OpenTA: week 18:

Lions Running Rambs:

a). In the original derivation of the Fokker-Planck equation, we used Itô's lemma:

$$df(x) = \cancel{\frac{\partial f}{\partial t}}^{=0} dt + \frac{\partial f}{\partial x} dx + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} dx^2$$

But now, we have:

$$df(x_1, x_2) = \cancel{\frac{\partial f}{\partial t}}^{=0} dt + \boxed{\frac{\partial f}{\partial x_1} dx_1 + \frac{1}{2} \frac{\partial^2 f}{\partial x_1^2} dx_1^2} + \boxed{\frac{\partial f}{\partial x_2} dx_2 + \frac{1}{2} \frac{\partial^2 f}{\partial x_2^2} dx_2^2}$$

$\Rightarrow$

$$\frac{\partial P(x_1, x_2, t)}{\partial t} = D \left(\boxed{\frac{\partial^2}{\partial x_1^2}} + \boxed{\frac{\partial^2}{\partial x_2^2}} \right) P(x_1, x_2, t).$$

b) $\begin{cases} x_1 = R + r/2 \\ x_2 = R - r/2 \end{cases} \Leftrightarrow \begin{cases} R = \frac{x_1 + x_2}{2} & : \text{centre of mass coord.} \\ r = x_1 - x_2 & : \text{relative coord.} \end{cases}$

$$\partial_{x_1} = \partial_R \cdot \underbrace{\frac{\partial R}{\partial x_1}}_{1/2} + \partial_r \cdot \underbrace{\frac{\partial r}{\partial x_1}}_{1} = \frac{1}{2} \partial_R + \partial_r$$

$$\partial_{x_2} = \partial_R \cdot \underbrace{\frac{\partial R}{\partial x_2}}_{1/2} + \partial_r \cdot \underbrace{\frac{\partial r}{\partial x_2}}_{-1} = \frac{1}{2} \partial_R - \partial_r.$$

$$\boxed{\partial_{x_1}^2 + \partial_{x_2}^2} = \frac{1}{4} \partial_R^2 + \cancel{\partial_R \partial_r} + \partial_r^2 + \frac{1}{4} \partial_R^2 - \cancel{\partial_R \partial_r} + \partial_r^2 = \boxed{\frac{1}{2} \partial_R^2 + 2 \partial_r^2}$$

So, the Fokker-Planck equation becomes:

$$\boxed{\frac{\partial P(R, r, t)}{\partial t} = \frac{D}{2} \partial_R^2 P(R, r, t) + 2D \partial_r^2 P(R, r, t).}$$

If we now assume that the probability distribution decouples as:

$$\boxed{P(R,r,t) = P_{com}(R,t)\cdot P_{rel}(r,t).}$$

And substituting in the Fokker-Planck equation:

$$\frac{\partial P_{com}}{\partial t}\cdot P_{rel} + P_{com}\cdot\frac{\partial P_{rel}}{\partial t} =$$

$$= \frac{D}{2}\cdot P_{rel}\cdot\partial_R^2 P_{com} + 2D\,P_{com}\,\partial_r^2 P_{rel} \Rightarrow$$

$$\Rightarrow \boxed{\frac{\partial P_{com}(R)}{\partial t}\frac{1}{P_{com}(R)} - \frac{D}{2}\frac{1}{P_{com}(R)}\cdot\partial_R^2 P_{com}(R)} \quad f(R)$$

$$= \boxed{-\frac{\partial P_{rel}(r)}{\partial t}\cdot\frac{1}{P_{rel}(r)} + 2D\,\frac{1}{P_{rel}(r)}\cdot\partial_r^2 P_{rel}(r)} \quad g(r)$$

$$\boxed{f(R)} = \boxed{g(r)} = C \sim \text{const.}$$

$$\Rightarrow \begin{cases} \dfrac{\partial P_{com}(R)}{\partial t} - \dfrac{D}{2}\,\partial_R^2 P_{com}(R) = C\,P_{com}(R). \\[2ex] \dfrac{\partial P_{rel}(r)}{\partial t} - 2D\,\partial_r^2 P_{rel}(r) = -C\,P_{rel}(r) \end{cases}$$

The equations are verified if both $P_{com}(R)$ and $P_{rel}(r)$ obey separate diffusion equations, with diffusion constants $\frac{D}{2}$ and $2D$, respectively, i.e.

$$\begin{cases} \dfrac{\partial P_{com}(R,t)}{\partial t} = \dfrac{D}{2}\,\partial_R^2 P_{com}(R,t) \\[2ex] \dfrac{\partial P_{rel}(r,t)}{\partial t} = 2D\,\partial_r^2 P_{rel}(r,t) \end{cases}$$

Which is verified if $\underline{C=0}$.

