Lecture 10 Mean First Passage Time (MFPT).

Examples Class #1 at 2pm today — Here.

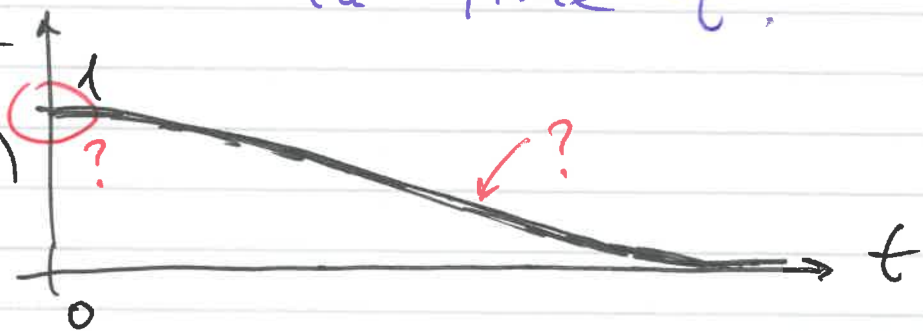
- What is the probability of escape in time t?
- Mean time of escape?

(For $\forall$ stochastic process)

Approach #1 : via Survival probability

$S(t)$ that it did not escape in time t.

Expect $S(t)$

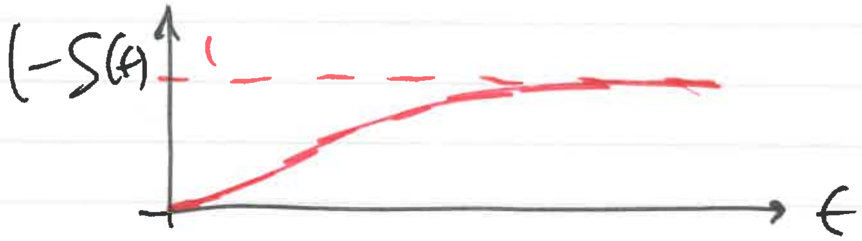


If we knew the full process probability $P(x,t)$, then

$$S(t) = \underbrace{\int_{\text{all values } x} P(x,t)\,dx}_{\text{Non-equilibrium process.}}$$

$\boxed{\int P(x,t)\,dx = 1 \text{ if normalised}}$

Then $1-S(t)$ is the probability to have escaped in time t.



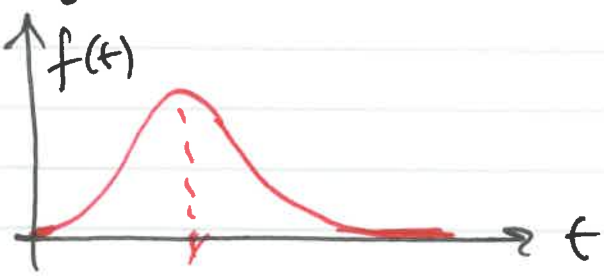
Consider a small step Δt:

$S(t) - S(t+\Delta t)$: number of escaped in Δt

Define the probability density to escape at t:

$$S(t) - S(t+\Delta t) = f(t)\cdot\Delta t$$

Hence $f(t) = -\dfrac{\partial S}{\partial t}$:



then $\langle t \rangle = \int_0^\infty t\, f(t)\, dt$

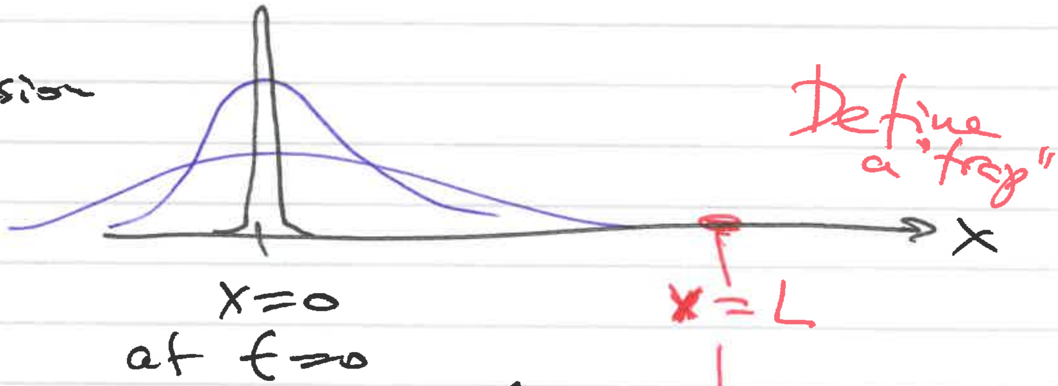
average time to escape

(by parts...)

