MMAE-502 ENGINEERING ANALYSIS II
FULL DERIVATION FOR 2D-DIFFUSION EQUATION

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BASICS

2D DIFFUSION EQUATION

2D – Determines the statistical randomness of moving particles across a medium.

Earliest known theory was in 1883 by Adolf Fick.

$\partial_t - k\,\nabla^2_{\mathrm{2D}}$	$\Theta(t)\left(\frac{1}{4\pi k t}\right)e^{-\rho^2/4kt}$

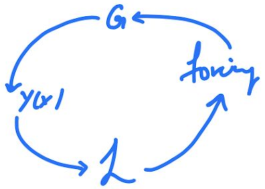
Problem Definition

$$\frac{\partial u}{\partial t} = D\nabla^2 u + f(\vec{r}+t)$$

or

$$\nabla^2 P - \frac{1}{D}\frac{\partial P}{\partial t} = 0$$ in cartesian coordinates

$y(x) = f(x)$



$\mathcal{L} = \partial t - K\nabla^2_{2D}$

D ↳ diffusion coefficient constant

↳ sometimes refered as K

$f(\vec{r}+t)$ → forcing function

back to the original problem

$$\nabla^2 P - \frac{1}{D}\frac{\partial P}{\partial t} = 0$$

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} - \frac{1}{D}\frac{\partial P}{\partial t} = 0$$

↪ linear PDE

↪ x and y do not mix so its separable

We begin with the 2D-FT in Cartesian solution.

Let $\hat{P}$ is the FT of our original function P

∴ Then

$$\hat{P}(k_x, k_y, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot P(x,y,t)\,dx\,dy$$

$$P(x,y,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \hat{P}(k_x, k_y, t)\,dk_x\,dk$$

- Symmetry in the Fourier Space

- Thus introduce integration by Parts

$$\int_a^b u\,dv = uv\Big|_a^b - \int_a^b v\,du$$

let $u = e^{-i2\pi(k_x \cdot x + k_y \cdot y)}$ and $v = \frac{\partial P}{\partial x}$

$du = \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} dx$ and $dv = \frac{\partial^2 P}{\partial x^2} dx$

by parts:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial^2 P}{\partial x^2} dx dy =$$

B.C $\frac{\partial P}{\partial(x,y)} = 0$ as $|x| = |y| \to \infty$

$$= e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \frac{\partial P}{\partial x}\Big|_{-\infty (x,y)}^{\infty} - \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x} dx dy$$

$$= e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \frac{\partial P}{\partial x}\Big|_{-\infty (x,y)}^{\infty} - \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x} dx dy$$

$$= \underbrace{e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \frac{\partial P}{\partial x}}_{0}\Big|_{-\infty (x,y)}^{\infty} + 2i\pi k_x \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x} dx dy$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial^2 P}{\partial x^2}\,dx\,dy = 2i\pi k_x \underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x}\,dx\,dy}_{\text{FT of } \frac{\partial P}{\partial x} \text{ therefore I follow the same manner}}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial^2 P}{\partial x^2}\,dx\,dy = 2i\pi k_x \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x}\,dx\,dy$$

$$= \underbrace{P \cdot e^{-i2\pi(k_x \cdot x + k_y \cdot y)}}_{0} \Big|_{-\infty(x,y)}^{\infty} + 2\pi i k_x \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P \cdot e^{-i2\pi(k_x \cdot x + k_y \cdot y)}$$

$P = 0$ as $|x| = |y| \to \infty$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot \frac{\partial P}{\partial x}\,dx\,dy = 2\pi i k_x \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P \cdot e^{-i2\pi(k_x \cdot x + k_y \cdot y)} \cdot dx\,dy$$

therefore

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x\cdot x+k_y\cdot y)}\cdot\frac{\partial^2 p}{\partial x^2}\,dx\,dy=(2\pi i k_x)^2\cdot\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p\cdot e^{-i2\pi(k_x\cdot x+k_y\cdot y)}\cdot dx\,dy$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi(k_x\cdot x+k_y\cdot y)}\cdot\frac{\partial^2 p}{\partial x^2}\,dx\,dy=(2\pi i k_x)^2\cdot\hat{p}$$

typically for n in general we would have:

$$\frac{\partial^n p}{\partial x^n}=(2\pi i k_x)^n\,\hat{p}$$

- since we used a spatial F.T function the derivative in time does not change.
- we can write the 2D-Diffusion Equation after FT

$$(2\pi)^2\,\hat{p}\cdot(k_x^2+k_y^2)+\frac{1}{D}\frac{\partial\hat{p}}{\partial t}=0$$

$$\frac{\partial\hat{p}}{\partial t}+D(2\pi)^2(k_x^2+k_y^2)\cdot\hat{p}=0$$

→ simple first order ODE with time

- We can Apply method of separation of variables
- assuming $\hat{P}(x,y,t) = T(t)X(x)Y(y)$ → product of functions

