w/ $D = D_1 + D_2$

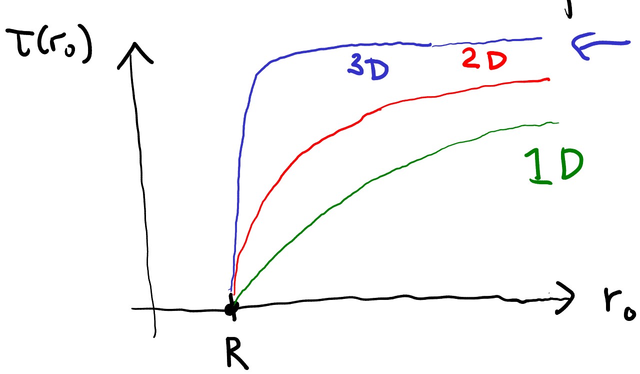


at contact $r = R_1 + R_2 \equiv R$

goal: calculate avg. time to contact when particles start at r_0:

capture time $\tau(r_0)$

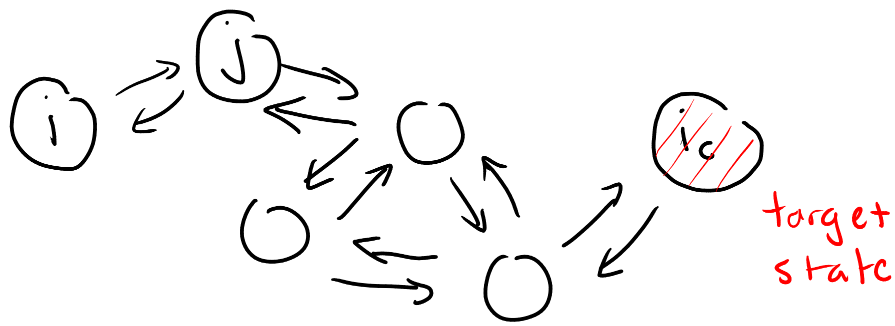
("mean first passage time")



asymptote due to finite volume

to calculate capture time, start more generally:

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



problem:

τ_i = avg. time to reach i_c from i for the first time

will prove: τ_i satisfies set of equations:

set of N equ's for N unknowns τ_i $i=1,\ldots,N$

$$\begin{cases} \sum_i \tau_i \Omega_{ij} = -1 & \text{for any } j \neq i_c \\ \tau_{i_c} = 0 \end{cases}$$

Convert to continuum picture
write down diff. equ. for $\tau(\vec{x})$