Analytical solution of Fourier/Fick's 2nd law (heat/diffusion equation)

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1 Diffusion by random walk

In a 1D transport, the net flux from plane 1 to plane 2 is

$$J = \Gamma_0 n_1 - \Gamma_0 n_2, \tag{1.1}$$

where Γ_0 is the jump rate between Planes 1 and 2, and n_1 and n_2 are the numbers of atoms on the two planes. The lattice plane distance between the two planes is λ. Thus, the concentrations on the two planes are

$$C_1 = \frac{n_1}{\lambda} \quad \text{and} \quad C_2 = \frac{n_2}{\lambda}. \tag{1.2}$$

Equation (1.1) is rewritten as

$$J = \Gamma_0 \lambda \big(C_1 - C_2 \big) = -\Gamma_0 \lambda^2 \frac{C_2 - C_1}{\lambda}. \tag{1.3}$$

When λ is very small, we obtain

$$J = -D \lim_{\lambda \to 0} \frac{C_2 - C_1}{\lambda} = -D \frac{\partial C}{\partial x}, \tag{1.4}$$

which is Fick's 1st law of diffusion, where $D = \Gamma_0 \lambda^2$ is the diffusion coefficient (or diffusivity). Note that an atom can jump in either positive or negative directions. Thus, Γ_0 is related to atoms' total jump rate (Γ) by

$$\Gamma_0 = \frac{\Gamma}{2}, \tag{1.5}$$

which leads to the diffusivity as

$$D = \frac{\Gamma \lambda^2}{2}. \tag{1.6}$$

In random walk, the number of processes that a walker landed at m position after a n number of jumps is

$$\Omega(n, m) = \frac{n!}{\big(\frac{n+m}{2}\big)! \big(\frac{n-m}{2}\big)!}. \tag{1.7}$$

The above expression is obtained by the following.

$$n = n_+ + n_- \quad \text{and} \quad m = n_+ - n_-,$$

where n_+ and n_- are the forward and backward jumps, respectively. Such that

$$n_+ = \frac{n+m}{2} \quad \text{and} \quad n_- = \frac{n-m}{2}.$$

$$\Omega = \frac{n!}{n_+!n_-!} = \frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!}.$$

The probability of finding a walker at location m is

$$P(n,m) = \left(\frac{1}{2}\right)^n \frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!}, \tag{1.8}$$

where the factor of $(1/2)^n$ originates from there are two possible results of each jump. We take logarithm of P:

$$\ln P = \ln\left(\frac{1}{2}\right)^n + \ln n! - \ln\left(\frac{n+m}{2}\right)! - \ln\left(\frac{n-m}{2}\right)!. \tag{1.9}$$

For large numbers of n and m, we can use

Stirling approximation:

$$\ln n! = n\ln n - n$$

to obtain

$$\begin{aligned}\ln P \approx n\ln\left(\frac{1}{2}\right) &+ n\ln n - n - \\ &\left[\left(\frac{n+m}{2}\right)\ln\left(\frac{n+m}{2}\right) - \frac{n+m}{2}\right] - \\ &\left[\left(\frac{n-m}{2}\right)\ln\left(\frac{n-m}{2}\right) - \frac{n-m}{2}\right],\end{aligned} \tag{1.10}$$

which can be reorganized to

$$\begin{aligned}\ln P \approx -\cancel{n\ln 2} &+ n\ln n - \cancel{n} \\ &-\left(\frac{n+m}{2}\right)\ln(n+m) + \cancel{\left(\frac{n+m}{2}\right)\ln 2} + \cancel{\frac{n+m}{2}} \\ &-\left(\frac{n-m}{2}\right)\ln(n-m) + \cancel{\left(\frac{n-m}{2}\right)\ln 2} + \cancel{\frac{n-m}{2}},\end{aligned} \tag{1.11}$$

i.e.,

$$\ln P \approx n\ln n - \frac{n+m}{2}\ln(n+m) - \frac{n-m}{2}\ln(n-m). \tag{1.12}$$

We then use

Taylor series

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} + ...$$

for $|x| \ll 1$.

