W09 - Random Walks

Brownian Movement (diffusion)

Brownian Motion

Brown (1829) movements of particles inside pollen grains

Lysozymes

$\delta = 10^{-10}$ cm

$\tau = 10^{-13}$ sec (time between collisions)

a lysozyme takes $N = \frac{1}{\tau} = 10^{13}$ steps per second!

$p = q$ $\qquad \langle x(t) \rangle = 0$

$$\langle x(t)^2 \rangle = \delta^2 \, Var(m)$$

$$= \delta^2 \, 4pqN$$

$$= \delta^2 \, 4pq\left(\frac{t}{\tau}\right)$$

$$= 4\left(\frac{t}{\tau}\right) p \cdot q \cdot \delta^2$$

$$= t \, \frac{\delta^2}{\tau} = 2Dt$$

$D \equiv \frac{1}{2} \frac{\delta^2}{\tau}$ diffusion coefficient

$$\langle x^2(t)\rangle = 2Dt$$

$$\sigma = \sqrt{2Dt}$$

$$P(x|t) \approx \frac{1}{\sqrt{4\pi Dt}}\, e^{-x^2/4Dt}$$

Generalization to 2D, 3D:

$$\langle x^2\rangle = \langle y^2\rangle = \langle z^2\rangle = 2Dt$$

$$P(r|t) = \frac{1}{\sqrt{4\pi Dt}}\, e^{-r^2/4Dt} \qquad r = x$$

$$P_{2D}(r|t) = \frac{1}{4\pi Dt}\, e^{-r^2/4Dt} \qquad r^2 = x^2+y^2.$$

$$P_{3D}(r|t) = \frac{1}{(4\pi Dt)^{3/2}}\, e^{-r^2/4Dt} \qquad r^2 = x^2+y^2+z^2$$

$$\langle x(t)\rangle = 0$$

$$\langle x^2(t)\rangle = 2Dt$$

for a lysozyme $\quad D = \frac{1}{2}\frac{\delta^2}{\tau} = 10^{-6}\, cm^2/sec$

How fast is Brownian motion?

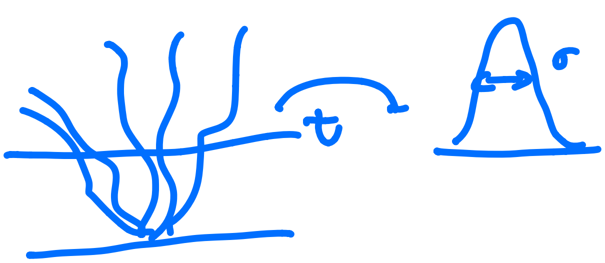
t	$\sqrt{x^2(t)}$	
1μ	10^{-4} cm	size of bacterium
1ms	10^{-3} cm	size of neuron's cell body
8 mins	0.1 mm	length of neuron's dendrite
6 days	1 cm	length of neuron's axon

In brownian motion:

$$\langle \sqrt{x^2(t)} \rangle = \sqrt{2Dt}$$

This is not a "velocity". There is no a "velocity of diffusion".

The mean-square deviation of the displacement



is proportional to the $\sqrt{t}$.

The Diffusion equations

Random walk behaviour when $\delta \to 0$ $\tau \to 0$

continuous space and time displacements

Diffusion eq. derived from the master eq.

$$P_{N+1}(m) = \frac{1}{2} P_N(m-1) + \frac{1}{2} P_N(m+1)$$

$$P_{N+1}(m) - P_N(N) = \frac{P_N(m-1) + P_N(m+1) - 2P(m)}{2}$$

$$\frac{\delta P(x,t)}{\delta t} = \lim_{\tau \to 0} \frac{P(x,t+\tau) - P(x,t)}{\tau}$$

$$\frac{\delta^2 P(x,t)}{\delta x^2} = \lim_{\delta \to 0} \frac{P(x+\delta, t) + P(x-\delta, t) - 2P(x,t)}{\delta^2}$$

$$\tau \frac{\delta P(x,t)}{\delta t} = \delta^2 \frac{1}{2} \frac{\delta^2 P(x,t)}{\delta x^2}$$

$$\frac{\delta P(x,t)}{\delta t} = \frac{1}{2} \frac{\delta^2}{\tau} \frac{\delta^2 P(x,t)}{\delta x^2}$$