$$\frac{1}{T}\frac{\partial T}{\partial t} + D(2\pi)^2(K_x^2+K_y^2) = 0$$ → sub & dividing by $\hat{P}$

$$\frac{1}{T}\frac{dT}{dt} = -D(2\pi)^2(K_x^2+K_y^2) = \text{constant} = \lambda$$ → or A (Norm)

$$\frac{1}{D}\frac{1}{T}\frac{dT}{dt} = -\lambda$$ and $$(2\pi)^2 D(K_x^2+K_y^2)X\cdot Y = -\lambda T\cdot X\cdot Y$$ sub & divide

$$T(t) = Ce^{-\lambda D t}$$

$$(2\pi)^2(K_x^2+K_y^2) = -\lambda$$

eigen value problem

$$X(t) = A\sin(K_x\cdot x)$$
$$Y(t) = B\sin(K_y\cdot y)$$

$$\hat{P}(x,y,t) = \sum_{n,m} C_{n,m}\sin(K_x n x)\sin(K_y\cdot m_y)e^{-D(2\pi)^2(K_x^2+K_y^2)t}$$

or

$$\hat{P} = \lambda e^{-D(2\pi)^2(K_x^2+K_y^2)t}$$ → Norm λ (or A) used for conservation of momentum

- Now back to the function

$$P = A\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-D(2\pi)^2(k_x^2+k_y^2)t} \cdot e^{i2\pi(k_x\cdot x + k_y\cdot y)} \cdot dk_x dk_y$$

↳ entire integral separation of variables

so:
$$P = A\left[\int_{-\infty}^{\infty} e^{i2\pi k_x\cdot x - D(2\pi k_x)^2 t} dk_x\right]\left[\int_{-\infty}^{\infty} e^{i2\pi k_y\cdot y - D(2\pi k_y)^2 t} dk_y\right]$$

One of the features of the original diffusion equation comes into play here; the entire integral is *separable* by spatial variable:

$$P = A\left(\int_{-\infty}^{\infty} e^{i2\pi k_x\cdot x - D(2\pi k_x)^2 t} dk_x\right)\cdot\left(\int_{-\infty}^{\infty} e^{i2\pi k_y\cdot y - D(2\pi k_y)^2 t} dk_y\right)$$

In general, the number of these separable integrals is directly related to the dimensionality of the diffusion equation; in three dimensions there would be three such integrals. This integral is not trivial…it requires completing the square of the exponent, rescaling the integration variable, and changing to polar coordinates. I will not cover it here, but it is just an integral, so Maple© it! Using Maple© v8.0 I got:

$$P(x,y,t) = A\frac{e^{\left(\frac{-(x^2+y^2)}{4D\cdot t}\right)}}{4\pi D\cdot t}$$

We're almost there! What about this normalization constant A? If we are calling this function P a probability distribution, then it makes sense that the particle must exist somewhere in the x-y plane from x and y to plus and

I WILL DERIVE THIS BY HAND AGAIN FULLY IN THE NEXT SLIDES back to our original function

$$P = \lambda \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-D(2\pi)^2(k_x^2+k_y^2)t} \cdot e^{i2\pi(k_x\cdot x + k_y\cdot y)} \cdot dk_x dk_y$$

↳ entire integral separation of variables

so:

$$P = \lambda \left[\int_{-\infty}^{\infty} e^{\underbrace{i2\pi k_x\cdot x - D(2\pi k_x)^2 t}_{1}} dk_x\right]\left[\int_{-\infty}^{\infty} e^{\underbrace{i2\pi k_y\cdot y - D(2\pi k_y)^2 t}_{2}} dk_y\right]$$

completing the square & integral changing to polar

polar $x^2+y^2=r^2$ for isotropic "independent of direction"

$$i2\pi k_x\cdot x - D(2\pi k_x)^2\cdot t = -4\pi^2 2Dt\left(k_x - \frac{ix}{(2\pi Dt)}\right)^2 - \frac{x^2}{4Dt}$$

let $u_x = k_x - \dfrac{ix}{2\pi Dt}$

$$-4\pi^2 Dt\, u_x^2 - \frac{x^2}{4Dt}$$

Similarly apply the same process to 2nd part and substitute u_y

$$\int_{-\infty}^{\infty} e^{(i2\pi k_x \cdot x - D(2\pi k_x)^2 \cdot t} dt = e^{\frac{-x^2}{4Dt}} \cdot \int_{-\infty}^{\infty} e^{-4\pi^2 Dt \cdot u_x^2} \cdot du_x$$

non elementary integral the Louiville -Ritt

say $v = 2\pi\sqrt{Dt}\, u$

$$\int_{-\infty}^{\infty} e^{\frac{-v^2}{4}} dv$$

$$\left[\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx\right]^2$$

$$= \left[\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx\right] \cdot \left[\int_{-\infty}^{\infty} e^{-\frac{y^2}{2}} dy\right]$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{(x^2+y^2)}{2}} dx\,dy$$