$$\boxed{\langle t \rangle = \int S(t)\, dt}$$

Let's test a simple example

1D diffusion

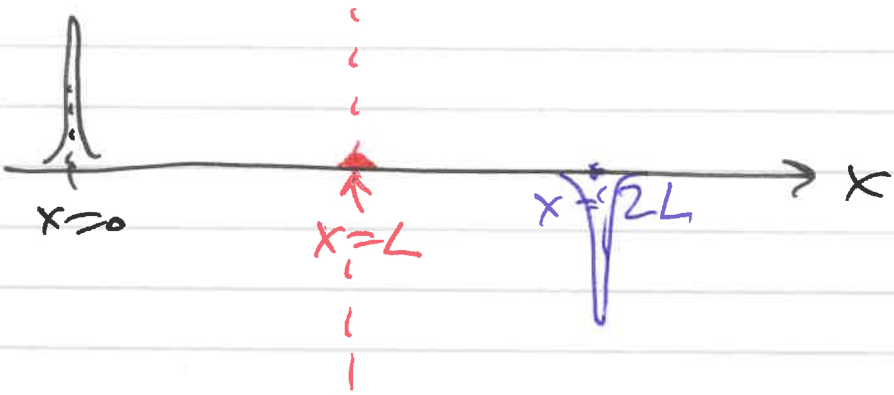


$$P(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}$$

We must find the correct $P(x,t)$ satisfying this B.C.

Absorbing Boundary Condition $P(L,t) = 0$

Here we can use Method of Images!

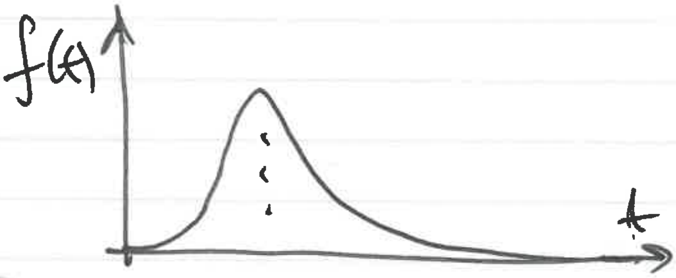


Find $P(x,t) = \frac{1}{\sqrt{4\pi D t}}\left(e^{-\frac{x^2}{4Dt}} - e^{-\frac{(x-2L)^2}{4Dt}}\right)$

Then $S(t) = \int_{-\infty}^{L} p(x,t)\,dx$ All available space!

$$\dots = \mathrm{Erf}\left[L/\sqrt{4Dt}\right]$$

Then we find $f(t) = -\frac{\partial S}{\partial t}$



$$f(t) = \frac{L}{\sqrt{4\pi D t^3}}\, e^{-\frac{L^2}{4Dt}}$$

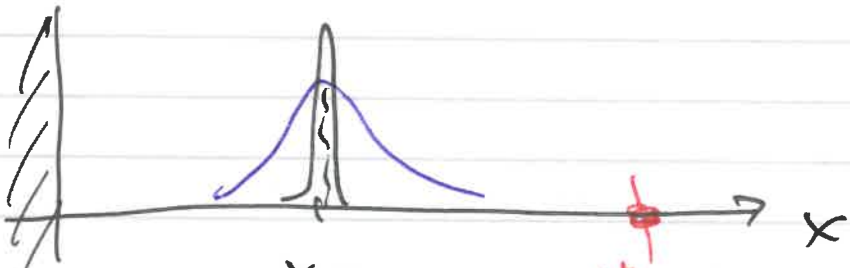
$$\text{MFPT} = \langle t \rangle = \int_0^\infty t\, \frac{L}{\sqrt{4\pi D t^3}}\, e^{-\frac{L}{4Dt}}\, dt$$

