Topics in Computational Science Report
Diffusion Equation

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1. Suppose a Diffusion Equation in 1D defined by:

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} \tag{1}$$

with initial position (assumption), $x = 0$, the solution for (1) defined by:

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

Show that (2) is the solution for (1)!

Answer:

First, taking first order partial time derivative of (2) we get,

$$\begin{aligned}
\rho_t(x,t) = \frac{\partial \rho(x,t)}{\partial t} &= -\frac{1}{2}4\pi D(4\pi Dt)^{-\frac{3}{2}}e^{-\frac{x^2}{4Dt}} + (4\pi Dt)^{-\frac{1}{2}}\frac{x^2}{(4Dt)^2}4De^{-\frac{x^2}{4Dt}} \\
&= \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\left(-\frac{1}{2}4\pi D\frac{1}{4\pi Dt} + \frac{x^2}{(4Dt)^2}4D\right) \\
&= \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\left(-\frac{1}{2t} + \frac{x^2}{4Dt^2}\right)
\end{aligned} \tag{3}$$

Then, taking first order partial space derivative of (2) we get,

$$\begin{aligned}
\rho_x(x,t) = \frac{\partial \rho(x,t)}{\partial x} &= -\frac{1}{\sqrt{4\pi Dt}}\frac{2x}{4Dt}e^{-\frac{x^2}{4Dt}} \\
&= -\frac{1}{\sqrt{4\pi Dt}}\frac{x}{2Dt}e^{-\frac{x^2}{4Dt}}
\end{aligned} \tag{4}$$

After that, we take partial space derivative of (4) we get,

$$\begin{aligned}
\frac{\partial \rho_x(x,t)}{\partial x} = \frac{\partial^2 \rho(x,t)}{\partial x^2} &= -\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\frac{1}{2Dt} + \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\frac{x^2}{(2Dt)^2} \\
&= \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\frac{1}{2Dt}\left(-1 + \frac{x^2}{2Dt}\right)
\end{aligned} \tag{5}$$

Substitute (5) and (3) into (1) we have,

$$
\begin{aligned}
\frac{\partial \rho(x,t)}{\partial t} &= D\frac{\partial^2 \rho(x,t)}{\partial x^2} \\
\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\Big(-\frac{1}{2t}+\frac{x^2}{4Dt^2}\Big) &= D\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\frac{1}{2Dt}\Big(-1+\frac{x^2}{2Dt}\Big) \\
\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\Big(-\frac{1}{2t}+\frac{x^2}{4Dt^2}\Big) &= \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\frac{1}{2t}\Big(-1+\frac{x^2}{2Dt}\Big) \\
\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\Big(-\frac{1}{2t}+\frac{x^2}{4Dt^2}\Big) &= \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\Big(-\frac{1}{2t}+\frac{x^2}{4Dt^2}\Big)
\end{aligned}
\tag{6}
$$

By (6) we have shown that (2) satisfies equation (1), therefore it is proved that (2) is the solution of (1).

2. What did you study in the Topics in Computational Science Class (Professor Nagao Course)?

Answer:

In this class, we study about the behaviour of particle as a single and many particle system. As a single particle system, the particle moves to the other side with probability P and the moves is a random walk with average of $\langle x(t)\rangle = 0$. Movement of a particle system also can be explained by Langevin Equation defined by:

$$m\frac{d^2x}{dt^2} = F - \varsigma\frac{dx}{dt} + \xi(t) \tag{7}$$

with:

(a) $m\frac{d^2x}{dt^2}$: Newton's Equation of Motion
(b) $\varsigma\frac{dx}{dt}$: Frictional force proportional to velocity
(c) $\xi(t)$: Random force (on Brownian dynamics)

and average of the Random force, $\langle\xi(t)\rangle = 0$ and ς is a constant number. While many particle system can be explained by Fick's Law with flux defined by:

$$J(x,t) = \rho(x,t)\left\langle\frac{dx}{dt}\right\rangle = \rho(x,t)\frac{F(x,t)}{\varsigma} \tag{8}$$

and Gradient of distribution of particle (density) is

$$J(x,t) = -D\frac{\partial\rho(x,t)}{\partial x} + \frac{F(x,t)}{\varsigma}, \quad F = 0 \rightarrow \text{Fick's law} \tag{9}$$

We also learn about Smoluchowski's equation which is an extension from the diffusion equation. At the last lecture, we also learn about the non-equilibrium system for example: biological system and cell universe. We can classify the non-equilibrium system by the relaxation process and the open system.

By relaxation process, we can classify non-equilibrium system into:

(a) Linear relaxation process $\Rightarrow$ fluctuation-dissipation theorem holds.
(b) Non-linear relaxation process : Internal degree of freedom

By the open system, non-equilibrium classified into:

(a) Non-equilibrium steady state : steady state presence of gradient of temperature, or density, or pressure.
(b) Non-equilibrium unsteady state : Distribution change with time.