DE-1

Schroedinger Eqn

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(xt) = -\frac{\hbar}{i}\frac{\partial \psi(xt)}{\partial t}$$

Diffusion Eqn $\rho(x\,t)$ = concentration at x,t

$T(x,t)$ = temperature at x,t

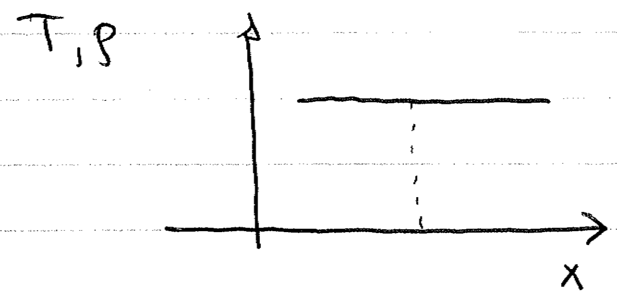
$$D\frac{\partial^2}{\partial x^2}\rho(xt) = \frac{\partial}{\partial t}\rho(xt)$$

NB $\int dx\, |\psi(xt)|^2 = 1$

but $\int dx\, \rho(x\,t) = 1$ ← conservation of particles/mass

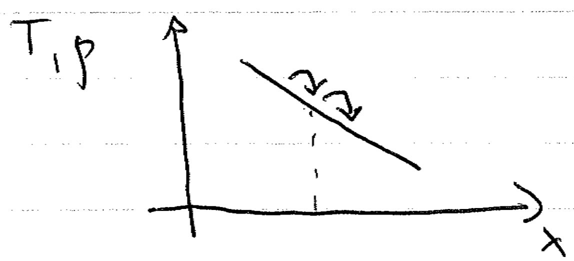
$\int dx\, T(x\,t) = 1$ ← conservation of energy

Why this form for diffusion Eqn



Do not expect particle or heat flow

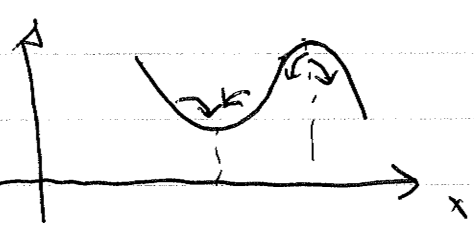
$$\frac{\partial \rho}{\partial t} = 0$$



similarly

$$\partial\rho/\partial t = 0$$

so $\partial\rho/\partial x \neq 0$ does not induce $\partial\rho/\partial t \neq 0$



Need $\frac{\partial^2 \rho}{\partial x^2} \neq 0$

Sign is also correct

DE-2

sec 2.4 of Griffiths, but easier!

HW problem: Given $\rho(x0) = \delta(x)$ compute $\rho(xt)$

Sol'n: $\rho(xt) = f(x) g(t)$

$$D f''(x)\, g = f\, g'(t)$$

$$D \frac{f''}{f} = \frac{g'}{g} = -Dk^2$$

$$f(x) = e^{ikx} \qquad g(t) = e^{-Dk^2 t}$$

general

$$\int a(k) e^{ikx - Dk^2 t} \frac{dk}{\sqrt{2\pi}} = \rho(x,t)$$

$$a(k) = \int \frac{dx}{\sqrt{2\pi}} e^{-ikx} \rho(x,0) \rightarrow \frac{1}{\sqrt{2\pi}} \text{ for } \delta(x)$$

$$\rho(xt) = \int \frac{dk}{2\pi} e^{ikx - Dk^2 t}$$

$$= \int \frac{dk}{2\pi} e^{-Dt\left(k^2 - \frac{ikx}{Dt}\right)}$$

$$= \int \frac{dk}{2\pi} e^{-Dt\left(k - \frac{ix}{2Dt}\right)^2} e^{+Dt\left(\frac{ix}{2Dt}\right)^2}$$

$$= \frac{1}{2\pi} \sqrt{\frac{\pi}{Dt}}\; e^{-x^2/4Dt}$$

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

Note still normalized

Numerical Soln to Diff Eqn

- we will do this in a few weeks after learning/reviewing C
- prelude to harder problem of numerical soln of Sch. Eqn!

Discretize $x \to dx$

$t \to dt$

$$f(x+dx) = f(x) + f'(x)dx + \tfrac{1}{2}f''(x)dx^2 + \ldots$$

$$f(x-dx) = f(x) - f'(x)dx + \tfrac{1}{2}f''(x)dx^2 + \ldots$$

$$\Rightarrow \quad f(x+dx) + f(x-dx) = 2f(x) + f''(x)dx^2$$

$$f''(x) = \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}$$

$$\Rightarrow \quad \frac{\rho(x,t+dt) - \rho(x,t)}{dt} = D\,\frac{\rho(x+dx,t) - 2\rho(x,t) + \rho(x-dx,t)}{dx^2}$$

$$\rho(x,t+dt) = \frac{D\,dt}{(dx)^2}\left[\rho(x+dx,t) - 2\rho(x,t) + \rho(x-dx,t)\right] + \rho(x,t)$$

~~Normalization?~~

DE -4

Change notation to emphasize discrete x, t

$x_n = n\,dx$ $\qquad$ $\cancel{p}$ $p(n,m)$ array

$t_m = m\,dt$

$$p(n, m+1) = \frac{D\,dt}{(dx)^2}\left[p(n+1,m) - 2p(n,m) + p(n-1,m)\right] + p(n,m)$$

Normalization $\quad \sum_n p(n, m+1) = \sum_n p(n,m)$

why?

Saves memory $\quad$ $p(n)$, $p_{new}(n)$ $\quad$ Just store p at two times.

$D\,dt/(dx)^2$ must be small

consider $D\,dt/(dx)^2 = \frac{1}{2}$

$$p(n, m+1) = \frac{1}{2}\left[p(n+1, m) + p(n-1, m)\right]$$

new value @ n = average of adjacent values earlier

		$n=-3$	-2	-1	0	1	2	3
$(t=0)$	$m=0$	0	0	0	1	0	0	0
		0	0	$1/2$	0	$1/2$	0	0
		0	$1/4$	0	$1/2$	0	$1/4$	0
		$1/8$	0	$3/8$	0	$3/8$	0	$1/8$

- Recognize this as binomial coefficients / Pascal's triangle ?

- Relation between diffusion and Random walk because if Random walk with $p(\text{Left}) = p(\text{right}) = \frac{1}{2}$ would get exact same table for probabilities of these final locations

- $D\,dt/(dx)^2 = \frac{1}{2}$ is too big : Diffusion does not have these zero values separating non zero values

DE-6

$$p(n, m+1) = 0.8\, p(n,m) + 0.1\left[p(n+1,m) + p(n-1,m)\right]$$

$D\, dt/(\Delta x)^2 = .1$

m	-3	-2	-1	0	1	2	3
0	0	0	0	1	0	0	0
1	0	0	0.1	0.8	0.1	0	0
2	0	0.01	0.16	0.66	0.16	0.01	0
3	.001	0.024	0.195	0.560	0.195	.024	.001

Much more reasonable for diffusion.