4) Diffusion equation:

4.1) A probabilistic derivation of the diffusion eq.:

Let us consider a random walk on the line of a particle that, at time $t=0$, starts at $x=0$.
Let us suppose that:

i) at each time-step the probability of jumping to the right is $p_r = \frac{1}{2}$ $\rightsquigarrow$ the walk is symmetric!

ii) time-step τ ; space-step h

Our aim is to find an equation satisfied by the limiting probability as $\tau, h \to 0$.

We first need some preliminary computations:

let $p(x,t)$ be the probability that the particle is at position x at time t.

Suppose: $\quad t = N\tau, \quad x = mh, \quad N \in \mathbb{N}, m \in \mathbb{Z}.$

In order to reach the pt x at time t, we have to make K steps to the right and $N-K$ to the left, where: $K = \frac{1}{2}(N+m)$ $\quad [m = K-(N-K)]$

The number of such a paths is

$$C_{N,K} = \frac{N!}{K!(N-K)!}.$$

The number of total paths is 2^N.

Before passing to the limit for $h, \tau \to 0$, we have to decide a scaling for them. For, we decide that we want to keep some properties of the random walk, mainly:

- the average of x after N steps
- the variance [recall that the standard deviation]

We see that:
- the average is $\langle x \rangle = \langle m \rangle h$
- the variance is $\langle (x - \langle x \rangle)^2 \rangle$

Now:

$$\langle m \rangle = 2 \langle K \rangle - N.$$

To find $\langle K \rangle$ we reason as follows:

$$\langle K \rangle = \sum_{K=1}^{N} K \frac{C_{N,K}}{2^N} = G'(1), \text{ where}$$

$$G(s) := \frac{1}{2^N} \sum_{K=1}^{N} C_{N,K}\, s^K = \frac{1}{2^N}(1+s)^N$$

Thus:

$$G'(s) = \frac{1}{2^N} \sum_{K=1}^{N} K\, C_{N,K}\, s^{K-1} = \frac{N}{2^N}(1+s)^{N-1}$$

$$\Downarrow$$

$$\langle K \rangle = G'(1) = \frac{N}{2}$$

$$\Downarrow$$

$$\langle m \rangle = 0$$

$$\Downarrow$$

$$\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle = \langle m^2 \rangle h^2$$

To find $\langle K^2 \rangle$, we use the fact that:

$$G''(s) = \frac{1}{2^N} \sum_{K=1}^{N} K(K-1) C_{N,K}\, s^{K-2} = \frac{N(N-1)}{2^N} (1+s)^{N-2}$$

$$\Downarrow$$

$$\frac{N(N-1)}{4} = G''(1) = \frac{1}{2^N} \sum_{K=1}^{N} K(K-1) C_{N,K}$$

$$= \frac{1}{2^N} \sum_{K=1}^{N} K^2 C_{N,K} - \frac{1}{2^N} \sum_{K=1}^{N} K C_{N,K}$$

$$= \langle K^2 \rangle - \langle K \rangle$$

$$\Rightarrow \quad \langle K^2 \rangle = \frac{(N-1)N}{4} + \langle K \rangle =$$

$$= \frac{(N-1)N}{4} + \frac{N}{2} = \frac{N(N+1)}{4}$$

So, we have that:

$$\langle m^2 \rangle = 4\langle K^2 \rangle - 4N\langle K \rangle + N^2$$
$$= N^2 + N - 2N^2 + N^2 = N \quad \Rightarrow \boxed{\sqrt{\langle x^2 \rangle} = \sqrt{N}\, h}$$

after $N\tau$ time-steps, the average distance from the origin is $\sqrt{N}\, h$

space $\sim \sqrt{\text{time}}$

$$\Downarrow$$

$$\boxed{h^2 \sim \tau}$$

We can now derive the limiting eq.: we have that

$$p(x,t+\tau) = \frac{1}{2}p(x-h,\tau) + \frac{1}{2}p(x+h,\tau).$$

By using Taylor's expansion:

