Diffusion equation

Fick's law's

(1.) Material never disappears.

$$\frac{\partial \rho(\vec{r},t)}{\partial t} + \nabla \cdot \vec{J} = 0$$

flux

(2.) Current flows from region of higher concentration to a lower concentration.

$$\Rightarrow \quad \vec{J} \propto -\nabla \rho(\vec{r},t).$$

$$\therefore \quad \vec{J} = -D \nabla \rho(\vec{r},t)$$

Thus, $$\frac{\partial \rho(\vec{r},t)}{\partial t} = D \nabla^2 \rho(\vec{r},t).$$

- Irreversibility ; 1^{st} order in time
- Parabolic partial differential equation.
- Diffusion eqn. $\longleftrightarrow$ Random walk problem

Diffusion eqn. in d-dimensional space

Boundary conditions: $\rho(\vec{r},t) \to 0$ as $r \to \infty$.

Initial condition: $\rho(\vec{r},0) = \delta^{(d)}(\vec{r})$ $\Big\}$ — (I)

for

$$\frac{\partial \rho(\vec{r},t)}{\partial t} = D\nabla^2 \rho(\vec{r},t). \quad \text{— (II)}$$

$$\mathcal{L}[\rho(\vec{r},t)] = \tilde{\rho}(\vec{r},s). \quad \text{— (III)}$$

Take Laplace transform on both sides

$$\Rightarrow \quad s\,\tilde{\rho}(\vec{r},s) - \rho(\vec{r},0) = D\nabla^2\tilde{\rho}(\vec{r},s) \quad \text{— (IV)}$$

$$\Rightarrow \quad (s - D\nabla^2)\,\tilde{\rho}(\vec{r},s) = \delta^{(d)}(\vec{r}). \quad \text{— (V)}$$

Fourier transform:

$$\tilde{\Phi}(\vec{k},s) = \int d^d r\, e^{-i\vec{k}\cdot\vec{r}}\,\tilde{\rho}(\vec{r},s) \,;\quad \tilde{\rho}(\vec{r},s) = \frac{1}{(2\pi)^d}\int d^d k\,\tilde{\rho}(\vec{k},s)\,e^{i\vec{k}\cdot\vec{r}}. \quad \text{— (VI)}$$

Implementing Fourier transform on eqn.

$$\therefore \quad (s + Dk^2)\,\tilde{\rho}(\vec{k},s) = 1. \quad \text{— (VII)}$$

$$\therefore \quad \tilde{\rho}(\vec{k},s) = \frac{1}{s + Dk^2}. \quad \text{— (VIII)}$$

If we take inverse Fourier transform first, we will come across various complications.

Lets take inverse Laplace transform first.

$$\Rightarrow \tilde{\rho}(\vec{k}, t) = \mathcal{L}^{-1}\left[\frac{1}{s+Dk^2}\right] = e^{-Dk^2t} \quad \text{—} \boxed{IX}$$

$$\left(\because \int_0^\infty \frac{1}{s+a} e^{st} ds = e^{-at}. \right)$$

Taking inverse Fourier transform on both sides,

$$\rho(\vec{r}, t) = \frac{1}{(2\pi)^d} \int d^dk \, e^{i\vec{k}\cdot\vec{r}} e^{-Dk^2t}.$$

$$= \left\{ \left(\frac{1}{2\pi}\right) \int_{-\infty}^{\infty} dk_1 \, e^{ik_1x_1 - Dk_1^2t} \right\} \cdots \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_d e^{ik_dx_d - Dk_d^2t} \right\}$$

$$\text{—} \boxed{X}$$

Consider the integral $\frac{1}{2\pi}\int_{-\infty}^{\infty} dk_1\, e^{ik_1x_1 - Dk_1^2 t}$.

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk_1\, e^{-Dt\left(k_1^2 - \frac{ik_1x_1}{Dt} + \left(\frac{ix_1}{2Dt}\right)^2 - \left(\frac{ix_1}{2Dt}\right)^2\right)}$$

$$= \frac{1}{2\pi} e^{-\frac{x_1^2}{4Dt}} \int_{-\infty}^{\infty} dk_1\, e^{-Dt\left(k_1 - \frac{ik_1x_1}{Dt}\right)^2}$$

$$= \frac{1}{2\pi} e^{-\frac{x_1^2}{4Dt}} \sqrt{\frac{\pi}{Dt}}$$

$$= \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x_1^2}{4Dt}} \quad \text{— XI:}$$

There are d-such terms in the product.

$$\therefore \quad \rho(\vec{r}, t) = \frac{1}{(4\pi Dt)^{d/2}} e^{-\frac{r^2}{4Dt}} ;$$

XII:

$$\left(\because \sum_i x_i^2 = r^2.\right)$$

$$\left.\begin{aligned} \langle r(t)\rangle &= 0 \\ \langle r^2(t)\rangle &= \sum_i \langle x_i^2\rangle = 2dDt. \end{aligned}\right\} \text{— XIII:}$$

$$\therefore \sigma \propto \sqrt{t}.$$

XIV: