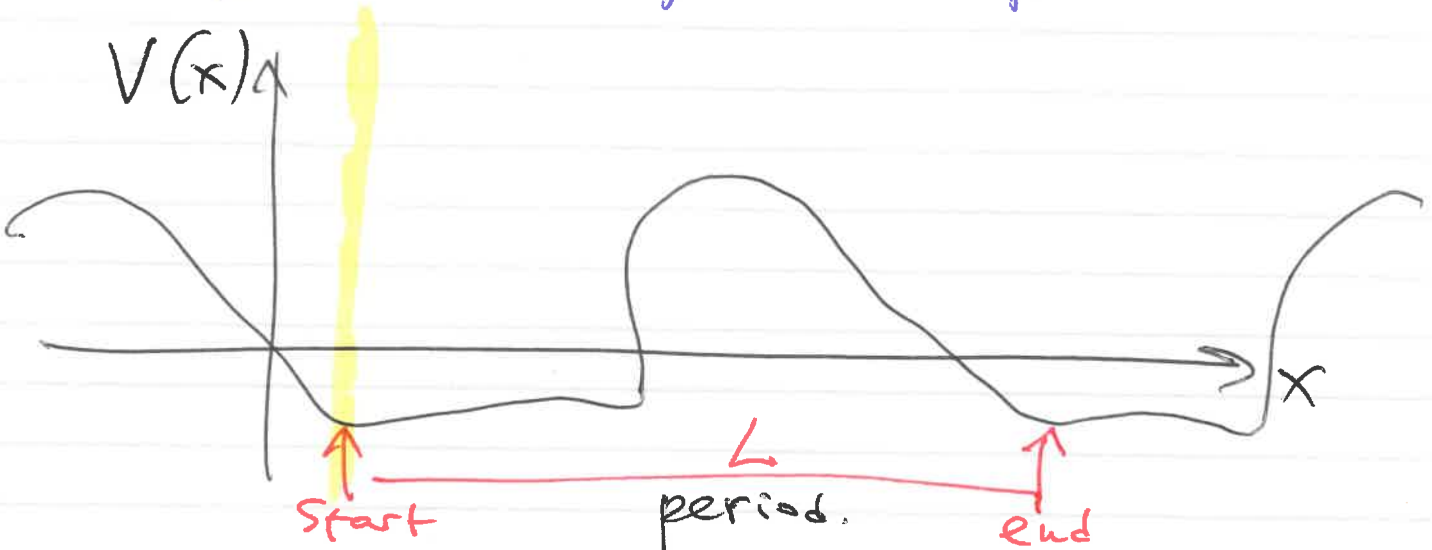
Lecture 12 – finishing MFPT ...

Diffusion in periodic potential



MFPT from "start" to "end"

$$\tau = \frac{1}{D} \int_{0}^{L} dx \, e^{\beta V(x)} \int_{0}^{x} e^{-\beta V(y)} dy$$

0 start — 0 left boundary

Define "effective diffusion" in time τ:

$$L^2 = 2 D_{eff} \cdot \tau,$$

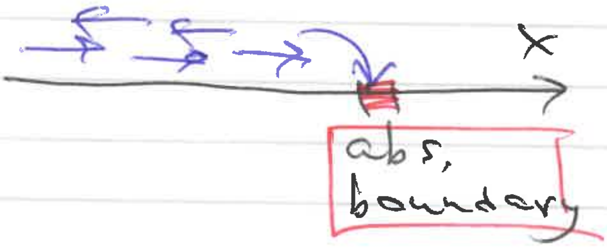
so
$$\boxed{D_{eff} = \frac{L^2}{2} D \frac{1}{\boxed{\int_0^L e^{\beta V(x)} \int_0^x e^{-\beta V(y)} dy}}}$$

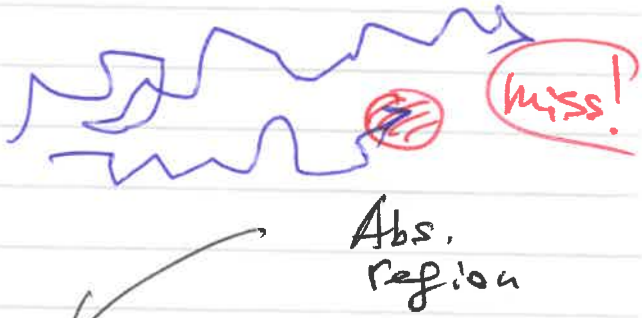
Always big...

Any potential:
$$D_{eff} \ll D$$

What we did in MFPT was strictly 1D ...

In higher-Dimensions, the issue arises!



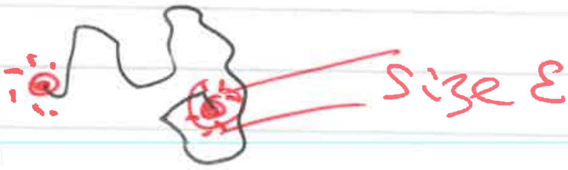


! (The MFPT must depend on the size of target.

Examples

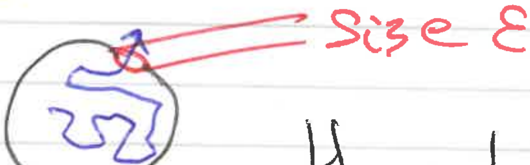
① "Forming a ring"

→ Szabo et. al. 1980



② "Narrow escape"

→ Holcman et. al. 2000



How long it takes to make contact?