such that

$$\ln(n+m) = \ln n\left(1 + \frac{m}{n}\right) = \ln n + \ln\left(1 + \frac{m}{n}\right) \approx \ln n + \frac{m}{n} - \frac{1}{2}\left(\frac{m}{n}\right)^2 \tag{1.13}$$

$$\ln(n-m) = \ln n\left(1 - \frac{m}{n}\right) = \ln n + \ln\left(1 - \frac{m}{n}\right) \approx \ln n - \frac{m}{n} - \frac{1}{2}\left(\frac{m}{n}\right)^2 \tag{1.14}$$

Thus, we can write

$$\begin{aligned}
\ln P &\approx \cancel{n\ln n} - \left(\frac{n+m}{2}\right)\left[\cancel{\ln n} + \frac{m}{n} - \frac{1}{2}\left(\frac{m}{n}\right)^2\right] - \left(\frac{n-m}{2}\right)\left[\cancel{\ln n} - \frac{m}{n} - \frac{1}{2}\left(\frac{m}{n}\right)^2\right] \\
&\approx -\left(\frac{n+m}{2}\right)\frac{m}{n} + \left(\frac{n+m}{2}\right)\frac{1}{2}\left(\frac{m}{n}\right)^2 + \left(\frac{n-m}{2}\right)\frac{m}{n} + \left(\frac{n-m}{2}\right)\frac{1}{2}\left(\frac{m}{n}\right)^2 \\
&\approx -\frac{m^2}{n} + n\frac{1}{2}\left(\frac{m}{n}\right)^2 = -\frac{m^2}{2n}.
\end{aligned} \tag{1.15}$$

Taking exponential of P, we obtain

$$P = \mathcal{A}\exp\left(-\frac{m^2}{2n}\right), \tag{1.16}$$

where

$$m = \frac{x}{\lambda} \quad \text{and} \quad n = \Gamma t = \frac{2D}{\lambda^2}t, \tag{1.17}$$

such that

$$P = \mathcal{A}\exp\left(-\frac{x^2}{4Dt}\right). \tag{1.18}$$

The normalization factor is obtained by

$$\int_{-\infty}^{\infty} P dx = 1 \implies \mathcal{A}\int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4Dt}\right)dx = 1 \implies A\left(\frac{\pi}{1/4Dt}\right)^{\frac{1}{2}} = 1 \implies A = \frac{1}{2\sqrt{\pi Dt}}. \tag{1.19}$$

Finally, we obtain

$$P = \frac{1}{2\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right). \tag{1.20}$$

which shows a **Gaussian distribution** of walkers in the x direction. This result indicates that a true random process will always lead to a Gaussian (normal) distribution.

We have used

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \left(\frac{\pi}{a}\right)^{\frac{1}{2}}$$

to obtain the value of $\mathcal{A}$.

2 Heat equation (diffusion equation)

The heat equation for heat conduction derived by Joseph Fourier in 1D reads as

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}. \tag{2.1}$$

For mass transport via diffusion, the governing equation is

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}. \tag{2.2}$$

These two equations have an identical form, i.e., mathematically there is no difference between them. Let us just use diffusion equation in the following derivation. It can be seen that this equation contains two independent variables: time (t) and space (x). To analytically solve it, we will start with separation of variables. Assuming the solution contains two independent functions: one for time and the other for space:

$$C(x,t) = X(x)T(t). \tag{2.3}$$

Here, $T(t)$ simply indicates a function of time, not temperature. Substituting Eq. (2.3) to Eq. (2.2), we obtain

$$X \frac{dT}{dt} = DT \frac{d^2 X}{dx^2}. \tag{2.4}$$

Dividing by XT, we get

$$\frac{1}{T}\frac{dT}{dt} = D \frac{1}{X}\frac{d^2 X}{dx^2}. \tag{2.5}$$

For this equation to remain valid, the right-hand side and the left-hand side must be equal to a separation constant. Here, we define

$$\frac{1}{T}\frac{dT}{dt} = -k^2 D \quad \Longrightarrow \quad \frac{dT}{T} = -k^2 D dt. \tag{2.6}$$

Taking integration, we have

$$\int \frac{dT}{T} = \int -k^2 D dt \quad \Longrightarrow \quad \ln T = -k^2 D t. \tag{2.7}$$