We have thus verified that $P(R,r,t)$ does indeed decouple in R and r.

(c). Solution to diffusion equation with initial condition $Prob(r, t=0) = \delta(r-R)$:

$$Prob(r,t) = \frac{1}{\sqrt{4\pi(2D)t}} \cdot e^{-\frac{(r-R)^2}{4(2D)t}}$$

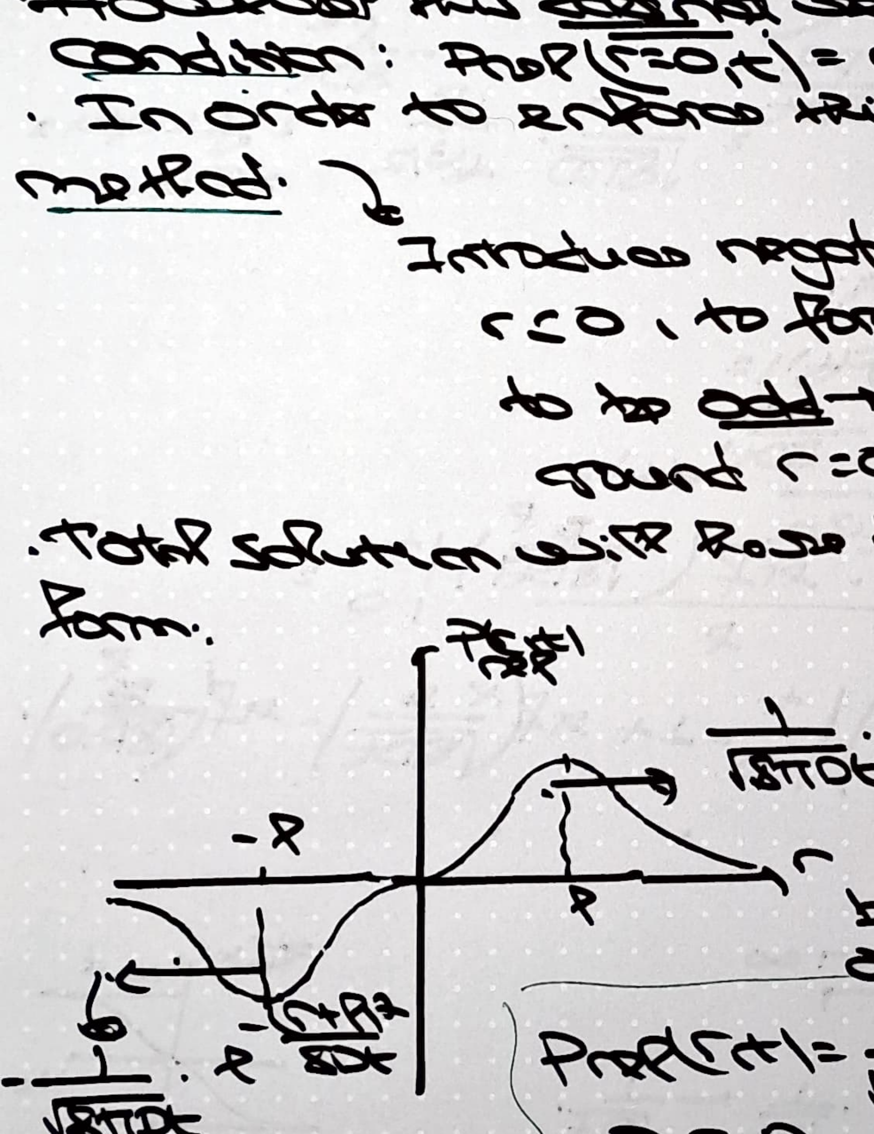
$D \to 2D$

$$= \frac{1}{\sqrt{8\pi D t}} \cdot e^{-\frac{(r-R)^2}{8Dt}}.$$

However this doesn't satisfy the boundary condition: $Prob(r=0,t)=0$.