- $p(x,t+\tau) = p(x,t) + p_t(x,t)\tau + o(\tau)$
- $p(x\pm h,t) = p(x,t) \pm p_x(x,t)\,h + \frac{1}{2}p_{xx}(x,t)\,h^2 + o(h^2)$

$$\Downarrow$$

$$p_t\,\tau + o(\tau) = \frac{1}{2}p_{xx}\,h^2 + o(h^2)$$

$$\Updownarrow$$

$$p_t + o(1) = \frac{1}{2}\frac{h^2}{\tau}p_{xx} + o\left(\frac{h^2}{\tau}\right)$$

Assume: $\boxed{\frac{h^2}{\tau} \to 2D}$, where D is called the <u>diffusion coefficient</u>

$$\boxed{\frac{h^2}{\tau} = \frac{\langle x^2\rangle}{t}} \to \text{the average distance per unit time is } \sqrt{2D}$$

$$\boxed{\begin{cases} p_t - D\,p_{xx} = 0 \\ p(x,0) = \delta(x) \end{cases}}$$

the <u>diffusion equation</u>

• **Note:** the limiting velocity of the particle is the limit

$$\frac{h}{\tau} = \underbrace{\frac{h^2}{\tau}}_{\to 2D} \frac{1}{h} \to +\infty \implies \boxed{\text{the velocity of the particle is } +\infty}$$

Not physical!

• Note: since the fundamental solution has exponential decay at ∞, this can still be used as an approximation of diffusion processes!

(*) 4.2.1)

4.2) Derivation of the heat Kernel:

4.2.1) A probabilistic derivation of the heat Kernel

We would like to find the limit of the probability $p_{h,\tau}$ as $h, \tau \to 0^+$, with $\frac{h^2}{\tau} \to 2D$.

For, $\boxed{\text{fix}}$ $x = mh$ and $t = N\tau$. Then:

$$p_{h,\tau}(x,t) = \begin{cases} \frac{C_{N,k}}{2^N} & \text{if } N+m \text{ is even,} \\ 0 & \text{otherwise.} \end{cases}$$

Let us recall that $k = \frac{m+N}{2}$, $C_{N,k} = \frac{N!}{k!(N-k)!}$.

When $h, \tau \to 0^+ \implies N \to +\infty$, $k \to +\infty$.

Thus, let us recall Stirling's formula:

$$\boxed{m! \sim \sqrt{2\pi m} \left(\frac{m}{e}\right)^m.}$$

So:

• $N! \sim \sqrt{2\pi N} \left(\frac{N}{e}\right)^N$

• $k! = \left(\frac{N+m}{2}\right)! \sim \sqrt{\pi(N+m)} \left(\frac{N+m}{2e}\right)^{\frac{N+m}{2}}$

• $(N-k)! = \left(\frac{N-m}{2}\right)! \sim \sqrt{\pi(N-m)} \left(\frac{N-m}{2e}\right)^{\frac{N-m}{2}}$

• $N = \frac{t}{\tau} = \frac{h^2}{\tau}\frac{t}{h^2} \sim \frac{t}{h^2} 2D$

• $m = \frac{x}{h}$

$\implies \boxed{N - m \xrightarrow[h \to 0]{} +\infty}$

Assume $N+m$ even. Then:

$$P_{h,\tau}(x,t) = \frac{1}{2^N}\frac{N!}{K!\,(N-K)!}$$

$$\sim \frac{1}{2^N}\sqrt{2\pi N}\left(\frac{N}{e}\right)^N \cdot \frac{1}{\sqrt{\pi(N+m)}\left(\frac{N+m}{2e}\right)^{\frac{N+m}{2}}}$$

$$\cdot \frac{1}{\sqrt{\pi(N-m)}\left(\frac{N-m}{2e}\right)^{\frac{N-m}{2}}}$$

$$= \left(\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{\frac{N+m}{2}}\sqrt{\frac{N-m}{2}}}\right)\cdot\left(\frac{1}{\left(1-\frac{m^2}{N^2}\right)^{N/2}}\right)\cdot\left(\frac{1}{\left(1+\frac{m}{N}\right)^{\frac{m}{2}}\left(1-\frac{m}{N}\right)^{-\frac{m}{2}}}\right)$$

