Lecture 11

2D wedge

absorbing boundaries

Survival prob. $S(t)$ – ? @ large t

$$c = c(r,\theta,t)$$

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{1}{r^2}\frac{\partial^2 c}{\partial \theta^2}\right)$$

BCs : $c = 0$ @ $\theta = 0, \alpha$

Green's function: $G(r,\theta,t) \sim \sum_{n=1}^{\infty} \sin\left(\frac{n\pi\theta}{\alpha}\right) \underbrace{\ldots}_{\text{decaying } t\text{-dependent part}}$

Large t : $n=1$ dominates, so choose an init. cond. w/ $n=1$ to begin with:

$$c(r,\theta,t=0) = \frac{\pi}{2\alpha r_0}\sin\left(\frac{\pi\theta}{\alpha}\right)\delta(r-r_0)$$

$$\int_0^{\alpha} d\theta \int_0^{\infty} r\,dr\, c(r,\theta,t=0) = \underline{\underline{1}}$$

Laplace domain:

$$s\,c(r,\theta,s) - c(r,\theta,t=0) =$$
$$= D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{1}{r^2}\frac{\partial^2 c}{\partial \theta^2}\right)$$

Try $c(r,\theta,s) = R(r,s)\sin\left(\frac{\pi\theta}{\alpha}\right)$

$$sR\,\cancel{\sin\left(\frac{\pi\theta}{d}\right)} - \frac{\pi}{2dr_0}\,\cancel{\sin\left(\frac{\pi\theta}{d}\right)}\,\delta(r-r_0) =$$

$$= D\,\cancel{\sin\left(\frac{\pi\theta}{d}\right)}\left[\frac{\partial^2 R}{\partial r^2} + \frac{1}{r}\frac{\partial R}{\partial r} - \frac{1}{r^2}\underbrace{\left(\frac{\pi}{d}\right)^2}_{\nu} R\right], \text{ or}$$

$$\frac{\partial^2 R}{\partial r^2} + \frac{1}{r}\frac{\partial R}{\partial r} - \frac{\nu^2}{r^2}R - \frac{s}{D}R = -\frac{\pi}{2dr_0 D}\,\delta(r-r_0).$$

$$x = r\sqrt{\frac{s}{D}} \quad \text{gives} \quad \begin{cases} r = x\sqrt{\frac{D}{s}}, \\ \frac{\partial}{\partial r} = \frac{\partial}{\partial x}\sqrt{\frac{s}{D}} \end{cases}$$

$$\frac{s}{D}R'' + \frac{s}{Dx}R' - \left(\frac{\nu^2}{r^2} + \frac{s}{D}\right)R = -\frac{\nu}{2\underbrace{r_0}_{x_0\sqrt{\frac{D}{s}}} D}\sqrt{\frac{s}{D}}\,\delta(x-x_0), \text{ or}$$

$$' \equiv \frac{d}{dx}$$

$$R'' + \frac{1}{x}R' - \underbrace{\qquad}_{\frac{D}{s}\left(\frac{s}{D} + \frac{\nu^2}{x^2\frac{D}{s}}\right) = \left(1 + \frac{\nu^2}{x^2}\right)} R = -\frac{\nu}{2x_0 D}\,\delta(x-x_0).$$

modified Bessel eq'n

$$R(x,s) = A\, I_\nu(x_<)\, K_\nu(x_>),$$

where A is given by:

$$R'\big|_{x=x_0+\epsilon} - R'\big|_{x=x_0-\epsilon} = -\frac{\nu}{2x_0 D}$$

$$\begin{cases} x_< = \min(x, x_0) \\ x_> = \max(x, x_0) \end{cases}$$

$$\Downarrow$$

$$A = \frac{\nu}{2D}$$

$$\begin{cases} I_\nu \text{ diverges as } x \to \infty \\ K_\nu \text{ diverges as } x \to 0 \end{cases}$$

Inverse Laplace transform:

$$R(r,t) = \frac{\nu}{4Dt}\, e^{-(r^2+r_0^2)/4Dt}\, I_\nu\left(\frac{r r_0}{2Dt}\right)$$

Finally, the <u>asymptotic</u> survival prob.

$$S(t) \sim \int_0^\alpha \sin(\nu\theta)\,d\theta \int_0^\infty r\,dr\; R(r,t)$$

$$t\to\infty:\; e^{-r_0^2/4Dt} \to 1 \quad (\text{but } \underline{\text{not}}\ e^{-r^2/4Dt})$$

$$I_\nu(x) \sim \left(\frac{x}{2}\right)^\nu \frac{1}{\Gamma(\nu+1)}.$$

Then $S(t) \sim \dfrac{2}{\nu\,\Gamma(\nu+1)} \displaystyle\int_0^\infty dr\, r\, \frac{\nu}{4Dt}\left(\frac{r r_0}{4Dt}\right)^\nu e^{-r^2/4Dt} \sim$

$$\cancel{\sim \int_0^{\sqrt{Dt}} r\,dr\,\frac{1}{Dt}\left(\frac{r r_0}{Dt}\right)^\nu \sim \frac{r_0^\nu}{(Dt)^{\nu+1}}\left(\sqrt{Dt}\right)^{\nu+2} \sim \left(\frac{r_0}{\sqrt{Dt}}\right)^\nu.}$$

$$\cancel{e^{-r^2/4Dt} = 1 \text{ at the front}}$$

So, $S(t) \sim t^{-\pi/2\alpha}$.