Then, we obtain the solution of the temporal part as

$$T = e^{-k^2 D t}. \tag{2.8}$$

For the spatial part, we have

$$D \frac{1}{X}\frac{d^2 X}{dx^2} = -k^2 D \quad \Longrightarrow \quad \frac{d^2 X}{dx^2} = -k^2 X, \tag{2.9}$$

for which, the analytical solution has a form of

$$X(x) = A\cos(kx) + B\sin(kx), \tag{2.10}$$

where k is the frequency. For the different values of k, the solution of C can be

$$C(x,t) = \sum_{k=1}^{\infty} \big[A(k)\cos(kx) + B(k)\sin(kx)\big] e^{-k^2Dt}. \tag{2.11}$$

At $t = 0$, we have the initial concentration profile as

$$C(x,0) = \sum_{k=1}^{\infty} \big[A(k)\cos(kx) + B(k)\sin(kx)\big]. \tag{2.12}$$

These A and B are Fourier coefficients and can be obtained using the Fourier transform:

$$A(k) = \frac{2}{L}\int_{-L/2}^{L/2} f(x')\cos(kx')dx', \tag{2.13}$$

$$B(k) = \frac{2}{L}\int_{-L/2}^{L/2} f(x')\sin(kx')dx', \tag{2.14}$$

where $f(x) = C(x,0)$ is the initial condition. Thus, Eq. (2.11) becomes

$$C(x,t) = \sum_{k=1}^{\infty}\left[\frac{2}{L}\int_{-L/2}^{L/2} f(x')\cos(kx')\cos(kx)dx' + \frac{2}{L}\int_{-L/2}^{L/2} f(x')\sin(kx')\sin(kx)dx'\right] e^{-k^2Dt}. \tag{2.15}$$

Use the following trigonometry formulae:

$$\cos(a)\cdot\cos(b) = \frac{1}{2}\big[\cos(a-b) + \cos(a+b)\big], \tag{2.16}$$

$$\sin(a)\cdot\sin(b) = \frac{1}{2}\big[\cos(a-b) - \cos(a+b)\big], \tag{2.17}$$

Eq. (2.15) becomes

$$C(x,t) = \sum_{k=1}^{\infty}\frac{2}{L}\int_{-L/2}^{L/2} f(x')\cos k(x'-x)dx'e^{-k^2Dt} = \frac{2}{L}\int_{-L/2}^{L/2} f(x')\sum_{k=1}^{\infty}\cos k(x'-x)e^{-k^2Dt}dx'. \tag{2.18}$$

A full wave length is L in length or 2π in radian, such that $2/L = 1/\pi$. We then have

$$C(x,t) = \frac{1}{\pi}\int_{-L/2}^{L/2} f(x')\sum_{k=1}^{\infty}\cos k(x'-x)e^{-k^2Dt}dx'. \tag{2.19}$$

Assuming that the increment of k is very small, we can replace the summation with integration. We also assume L to be very large, and we then arrive at

$$C(x,t) = \frac{1}{\pi}\int_{-\infty}^{\infty} f(x')\int_{0}^{\infty}\cos k(x'-x)e^{-k^2Dt}dkdx'. \tag{2.20}$$

Now, we transform the variables by defining $y^2 = k^2 Dt$, such that $k = y/\sqrt{Dt}$ and $dk = dy/\sqrt{Dt}$. Equation (2.20) becomes

$$C(x,t) = \frac{1}{\pi}\int_{-\infty}^{\infty} f(x')\int_0^{\infty}\cos\frac{y}{\sqrt{Dt}}(x'-x)e^{-y^2}\frac{1}{\sqrt{Dt}}dydx'. \tag{2.21}$$

We define another variable: $z = \big(x'-x\big)/\sqrt{Dt}$. Then, we have

$$C(x,t) = \frac{1}{\pi}\int_{-\infty}^{\infty} f(x')\frac{1}{\sqrt{Dt}}\int_0^{\infty}\cos(yz)e^{-y^2}dydx'. \tag{2.22}$$

Here, we define the 2nd integral term in Eq. (2.22) as

$$I(z) = \frac{1}{\sqrt{Dt}}\int_0^{\infty} e^{-y^2}\cos(yz)dy, \tag{2.23}$$

for which, the derivative with respect to z is

$$\frac{dI(z)}{dz} = \frac{-1}{\sqrt{Dt}}\int_0^{\infty} e^{-y^2}y\sin(yz)dy = \frac{-1}{\sqrt{Dt}}\int_0^{\infty}\sin(yz)e^{-y^2}ydy. \tag{2.24}$$