Let us analyze each term separately.
Recall that,

$$N \sim \frac{t}{h^2}\,2D$$

$$m = \frac{x}{h}$$

So:

- $$\frac{1}{\sqrt{2\pi}} \frac{\sqrt{N}}{\sqrt{\frac{N+m}{2}}\sqrt{\frac{N-m}{2}}} = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{N}}{\sqrt{\frac{1}{4}(N^2-m^2)}}$$

$$\sim \frac{1}{\sqrt{2\pi}} \frac{\sqrt{2Dt}}{h} \frac{1}{\sqrt{\frac{1}{4}\left(\frac{t^2}{h^4}4D^2 - \frac{x^2}{h^2}\right)}}$$

$$= \sqrt{\frac{Dt}{\pi}} \cdot \frac{h}{\sqrt{t^2D^2 - h^2x^2}} \sim \frac{h}{\sqrt{Dt\pi}}$$

t and x are fixed; $h \to 0$

- $$\left(1 - h^2\frac{x^2}{4D^2t^2}\right)^{\frac{t}{h^2}D} = \underbrace{\left(1 - h^2\frac{x^2}{4D^2t^2}\right)^{\frac{1}{h^2}\frac{4D^2t^2}{x^2}}}\cdot\frac{x^2}{4tD}$$

$$s := h^2\frac{x^2}{4D^2t^2} \rightsquigarrow (1-s)^{\frac{1}{s}\frac{x^2}{4tD}} \xrightarrow[s\to 0]{} e^{-\frac{x^2}{4tD}}$$

- $$\left(1 + h\frac{x}{2Dt}\right)^{\frac{x}{2h}} = \underbrace{\left(1 + h\frac{x}{2Dt}\right)^{\frac{2Dt}{hx}}}\cdot\frac{x^2}{4Dt}$$

$$s := h\frac{x}{2Dt} \rightsquigarrow (1+s)^{\frac{1}{s}\frac{x^2}{4Dt}} \longrightarrow e^{+\frac{x^2}{4Dt}}$$

- $$\left(1 - h\frac{x}{2Dt}\right)^{-\frac{x}{2h}} \longrightarrow e^{-\frac{x^2}{4Dt}}$$

Thus:

$$p_{h,\tau}(x,t) \sim \frac{h}{\sqrt{2\pi D t}} e^{-\frac{x^2}{4Dt}}.$$

Of course, if we simply let $h \to 0$, we get $p_{h,\tau} \equiv 0$. This is because, when passing to the limit, we have to consider no more the probability of being in a specific pt, but the probability of being in an interval (a,b). So, let us fix an interval (a,b) and, for each h, let I_h be the set of pts $x_i = mh \in (a,b)$, for some $m \in \mathbb{Z}$. Then:

$$p_{h,\tau}(x \in (a,b), t) = \sum_{i \in I_h} p_{h,\tau}(x_i, t) \sim$$

$$\sim \sum_{i \in I_h} h \frac{1}{\sqrt{\pi D t}} e^{-\frac{x_i^2}{4Dt}}$$

$$\xrightarrow{h \to 0^+} \int_a^b \frac{1}{\sqrt{\pi D t}} e^{-\frac{x^2}{4Dt}} dx$$

this is a <u>Riemann sum</u>:

$$\int_a^b f(x)\,dx \sim \sum_{i \in I} h f(x_i)$$

Thus, the limiting probability, recalling that $p_{h,\tau} = 0$ if $N+m$ is odd, turns out to be:

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

the <u>heat Kernel</u>