

How a non-equilibrium system evolve over time

Theory of diffusion

2 assumptions

1. A substance will move down to its concentration gradient (Fick's first law)

$$\vec{J} = -D \nabla C \rightarrow \text{concentration} \quad 1D: J = -D \frac{\partial C}{\partial x}$$

↓
flux
diffusion
constant

2. conservation of matter

$$\frac{\partial C}{\partial t} = -\nabla \cdot \vec{J} \quad 1D: \frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}$$

↓
divergence

All together, we get Diffusion equation

$$\frac{\partial C}{\partial t} = D \nabla^2 C \quad 1D: \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

↓
Laplacian
operator

Diffusion equation: a partial differential equation
how a spatial distribution of material changes over time

Define solution $\begin{cases} \text{initial conditions} \\ \text{boundary conditions} \end{cases}$

One-dimensional diffusion from a point

Initial conditions: $C = M \underbrace{\delta(x)}_{[L]} @ t=0$ which means $\int_{-\infty}^{\infty} C(x) dx = M$

boundary conditions: length = ∞

Brown part: If not familiar with complex form of Fourier transformation

Periodic functions: expand to Fourier series

Non-periodic functions: functions of no period \Rightarrow Fourier integrals
frequency: $0 \rightarrow \infty$

$$F(x) = \int_0^{\infty} A(s) \sin(xs) ds + \int_0^{\infty} B(s) \cos(xs) ds \quad \text{where} \quad \begin{cases} A(s) = \frac{1}{\pi} \int_{-\infty}^{\infty} F(x) \sin(xs) dx \\ B(s) = \frac{1}{\pi} \int_{-\infty}^{\infty} F(x) \cos(xs) dx \end{cases}$$

$$\begin{cases} \cos(xs) = \frac{1}{2}(e^{ixs} + e^{-ixs}) \\ \sin(xs) = \frac{1}{2i}(e^{ixs} - e^{-ixs}) \end{cases}$$

$$F(x) = \int_0^{\infty} \frac{1}{2} [B(s) - iA(s)] e^{ixs} ds + \int_0^{\infty} \frac{1}{2} [B(s) + iA(s)] e^{-ixs} ds$$

$$\downarrow$$

$$\int_0^{\infty} \frac{1}{2} [A(|w|) + iB(|w|)] e^{isx} ds$$

$$\text{set } G(s) = \begin{cases} \frac{1}{2}[B(w) - iA(w)] & (s \geq 0) \\ \frac{1}{2}[B(|w|) + iA(|w|)] & (s < 0) \end{cases}$$

$$F(x) = \int_{-\infty}^{\infty} G(s) e^{ixs} ds \quad \text{transformation between two domains: } (x, s)$$

Fourier integrals in complex form

$$F(x) = \int_{-\infty}^{\infty} G(s) e^{ixs} ds$$

$$\text{For } s \geq 0, \quad G(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) [\cos(xs) - i\sin(xs)] dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) e^{-ixs} dx$$

$$\text{For } s < 0, \quad G(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) [\cos(|s|x) + i\sin(|s|x)] dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) e^{ixs} dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) e^{-ixs} dx$$

$$\int_{-\infty}^{\infty} F(x) e^{-ixs} dx = 2\pi \int_{-\infty}^{\infty} G(s) g(s-s') ds$$

(A3.10) should be

$$G(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(x) e^{-ixs} dx$$