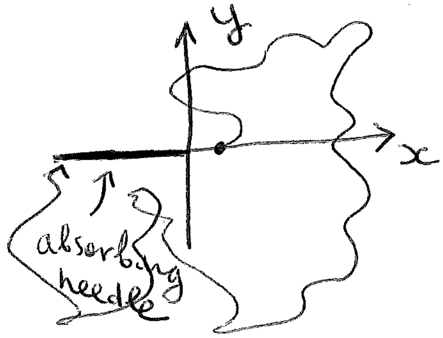
$$x = \frac{r}{\sqrt{4Dt}} \Rightarrow S(t) \sim \cancel{\sqrt{4Dt}} \int_0^\infty dx\, \frac{x}{\cancel{\sqrt{4Dt}}}\left(\frac{x r_0}{\sqrt{4Dt}}\right)^\nu e^{-x^2} \sim$$

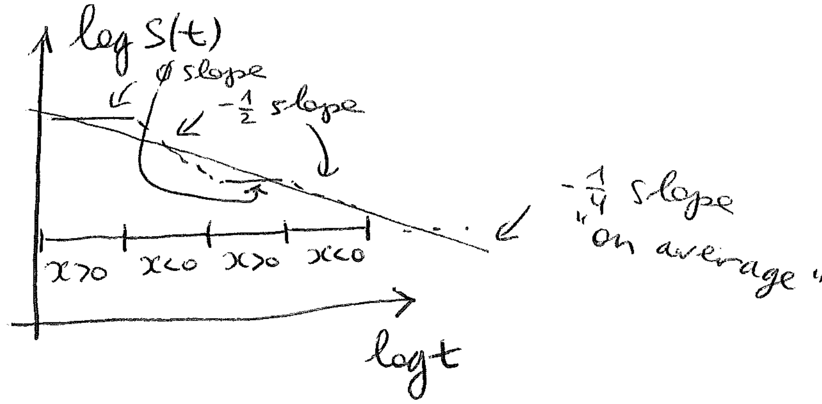
$$\sim t^{-\frac{\nu}{2}} = t^{-\pi/2\alpha}.$$

$\alpha = 2\pi \Rightarrow$ "absorbing needle"

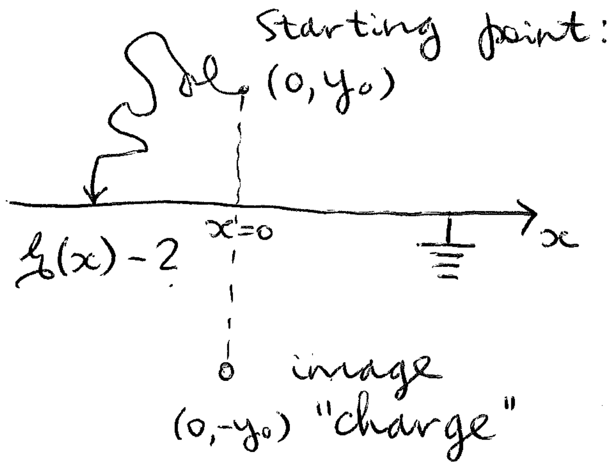
$$S(t) \sim t^{-1/4}$$

Decompose diffusion into x & y components. If $x<0$, we have a trapping point @ $y=0 \Rightarrow S(t) \sim t^{-1/2}$. If $x>0$, there's no trapping. With time, $x \sim t^{1/2}$


y
x
absorbing needle


log S(t)
ϕ slope
$-\frac{1}{2}$ slope
$-\frac{1}{4}$ slope
"on average"
x>0
x<0
x>0
x<0
log t

Diffusion in a 2D system with a boundary



$y=0$ is the absorbing boundary

We have

$$C(x,y,t) = \frac{1}{4\pi D t}\Big[e^{-(x^2+(y-y_0)^2)/4Dt} - \\ - e^{-(x^2+(y+y_0)^2)/4Dt}\Big]$$

Then
$$|j(x,t)| = D\left.\frac{\partial c}{\partial y}\right|_{y=0} = \frac{1}{4\pi D t} D \frac{1}{4Dt} \times \\ \times \Big[2y_0\, e^{-(x^2+y_0^2)/4Dt} + 2y_0\, e^{-(x^2+y_0^2)/4Dt}\Big] = \\ = \frac{1}{4\pi D t}\,\frac{y_0}{t}\, e^{-(x^2+y_0^2)/4Dt}$$

