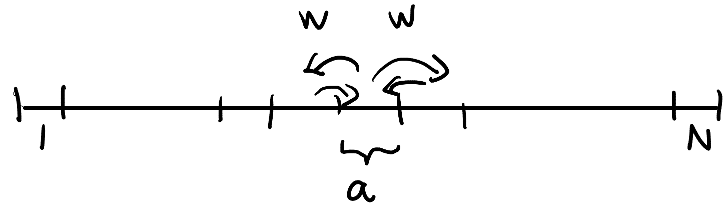


$a \to 0$

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

$D = wa^2 \rightsquigarrow$ D is related to a physical observable & should be indep. of grid choice a

$\langle \Delta_i^2 \rangle_t = 6Dt$

$w = \frac{D}{a^2}$ ← const.

as $a \to 0$, w increases (easier to leave a small box)

master equ:

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

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

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

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

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

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

plug into (1): $\frac{\partial p(x,t)}{\partial t} = \underbrace{wa^2}_{D}\frac{\partial^2}{\partial x^2}p(x,t)$

$$\Rightarrow \quad \boxed{\frac{\partial p}{\partial t} = D \frac{\partial^2}{\partial x^2} p}$$

diffusion equation

$$wa^3 = wa^2 \cdot a = Da \to 0 \quad \text{as} \quad a \to 0$$

higher order terms vanish as $a \to 0$

(2) : $\frac{\partial p}{\partial t}(a,t) = wa \frac{\partial p}{\partial x}(a,t) + \frac{1}{2} wa^2 \frac{\partial^2}{\partial x^2} p(a,t) + \cdots$

$p_1(t) \to p(a,t)$

$x = ia \quad i = 1$

$$\cancel{a \frac{\partial p}{\partial t}(a,t)} = \underbrace{wa^2}_{D} \frac{\partial p}{\partial x}(a,t) + \frac{1}{2} \cancel{wa^3 \frac{\partial^2}{\partial x^2} p(a,t)} + \cdots$$

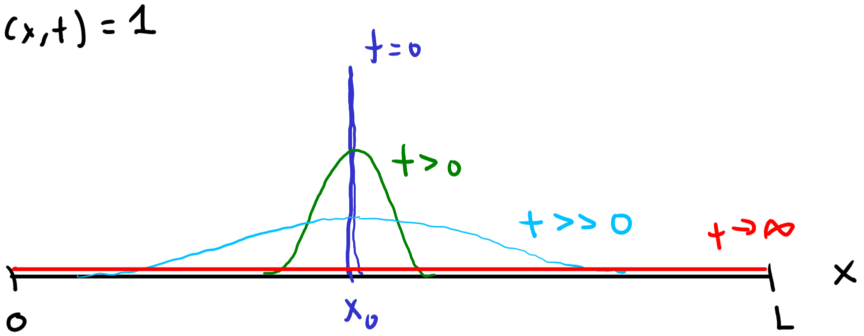
0 0

$a \to 0$: $\boxed{0 = D \frac{\partial p}{\partial x}(0,t)} \Rightarrow \frac{\partial p}{\partial x}(0,t) = 0$

(3) $\Rightarrow \quad \boxed{\frac{\partial p}{\partial x}(L,t) = 0}$ $\quad x = Na \equiv L$

Boundary conditions

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



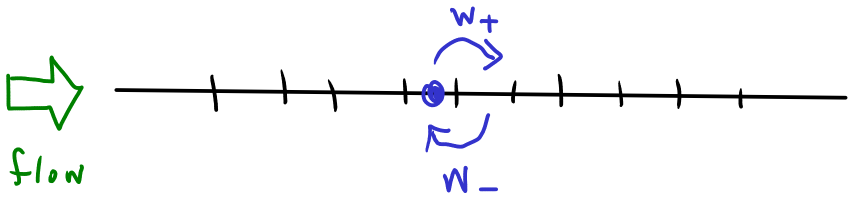
$p(x, t=0) = \delta(x - x_0)$

$x_0 = i_0 a$

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

Gaussian at x_0 w/ width $\propto \sqrt{Dt}$

another example:



$W_+ > W_-$ b/c flow biasing transitions

same derivation:

