(1) $\quad 1 < i < N: \quad \dfrac{dp_i}{dt} = -2wp_i + w(p_{i+1} + p_{i-1})$

(2) $\quad i = 1: \quad \dfrac{dp_1}{dt} = -wp_1 + wp_2$

(3) $\quad i = N: \quad \dfrac{dp_N}{dt} = -wp_N + wp_{N-1}$

$$p_i(t) \rightarrow p(x,t)$$

$$p_{i+1}(t) \rightarrow p(x+a,t) \approx p(x,t) + a\frac{\partial p}{\partial x} + \frac{1}{2}a^2\frac{\partial^2 p^2}{\partial x^2}$$

$$p_{i-1}(t) \rightarrow p(x-a,t) \approx p(x,t) - a\frac{\partial p}{\partial x} + \frac{1}{2}a^2\frac{\partial^2 p^2}{\partial x^2}$$

$a$ small, $\quad D = wa^2 = \text{const.}$

(1) $\Rightarrow \quad \boxed{\dfrac{\partial p}{\partial t} = D\dfrac{\partial^2}{\partial x^2}p} \quad$ continuum diffusion equation

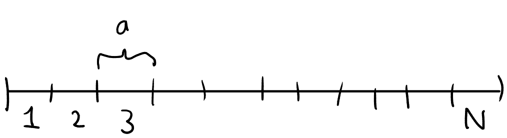
(2) $\Rightarrow \quad \dfrac{\partial p}{\partial t}(a,t) = wa\dfrac{\partial p}{\partial x}(a,t) + \dfrac{1}{2}wa^2\dfrac{\partial^2}{\partial x^2}p(a,t)$

$x = ia$
$i = 1$

$$\underbrace{\cancel{a\frac{\partial p}{\partial t}}}_{0} = \underbrace{wa^2}_{D}\frac{\partial p}{\partial x} + \underbrace{\cancel{\frac{1}{2}wa^3}}_{0 \quad \frac{1}{2}Da}\frac{\partial^2}{\partial x^2}p$$

$a \to 0$:

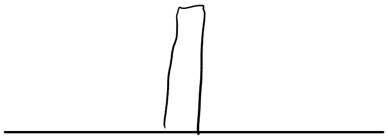
$$0 = D\frac{\partial p}{\partial x}(0,t) \quad \text{boundary condition at } x=0$$

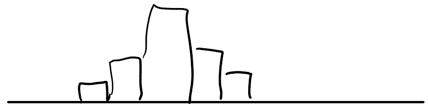



$L = Na$

eq. (2): $\quad \boxed{\dfrac{\partial p}{\partial x}(0,t) = 0}$

eq. (3): $\quad \boxed{\dfrac{\partial p}{\partial x}(L,t) = 0}$

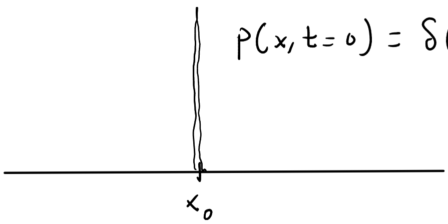




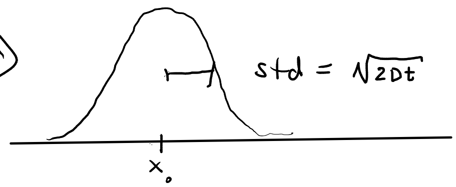
discrete cells of width

$t > 0$

continuous:




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




std $= \sqrt{2Dt}$

$\text{std}^2 = \text{MSD}$

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

$t \to \infty$ $\quad p(x,t) = \dfrac{1}{L}$ flat

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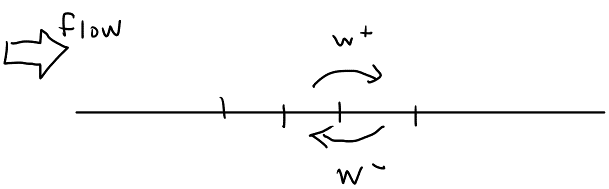
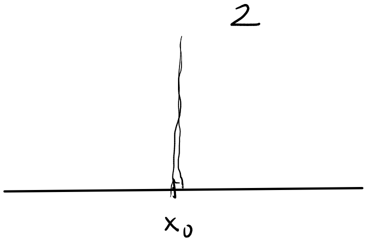