MFPT: 1D $\tau \sim \frac{L^2}{D}$

2D $\tau \sim \frac{L^2}{D} \ln(1/\varepsilon)$

3D $\tau \sim \frac{L^3}{D\varepsilon}$

Last topic

"Multiplicative Noise"

i.e., $dx = \mu(x,t)\,dt + \sigma(x)\,dW$

(E.g. in GBM)

Corresponding F.-P. equation

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\mu(x,t)\cdot P\right) + \underbrace{\frac{1}{2}\frac{\partial}{\partial x^2}\left(\sigma^2(x) P\right)}_{\text{2nd Kramers-Moyal cf.}}$$

or is it

$$\longrightarrow \frac{\sigma^2(x)}{2}\frac{\partial^2 P}{\partial x^2}$$

or is it

$$\longrightarrow \frac{1}{2}\sigma(x)\frac{\partial}{\partial x}\left(\sigma(x)\frac{\partial P}{\partial x}\right)$$

$\boxed{\text{or something else}}$

Let's re-examine the Kramers-Moyal process: evaluate $\langle \Delta x^n \rangle$

$$\langle \Delta x \rangle = \int_t^{t+\Delta t} \left(\mu(s) + \sigma(s)\,\xi(s)\right) ds$$

Average in another way: time average

slow variation

$$= \mu(x,t)\,\Delta t + \sigma(x[t]) \int \xi(s)\,ds$$

$\longrightarrow 0$

Wiener ...

We need to decide at which point on interval $t \div t+\Delta t$ do we evaluate $G(x[t])$

Mathematically consistent (Itoh)

- version is: evaluate at t, (start of interval)

$$\underbrace{G(x[t])}\int_t^{t+\Delta t}\underbrace{dW}$$

Statistically independent!

- Stratonovich version: evaluate at the middle

$$\int G(x[t+\tfrac{1}{2}\Delta t])\,\xi(t)\,dt$$

- More recently: evaluate at an arbitrary point

$$G(x[t+\alpha\Delta t])$$

and compare with experiment

Itoh: $\alpha=0$

Stratonovich: $\alpha=\frac{1}{2}$

Lau-Lubensky: $\alpha=1$ (end of...)

If we follow Itoh process:

$\alpha = 0$

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}(\mu P) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left(\sigma^2(x) P\right)$$

If we follow Stratonovich process:

$\alpha = 1/2$

$$\text{———} \;\; '' \;\; \text{———} \;\; \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma(x)\frac{\partial}{\partial x}\left[\sigma(x) P\right]\right)$$

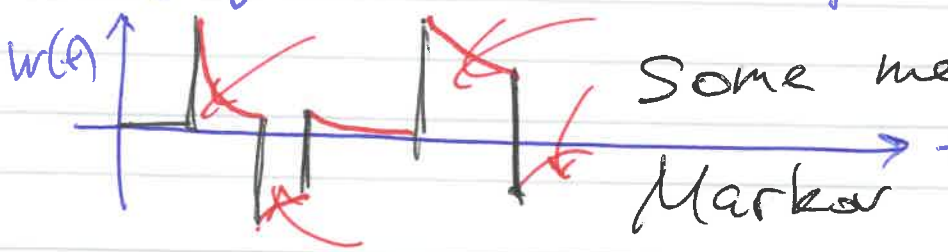
If we follow Lau-Lubensky:

$\alpha = 1$

$$\text{———} \;\; '' \;\; \text{———} \;\; \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma^2(x)\frac{\partial P}{\partial x}\right)$$

The formal accepted resolution of this is via a more careful look at the approximation leading to the Wiener process ...

Physical (e.g. thermal noise) process



Some memory?

Markov assumption

- Wong-Zakai Theorem:

applies when a physical process behind the approximate $W(t)$ is a sequence of deterministic events "W_n"

we must modify the SDE

$$dx = \left(\mu(x,t) + \underline{\tfrac{1}{2}\sigma(x)\tfrac{\partial\sigma}{\partial x}}\right)dt + \sigma(x)\,dW$$

Must have an additive drift term

We then work with proper Itoh process (statistically independent $\sigma(x)$ and dW)

$$\rightarrow \frac{\partial P(x,t)}{\partial t} = \underbrace{-\frac{\partial}{\partial x}(\mu \cdot P) - \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma\frac{\partial\sigma}{\partial x}\cdot P\right)}_{1^{st}\text{ Kramers-Moyal term}}$$

$$+ \underbrace{\frac{1}{2}\frac{\partial^2}{\partial x^2}\left(\sigma^2(x)P\right)}_{2^{nd}\text{ Kramers-Moyal}}$$

Simple algebra gives:

$$\boxed{\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big(\mu(x,t)\,P\Big) + \frac{1}{2}\frac{\partial}{\partial x}\Big[\underbrace{\sigma(x)\frac{\partial}{\partial x}\Big(\sigma(x)P\Big)}_{\text{exactly the Stratonovich version!}}\Big]}$$

When $\sigma = \text{const}$: $D = \frac{1}{2}\sigma^2$, we had

$$J = -D e^{-\beta V(x)} \frac{\partial}{\partial x}\left(e^{\beta V(x)} P(x,t)\right)$$

Now we have the flux:

$$\boxed{J = -\frac{1}{2}\sigma(x) e^{-\beta V(x)} \frac{\partial}{\partial x}\left(\sigma(x) \cdot e^{\beta V(x)} \cdot P\right)}$$

As long as we identify the "friction constant" as

$$\boxed{\gamma(x) = \frac{2kT}{\sigma^2(x)}}$$ a version of F.D.T.

then $D(x) = \frac{kT}{\gamma(x)} = \frac{1}{2}\sigma^2(x)$ is still valid.