Mathematica

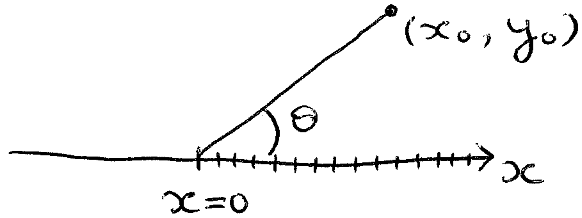
Finally, $g(x) = \int_0^\infty dt\, |j(x,t)| = \frac{1}{\pi}\frac{y_0}{y_0^2+x^2}$

Cauchy distr'n

$\sim \frac{1}{x^2}$ as $x \to \pm\infty$

No finite moments of any order, incl. the mean

More generally, consider



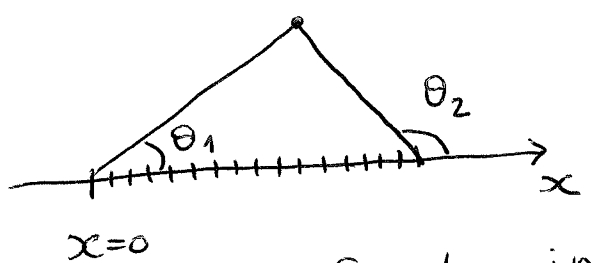
Here, $\mathcal{P}(x) = \dfrac{1}{\pi} \dfrac{y_0}{y_0^2 + (x-x_0)^2}$.

The prob. of hitting the $x \geq 0$ semi-axis is given by

$$\int_0^\infty dx\, \mathcal{P}(x) = \frac{1}{\pi} \int_0^\infty dx \frac{y_0}{y_0^2 + (x-x_0)^2} =$$

$$= 1 - \frac{1}{\pi} \tan^{-1}\left(\frac{y_0}{x_0}\right) = 1 - \frac{\theta}{\pi}.$$

Finally,



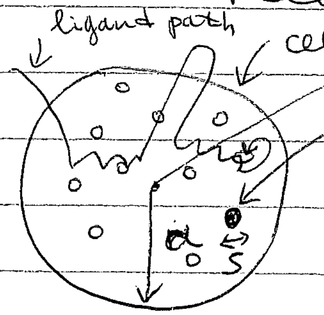
Prob (hitting finite interval) =

$$= \frac{\theta_2 - \theta_1}{\pi}.$$

1977

Berg & Purcell result for cell receptors

Howard Berg



r - starting radius, > a

N receptors ~ 10^4

$a \sim 10^{-6}$ m

$s \sim 10^{-9}$ m

k_{3D}
$$\begin{cases} \nabla^2 C = 0 \\ C(r=a) = 0 \\ C(r\to\infty, t) = 1 \end{cases}$$

$C(r) = \left[1 - \left(\frac{a}{r}\right)^{d-2}\right]$

$k = \int_{\partial S} d^{d-1}\Omega\, D\, \nabla C = 4\pi D a.$ ($\nabla C \sim \frac{\partial C}{\partial r}\big|_{r=a}$)

$\frac{\partial C(r)}{\partial r}\Big|_{r=a} = +(d-2)\, a^{d-2}\, r^{1-d}\big|_{r=a} = \frac{d-2}{a}$

$d=3$: $\to \frac{1}{a}$

Hitting prob.(r): $= \frac{a}{r}$ ($d=3$)

"electrostatic potential distance r away"

Scale of the problem: s (receptor size)

Consider

p_s = hitting prob $(a+s) = \frac{a}{a+s}$

"Hit the sphere from r, bounce up to a+s, hit again..."

P_n = prob. of n indep. hits =

$= p_s^n (1-p_s)$

$\langle n \rangle = \sum n p_s^n (1-p_s) = \frac{p_s}{1-p_s} = \frac{a/(a+s)}{s/(a+s)} = \frac{a}{s}$

H = prob. to hit receptor $= \frac{N\pi s^2}{4\pi a^2} = \frac{Ns^2}{4a^2}$

M = prob. to miss receptor $= 1 - \frac{Ns^2}{4a^2}$

$H + M = 1$

$P_{esc} = \sum_{n=0}^{\infty} (M p_s)^n (1-p_s) = \frac{1-p_s}{1-Mp_s} = \frac{s/(a+s)}{1-\left(1-\frac{Ns^2}{4a^2}\right)\frac{a}{a+s}} = \frac{s/(a+s)}{s/(a+s) + \frac{Ns^2}{4a(a+s)}} \stackrel{\circ}{=} \frac{1}{1+\frac{Ns}{4a}} = \frac{4a}{4a+Ns}$

$\mathcal{H}$ = eventual hitting prob =

$= 1 - P_{esc} = \frac{Ns}{4a+Ns}$

$s \to 0 \Rightarrow \mathcal{H} \to 0$

oh no

So, $\boxed{k_{cell} = 4\pi D a \left(\frac{Ns}{Ns+4a}\right)}$

$$\frac{Ns}{4a+Ns} \sim \frac{10^4 10^{-9}}{4\times10^{-6}+10^{+4}10^{-9}} \sim 0.7!$$

Area fraction covered:

$$\frac{Ns^2}{4a^2} \sim 10^{-3}$$, much smaller than 0.7