$$= \int_{0}^{2\pi}\int_{0}^{\infty} e^{-\frac{r^2}{2}} r\,dr\,d\theta$$

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}$$

here

$$\left.\begin{aligned} x &= r\cos\theta \\ y &= r\sin\theta \\ x^2+y^2 &= r^2 \\ dx\,dy &= r\,dr\,d\theta \end{aligned}\right\} \text{polar}$$

make a sub $u = r^2/2$

$$= 2\pi \left[e^{-u} \right]_0^\infty$$

$$= 2\pi$$

$$\left[\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx \right]^2 = \int_{-0}^{2\pi} \int_0^{2\pi} e^{-\frac{r^2}{2}} r\,dr\,d\theta = 2\pi$$

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{2\pi}$$

Thus

$$\int_{-\infty}^{\infty} e^{-4\pi^2 D \cdot t \cdot u^2} du = \int_{-\infty}^{\infty} e^{-\frac{v^2}{4}} dv = 2\sqrt{\pi}$$

sub back for v and multiply be $e^{-\frac{x^2}{4Dt}}$.

$$= \sqrt{\frac{\pi}{4Dt}}\, e^{-\frac{x^2}{4Dt}}$$

$$\int_{-\infty}^{\infty} e^{(i2\pi k_x \cdot x - D(2\pi k_x)^2 \cdot t} dt = e^{\frac{-x^2}{4Dt}} \cdot \int_{-\infty}^{\infty} e^{-4\pi^2 Dt \cdot u_x^2} \cdot du_x$$

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

$$\int_{-\infty}^{\infty} e^{(i2\pi k_y \cdot y - D(2\pi k_y)^2 \cdot t} dt = e^{\frac{-y^2}{4Dt}} \int_{-\infty}^{\infty} e^{-4\pi^2 Dt \cdot u_y^2} \cdot du_y$$

$$= \frac{\sqrt{4}}{4Dt} \cdot e^{\frac{-y^2}{4Dt}}$$

→ non elemento integral the Louiville -Ritt

Combine all

$$p(x,y,t) = \frac{A}{4\pi Dt} \left[e^{\frac{-(x^2+y)}{4Dt}} \right]$$

$x^2 + y^2 = r^2$ in polar coordinates

but what is $A = ?$

A $\longrightarrow$ how many non-interacting particles we have in the system.

Impose a condition by making the total probability sum to 1. i.e.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y,t)\,dx\,dy = 1 \longrightarrow \text{Unity function}$$

Therefor

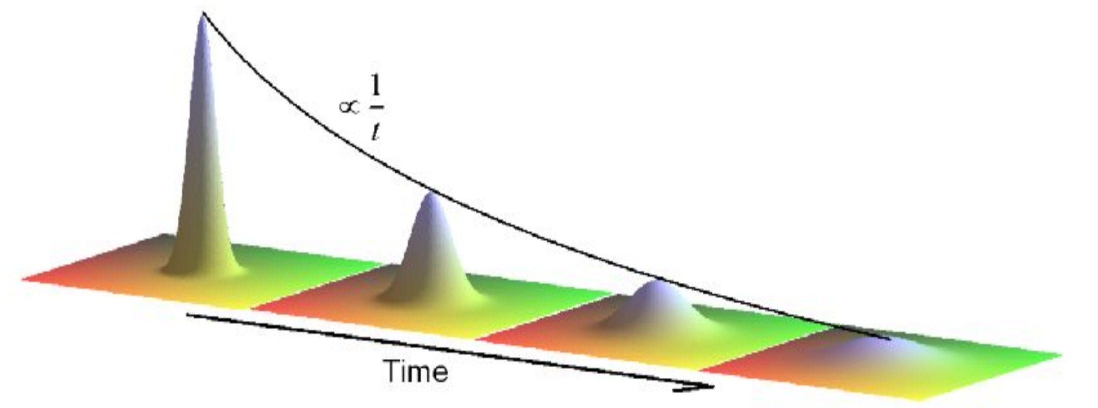
$$\boxed{p(r,t) = \frac{e^{\frac{-(r^2)}{4DT}}}{4\pi D t}}$$

- But what is diffusion coefficient D?
- has units of $\frac{L^2}{t}$
- relates to the rate of increase the mean distance of the particles with time.

$$D \propto \frac{k_B T}{\eta \cdot R} \Rightarrow D = \frac{k_B T}{6\pi\eta \cdot R}$$ spherical

- Helps determine the medium viscousity.

This is called a normalized Gaussian function. The first plot below shows diffusion at early times; notice how high the peak is, meaning the particles are localized around the area where they were first introduced. The remaining plots demonstrate how the particles spread out from their original entry point with time:



Source: Prof. Urser Caltech

QUESTIONS