Introduce $D =: \frac{1}{2} \frac{\delta^2}{\tau}$ " the diffusion coefficient

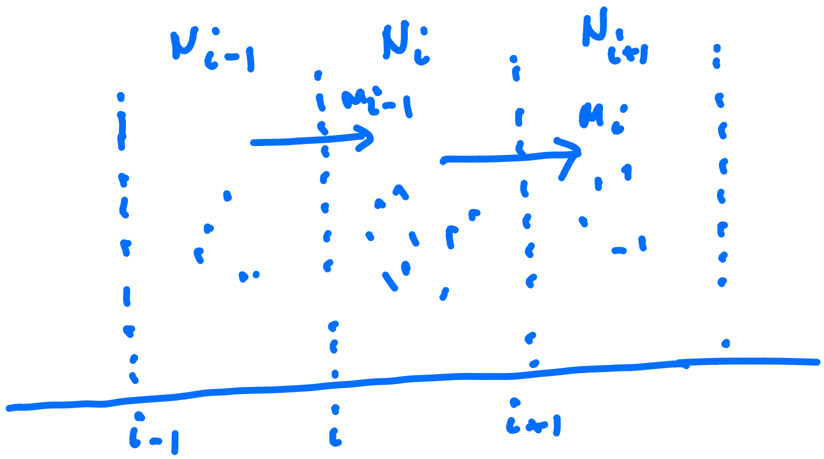
then: $$\boxed{\frac{\delta P(x,t)}{\delta t} = D \frac{\delta^2 P(x,t)}{\delta x^2}}$$

the diffusion equation

Diffusion eq. take 2. (Berg Chapter 2)

N_j = # particles

from i to $i+1$



M_i = net crossing from i to $i+1$

ΔN_i = concentration change

$$M_i = \frac{1}{2} N_i - \frac{1}{2} N_{i+1}$$

$$\Delta N_i = -M_i + M_{i+1}$$

- Flux: $\quad J_i = \frac{M_i}{\tau}$

  particles crossing per unit time

· concentration

$$c_i = \frac{N_i}{\delta}$$

particles per unit length at position i

$$J_i = \frac{M_i}{\tau}$$

$$= -\frac{1}{2\tau}\left(N_{i+1} - N_i\right)$$

$$= -\frac{1}{2\tau}\left(\delta c_{i+1} - \delta c_i\right)$$

$$= -\frac{\delta}{2\tau}\left(c_{i+1} - c_i\right)$$

$$= -\frac{\delta^2}{2\tau}\,\frac{c_{i+1} - c_i}{\delta}$$

$$= -D\,\frac{\delta c_i}{\delta t} \rightarrow \boxed{J_i = -D\,\frac{\delta c_i}{\delta t}}$$

first Fick equation:

First Fick eq: $$J_i = -D \frac{\delta c_i}{\delta t}$$

the net flux is proportional to the change in concentration and the D constant

The second eq

$$\Delta N_i = -M_i + M_{i+1}$$

can be re-written as

$$\frac{\Delta N_i}{\delta} = -\frac{1}{\delta}(M_i - M_{i-1})$$

$$\Delta c_i = -\frac{1}{\delta}(M_i - M_{i-1})$$

$$\frac{\Delta c_i}{\tau} = -\frac{1}{\delta}\,\frac{M_i - M_{i-1}}{\tau}$$

$$\frac{\delta c_i}{\delta t} = -\frac{J_i - J_{i-1}}{\delta} = -\frac{\delta J_i}{\delta x}$$

the second fick eq

$$\boxed{\frac{\delta c_i}{\delta t} = -\frac{\delta J_i}{\delta x}}$$

Putting both eq together

$$J_i = -D\frac{\delta c_i}{\delta x}$$

$$\frac{\delta c_i}{\delta t} = -\frac{\delta J_i}{\delta x}$$

results in

$$\frac{\delta c_i}{\delta t} = -\frac{\delta}{\delta x}\left(-D\frac{\delta c_i}{\delta x}\right) = D\frac{\delta^2 c_i}{\delta x^2}$$

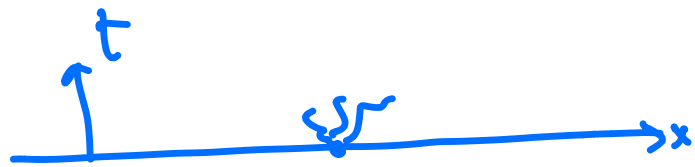
$$\boxed{\frac{\delta c_i}{\delta t} = D\frac{\delta^2 c_i}{\delta x^2}}$$