$$\sim \int^\infty \frac{1}{\sqrt{t}}\, dt \to \infty$$

This is not a well-posed problem

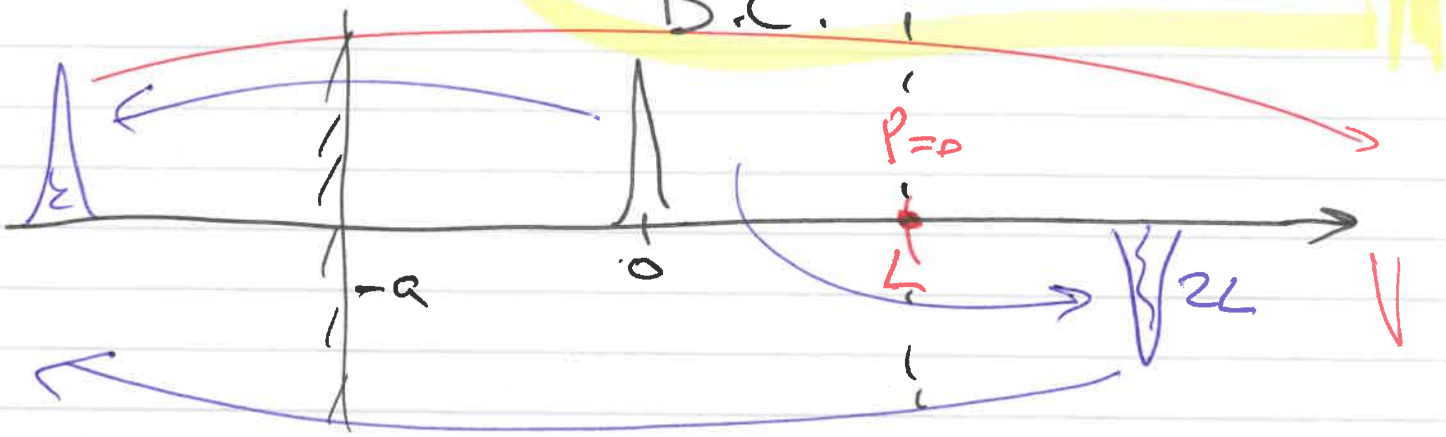
(∞ time of travel to $x \to -\infty$ and back)

Make it well-posed:



i.e. $\boxed{\dfrac{\partial p}{\partial x}=0}$

How to find $P(x,t)$ that satisfies both B.C.



⊙ Build an ∞ series of ± images reflecting $e^{-\frac{x^2}{4Dt}}$

OR...

⊙ Just solve the diffusion equation $\dot{p} = Dp''$ with these two B.C.

$\rightarrow \infty$ series of $\sum_n \sin\left(\frac{n\pi x}{L+a}\right) e^{-?Dt}$

....

Once $P(x,t)$ is found

$$\longrightarrow S(t) = \int_{-a}^{L} P(x,t)\, dx$$

All available space

$$\downarrow$$

$$MFPT = \frac{L(L+2a)}{2D}$$ for start at $x=0$

if $a=0$ | $MFPT = L^2/2D$ } Diffusion time (mean) over L

But if the initial condition is an arbitrary $x = x_0$ (at $t=0$), then MFPT is a function of x_0 (E.g. if $x_0 = L$ MFPT $= 0$)

Now a different approach to MFPT, for Wiener process.

#2: Via Adjoint Fokker-Planck operator

We saw the Smoluchowski equation (a case of Fokker-Planck equation set)

$$\boxed{\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma}\rho\right) + D\frac{\partial^2 \rho}{\partial x^2}}$$

$$\left(\text{or} \quad -\frac{\partial}{\partial x}\left(\mu(x,t)\,p\right) + \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}\right)$$

Define a Fokker-Planck operator acting on X.

$$\frac{\partial p}{\partial t} = -\hat{L}_{FP}\, P(x,t)$$

We saw the alternative form of it:

$$\hat{L}_x = D\frac{\partial}{\partial x}\left(e^{-\beta V(x)}\frac{\partial}{\partial x}\left[e^{\beta V(x)}\,p(x,t)\right]\right)$$

this operator acts on x!

$$\boxed{P(x,t) = e^{-\hat{L}_x t}\, P(x,0)}$$

If we want MFPT:

$$MFPT = \int_0^\infty S(t)\, dt$$

$$= \int_0^\infty dt \underbrace{\int dx}_{\text{vol.}} P(x,t \,|\, x_0, 0)$$

initial condition

$$\equiv \tau(x_0)$$

Could we find an equation that would return $\tau(x_0)$?

To find that, we need operators that act on the initial condition

(that's not what we are used to)

Need Kolmogorov - Chapman

$$P(x,t \,|\, x_0, 0) = \int G(x,t \,|\, y, t')\, P(y,t' \,|\, x_0, 0)\, dy$$

Here

Since $\frac{\partial P}{\partial t} = -\hat{L}_x P(x,t)$ then $\boxed{\frac{\partial G}{\partial t} = -\hat{L}_x G}$

Acting on x

Kolmogorov–Chapman

Let me differentiate w.r.t. t'

$$\frac{\partial}{\partial t'} P(x,t|x_0,0) \equiv 0$$

$$0 = \int \left[G(x,t|y,t') \boxed{\frac{\partial P(y,t'|x_0,0)}{\partial t'}} + P(y,t'|x_0,0) \frac{\partial G(x,t|y,t')}{\partial t'} \right] dy$$

$$= \int G(x,t|y,t') \cdot \left[-\hat{L}_y P(y,t'|x_0,0) \right]$$

Continue next ....

deal with this...