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

$$v = a(w_+ - w_-)$$

avg. speed to the right

simple case of more general class of equations: Fokker-Planck equ's

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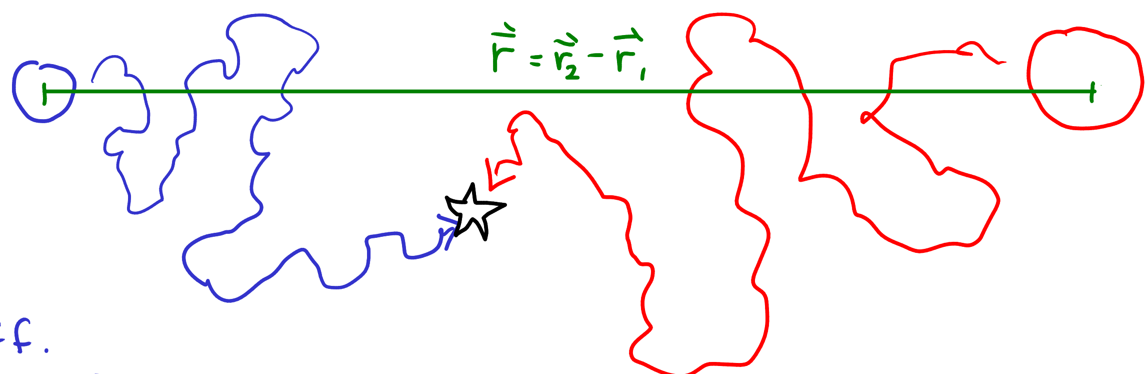
molec. 1 starts at $\vec{r}_1^{\,0}$ w/ diff. constant D_1



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

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

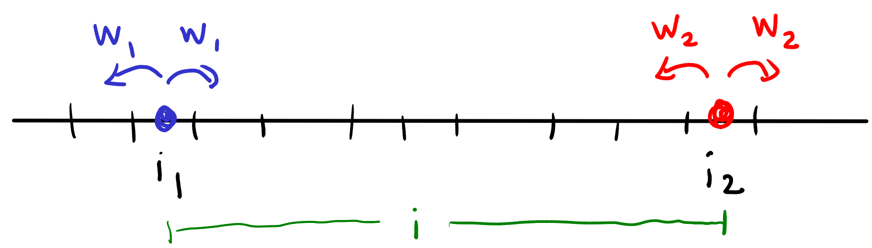
$$\langle (\vec{r}_2 - \vec{r}_2^{\,0})^2 \rangle_t = 6 D_2 t \qquad D_2 = w_2 a^2$$

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

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

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

dynamics: what happens to i in one time step?



prob

case: $i \to i+1$

mol. 1 jumps   mol. 2 stays   2 jump   1 stays

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

$+$ lots of other cases

$$\approx \boxed{(w_1 + w_2)\, \delta t} + O(\delta t^2) + O(\delta t^3) + \cdots$$

$i \to i-1$: $(w_1 + w_2)\, \delta t + \cdots$

$i \to i+2$: $O(\delta t^2)$ or higher

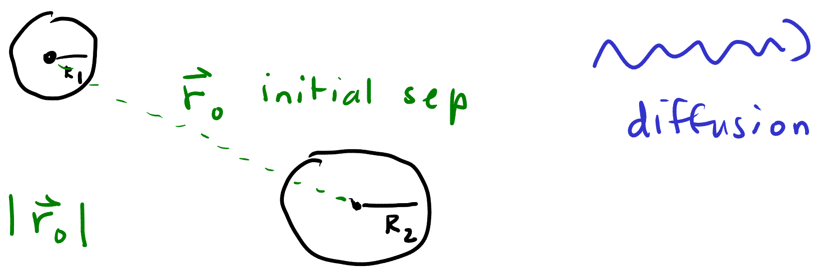
$i \to i$: $1 - 2(w_1 + w_2)\, \delta t + \cdots$

same prob's as one particle diff:
with $w = w_1 + w_2$

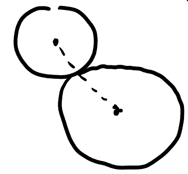
Separation of two particles behaves like one part. diffusion w/ $w = w_1 + w_2$

$$D = w a^2 = (w_1 + w_2) a^2 = D_1 + D_2$$

restate problem:



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



at contact
$r = |\vec{r}|$
$= R_1 + R_2$
$\equiv R$

GOAL: calculate avg. time to reach contact when particles start at r_0: capture time $\tau(r_0)$
"mean first passage time"