Note that

$$\frac{d}{dy}e^{-y^2} = -2ye^{-y^2} \quad\Longrightarrow\quad d(e^{-y^2}) = -2e^{-y^2}ydy. \tag{2.25}$$

Such that Eq. (2.24) becomes

$$\frac{dI(z)}{dz} = \frac{1}{2\sqrt{Dt}}\int_0^{\infty}\sin(yz)d(e^{-y^2}). \tag{2.26}$$

Recall the identity of integration by parts:

$$\int udv = u\cdot v - \int vdu \tag{2.27}$$

such that

$$\begin{aligned}\int_0^{\infty}\sin(yz)d(e^{-y^2}) &= \sin(yz)\cdot e^{-y^2}\Big|_0^{\infty} - \int_0^{\infty} e^{-y^2}d(\sin(yz)) = \\ &\Big[\cancelto{0}{\sin(yz)e^{-\infty^2}} - \cancelto{0}{\sin(0)e^{-0^2}}\Big] - \int_0^{\infty} e^{-y^2}\big[z\cos(yz)dy\big] = \\ &-z\int_0^{\infty} e^{-y^2}\cos(yz)dy = -z\sqrt{Dt}I(z).\end{aligned} \tag{2.28}$$

Equation (2.26) becomes

$$\frac{dI}{dz} = \frac{1}{2\sqrt{Dt}}\cdot\big(-z\sqrt{Dt}I\big) = -\frac{z}{2}I \quad\Longrightarrow\quad \frac{dI}{I} = -\frac{z}{2}dz. \tag{2.29}$$

Taking integration, we obtain

$$\ln I = -\frac{z^2}{4} + \mathcal{C} \quad\Longrightarrow\quad I = \mathcal{C}\exp\left(\frac{-z^2}{4}\right), \tag{2.30}$$

where $\mathcal{C}$ is an integration constant. At $z = 0$,

$$I(0) = \frac{1}{\sqrt{Dt}}\int_0^{\infty} e^{-y^2}\cos(0)dy = \frac{1}{\sqrt{Dt}}\int_0^{\infty} e^{-y^2}\cdot 1\cdot dy = \frac{1}{2}\left(\frac{\pi}{Dt}\right)^{1/2} = \mathcal{C}. \tag{2.31}$$

Note that we have used integration table:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \left(\frac{\pi}{a}\right)^{\frac{1}{2}} \quad \Longrightarrow \quad \int_{0}^{\infty} e^{-y^2} dy = \frac{1}{2}\left(\frac{\pi}{1}\right)^{\frac{1}{2}}. \tag{2.32}$$

Thus, we obtain

$$I(z) = \mathcal{C} \exp\left(-\frac{z^2}{4}\right) = \frac{1}{2}\left(\frac{\pi}{Dt}\right)^{\frac{1}{2}} \exp\left[\frac{-(x'-x)^2}{4Dt}\right]. \tag{2.33}$$

Finally, the solution of $C(x,t)$ is

$$\begin{aligned} C(x,t) =& \frac{1}{\pi}\int_{-\infty}^{\infty} f(x')\frac{1}{2}\left(\frac{\pi}{Dt}\right)^{\frac{1}{2}} \exp\left[\frac{-(x'-x)^2}{4Dt}\right] dx' = \\ & \frac{1}{2\sqrt{\pi Dt}} \int_{-\infty}^{\infty} f(x') \exp\left[\frac{-(x'-x)^2}{4Dt}\right] dx'. \end{aligned} \tag{2.34}$$

If the initial condition $f(x')$ is a Dirac delta function, we then have

$$C(x,t) = \frac{1}{2\sqrt{\pi Dt}} C_0 \exp\left(\frac{-x^2}{4Dt}\right). \tag{2.35}$$

This analytical solution has a form of Gaussian function.

Note that we have used the property of a Dirac delta function:

$$\int_{-\infty}^{\infty} g(x)\delta(x) dx = g(x). \tag{2.36}$$

For $f(x') = C_0\delta(x'-0)$,

$$\int_{-\infty}^{\infty} C_0\delta(x'-0) \exp\left[\frac{-(x'-0)^2}{4Dt}\right] dx' = C_0 \exp\left(\frac{-x^2}{4Dt}\right). \tag{2.37}$$