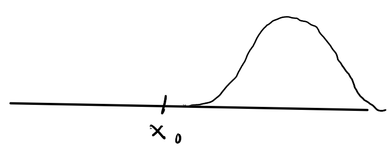

$w^+ > w^-$ b/c of flow biasing diffusion

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

$v = a(w_+ - w_-)$ = avg. speed of moving to right

$D = \dfrac{(w_+ + w_-)}{2} a^2$

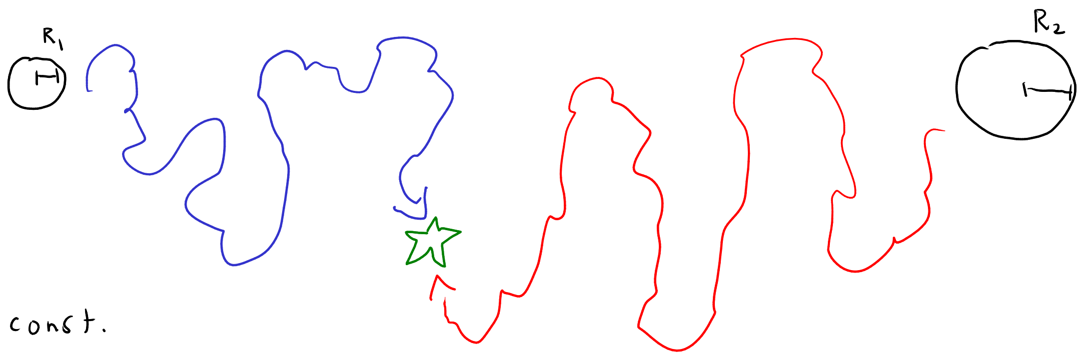



simple of example: Fokker - Planck equ.

Next step: consider 2 particles

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




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

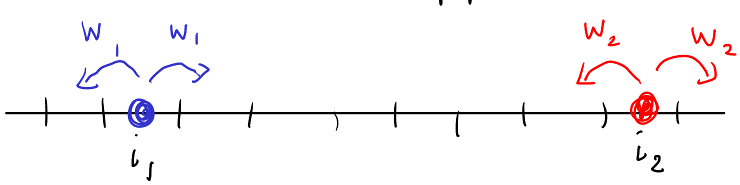
know so far: $\langle (\vec{r}_1 - \vec{r}_1^{\,0})^2 \rangle_t = 6 D_1 t \qquad D_1 = w_1 a^2$

$$\langle (\vec{r}_2 - \vec{r}_2^{\,0})^2 \rangle_t = 6 D_2 t \qquad D_2 = w_2 a^2$$

$$\vec{r}_1 = a(i_1, j_1, k_1)$$
$$\vec{r}_2 = a(i_2, j_2, k_2)$$

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

dynamics: what happens to $i$ in one time step?




$$i = i_2 - i_1$$

<u>transition</u> <u>prob.</u>

$i \to i+1$

$$\underbrace{w_1 \delta t}_{\text{part. 1 jumps}} \underbrace{(1 - 2 w_2 \delta t)}_{\text{part. 2 stays}} + \underbrace{w_2 \delta t}_{\text{part. 2 jumps}} \underbrace{(1 - 2 w_1 \delta t)}_{\text{part. 1 stays}}$$

+ other possibilities (higher order in $\delta t$)

ignore

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

$i \to i-1$

$$\approx (w_1 + w_2)\delta t$$

$i \to i+2$ etc. $\qquad \approx O(\delta t^2)$ or higher : ignore

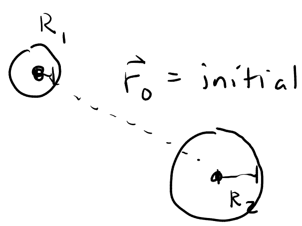
$i \to i \qquad 1 - 2(w_1 + w_2)\,\delta t$

<u>Same</u> dynamics as a single particle but w/
$w = w_1 + w_2$

$\Rightarrow$ separation of two particles obeys single particle diffusion math w/

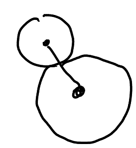
$$D = wa^2 = w_1 a^2 + w_2 a^2 = D_1 + D_2$$

restate problem:




$t = 0$

diffusion
w/ $D = D_1 + D_2$

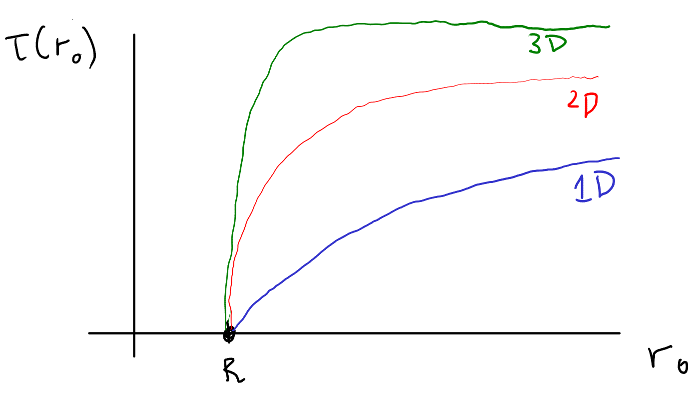


at contact
$r = R_1 + R_2$
$= R$

goal: calculate avg. time to first reach contact when particles start at $\vec{r}_0$:

capture time $\tau(r_0)$ — func. of $r_0 = |\vec{r}_0|$ by symmetry

"mean first passage time"




$\tau(r_0)$ in 3D reaches a max. value for $r_0$ just a little above R