Particular Solutions

Initial condition is a pulse

$$\left.\begin{array}{l} C(x\neq 0, t=0)=0 \\ C(x=0, t=0)=1 \end{array}\right\}$$

$$C(x, t=0) = \delta(x=0)$$



$$C(x,t) = N\,P(x,t) = N \cdot \mathcal{N}(x \mid \mu=0, \sigma^2=2Dt)$$

$$C(x,t) = \frac{N}{\sqrt{4\pi Dt}}\, e^{-x^2/4Dt}$$

→ you can verify that this $c(x,t)$ §

Sections

i) $C(x, t=0) = N$

ii) $\frac{\delta C(x,t)}{\delta t} = D \frac{\delta^2 C(x,t)}{\delta x^2}$

This initial conditions apply to a pipette filled with fluid, that injects dye at $t=0$

Other properties

- the concentration remains highest at $t=0$

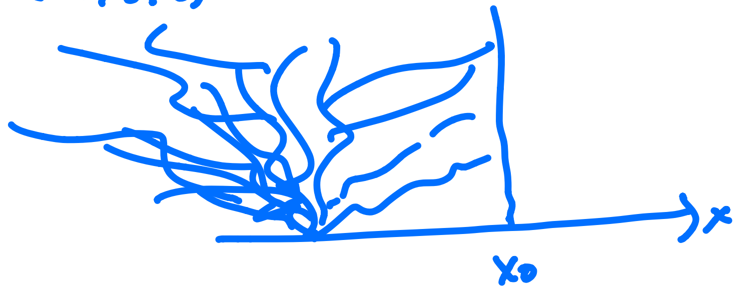
- the concentration decays with

$$\frac{1}{\sqrt{t}} \text{ if 1D}$$

$$\frac{1}{t^{3/2}} \text{ if 3D} \qquad \text{fast!}$$

Absorbtion and Reflection

- Absorbtion $\quad C(x_0,t)=0 \ \forall t \quad C=0$

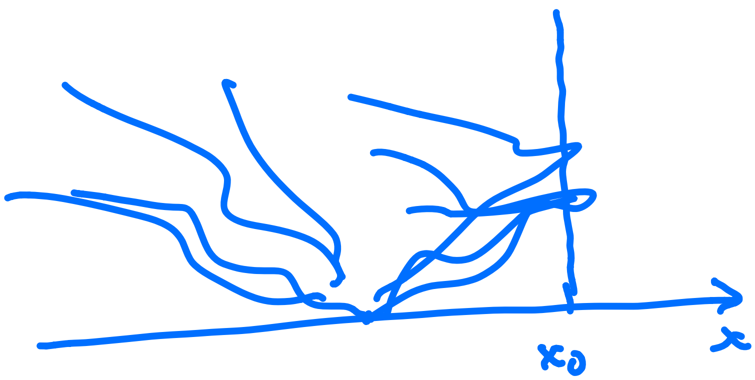


- Reflection $\quad J(x_0,t)=0 \ \forall t$

$J(x,t)=\frac{\delta C}{\delta x}$

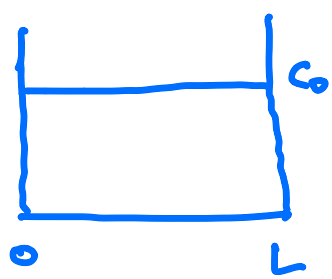
$J(x_0,t)=0 \Rightarrow$

$C(x_0)=C$

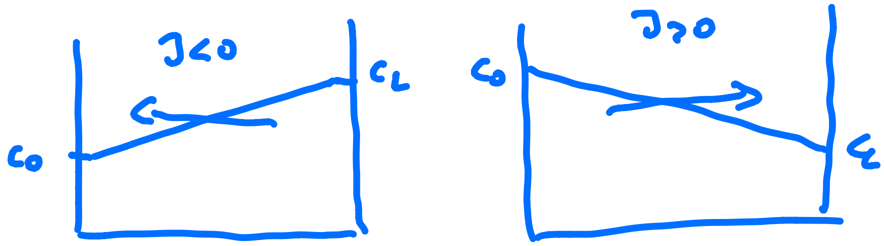


Steady state

$$\frac{\delta C}{\delta t}=0 \quad \text{or} \quad \frac{\delta^2 C}{\delta x^2}=0$$



- $C(x,t)=C_0 \rightarrow J=0$
- $C(x,t)=C_0+x\frac{C_L-C_0}{L} \rightarrow J=-D\frac{\delta C}{\delta x}=-D\frac{C_L-C_0}{L}$



$$J = -D\,\frac{c_L - c_0}{L}$$