In order to enforce this, we use the image method. → Introduce negative probabilities for $r\leq 0$, to force the total function to be odd → Antisymmetric around $r=0$, with $Prob(0)=0$.

Total solution will have the following form:



If we superimpose both solutions, we obtain:

$$\boxed{Prob(r,t) = \frac{1}{\sqrt{8\pi D t}}\left(e^{-\frac{(r-R)^2}{8Dt}} - e^{-\frac{(r+R)^2}{8Dt}}\right)}$$

Q.E.D.

(d). J → probability current density: Probability / unit time.

In 1D, this one is just a point, so we have units of Prob./time → probability which goes into $r=0$ per unit of time at time t.

$$f(t) = 2D \frac{\partial}{\partial x} P_{abs}(x,t)\Big|_{x=0} =$$

$$= \frac{2D}{\sqrt{8\pi Dt}} \frac{\partial}{\partial x}\left(e^{-\frac{(x-x_0)^2}{8Dt}} - e^{-\frac{(x+x_0)^2}{8Dt}} \right)\Big|_{x=0} =$$

$$= \frac{2D}{\sqrt{8\pi Dt}} \cdot \frac{1}{8Dt}\left(-e^{-\frac{(x-x_0)^2}{8Dt}} \cdot \underset{-2x_0}{2(x-x_0)} + e^{-\frac{(x+x_0)^2}{8Dt}} \cdot \underset{2x_0}{2(x+x_0)} \right)$$

$$= \frac{4Dx_0}{8Dt} \cdot \frac{1}{\sqrt{8\pi Dt}} \left(e^{-\frac{x_0^2}{8Dt}} + e^{-\frac{x_0^2}{8Dt}} \right) =$$

$$= \frac{4 \cdot 2 \cdot x_0}{8t\sqrt{8\pi Dt}} e^{-\frac{x_0^2}{8Dt}} = \boxed{\frac{x_0}{\sqrt{8\pi D}} \cdot \frac{e^{-\frac{x_0^2}{8Dt}}}{t^{3/2}} = f(0,t) = F(t)}$$

Survival probability:

$$S(t) = 1 - \int_0^t dt' \, F(t') =$$

$$= 1 - \frac{x_0}{\sqrt{8\pi D}} \int_0^t \frac{e^{-\frac{x_0^2}{8Dt'}}}{t'^{3/2}} dt' =$$

$$= 1 + \frac{x_0}{\sqrt{8\pi D}} \left(\frac{\sqrt{8\pi D} \cdot \operatorname{erf}\left(\frac{x_0}{\sqrt{8Dt'}}\right)}{x_0} \right)\Big|_0^t =$$

$$= 1 + \operatorname{erf}\left(\frac{x_0}{\sqrt{8Dt'}}\right)\Big|_0^t = 1 + \operatorname{erf}\left(\frac{x_0}{\sqrt{8Dt}}\right) - \underbrace{\cancel{\operatorname{erf}\left(\frac{x_0}{\sqrt{8D \cdot 0}}\right)}}_{1}$$

(gaussian integral)

$$= \operatorname{erf}\left(\frac{x_0}{\sqrt{8Dt}}\right).$$

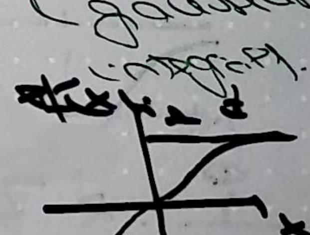
$$S(t) = \operatorname{erf}\left(\frac{x_0}{\sqrt{8Dt}}\right) \xrightarrow{t \to \infty}$$

Q.E.D

$$\rightarrow \underbrace{\frac{2}{\sqrt{\pi}} \cdot \frac{x_0}{\sqrt{8Dt}}}_{} = \frac{x_0}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{Dt}} \boxed{\sim \frac{1}{\sqrt{Dt}}}$$

Maclaurin series of "erf" function, where I keep just the first term!

$\operatorname{erf}(x)$



$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

Proof.