Lecture 26

Last time we derived heat conduction eq'n, which has the same form as the diffusion eq'n

$$\frac{\partial T}{\partial t} = D_T \nabla^2 T \qquad D_T = \frac{K}{\hat{c}_v} = \frac{1}{3}\bar{v}\ell$$

$$\frac{\partial n}{\partial t} = D \nabla^2 n \qquad D = \frac{1}{3}\bar{v}\ell$$

Diffusivity or Diffusion coefficient

Same eq'n describes heat flow between different temperatures and particle flow between different chemical potential

Note difference with wave eq'n:

$$\frac{\partial^2 u}{\partial t^2} = c\nabla^2 u \qquad c = \text{speed of propagation}$$

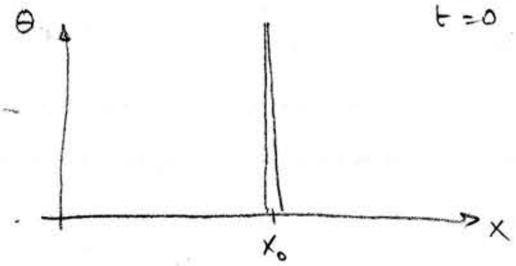
Solutions to diffusion equation are not propagating waves

Diffusion eq'n is very rich, has lot's of solutions depending on initial conditions $(t=0)$ and boundary conditions

Ex: development of a pulse (1-D)

$$\frac{\partial \theta}{\partial t} = D\frac{\partial^2 \theta}{\partial x^2}$$

at $t=0$ $\theta(x, t=0) = \delta(x-x_0)$ "pulse"
but no constraints in x $(-\infty < x < \infty)$



This could apply to
- a heating pulse using a laser or e^- beam at x_0
- a pulse of particles at x_0

How does this pulse evolve over time?

Solve this using Fourier transforms *

$$\tilde{\theta}(k,t) = \int_{-\infty}^{\infty} dx \; e^{-ikx} \, \theta(x,t)$$

$$\theta(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \; e^{ikx} \, \tilde{\theta}(k,t)$$

In Fourier space, diffusion eq'n becomes

$$\frac{\partial \tilde{\theta}}{\partial t} = -D k^2 \tilde{\theta} \qquad \therefore \qquad \tilde{\theta} = A(k) e^{-k^2 D t}$$

At $t=0$ $\qquad \theta(x, t=0) = \delta(x - x_0)$

$$\therefore \quad \tilde{\theta}(k, t=0) = \int_{-\infty}^{\infty} dx \; e^{-ikx} \, \delta(x - x_0) = e^{-ikx_0}$$

$$\Rightarrow \quad \tilde{\theta}(k,t) = e^{-ikx_0} \, e^{-k^2 D t}$$

Now inverse transform to go back to x

$$\theta(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \; \underbrace{e^{ik(x-x_0)} \, e^{-k^2 D t}}$$

Exponent is of the form $\quad -\alpha k^2 + i\beta k$

can turn into $\quad = -\alpha \left(k^2 - \frac{i\beta k}{\alpha} + \left(\frac{i\beta}{2\alpha}\right)^2 \right) - \frac{\beta^2}{4\alpha}$

$$= -\alpha \left(k - \frac{i\beta}{2\alpha} \right)^2 - \frac{\beta^2}{4\alpha}$$

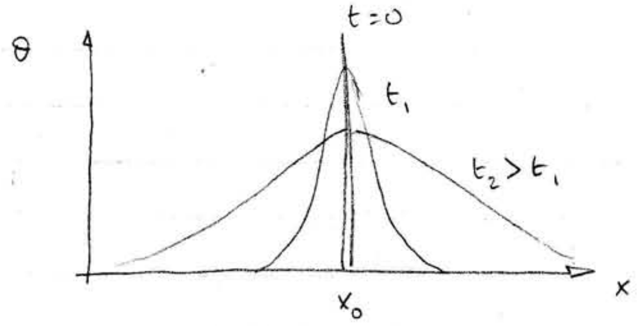
$$\therefore \quad \theta(x,t) = \frac{1}{2\pi} e^{-\beta^2/4\alpha} \int_{-\infty}^{\infty} dk \; e^{-\alpha(k - i\beta/2\alpha)^2}$$

$$= \frac{1}{2\pi} e^{-\beta^2/4\alpha} \underbrace{\int_{-\infty}^{\infty} dk' \; e^{-\alpha k'^2}}_{\text{Gaussian integral } \sqrt{\frac{\pi}{\alpha}}} \qquad k' \equiv k - \frac{i\beta}{2\alpha}$$

$\alpha \equiv Dt \;, \quad \beta \equiv (x - x_0)$

$$\therefore \quad \boxed{\theta(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-(x-x_0)^2/4Dt}}$$

Plot:



Pulse spreads symmetrically about x_0

Note that $\int_{-\infty}^{\infty} \theta(x,t) = 1$

$$\langle (x-x_0)\rangle = \int_{-\infty}^{\infty} (x-x_0)\,\theta(x,t) = \int_{-\infty}^{\infty} \underbrace{\frac{(x-x_0)}{\sqrt{4Dt}}}_{\text{odd}}\ \underbrace{e^{\frac{-(x-x_0)^2}{4Dt}}}_{\text{even}}\, dx = 0$$

$\therefore$ center of pulse remains fixed at x_0

$$\langle (x-x_0)^2\rangle = \int_{-\infty}^{\infty} \frac{(x-x_0)^2}{\sqrt{4Dt}}\, e^{-\frac{(x-x_0)^2}{4Dt}}\, dx = 2Dt$$

$\therefore$ The standard deviation (width of pulse) <u>increases</u> as $\Delta x_{rms} = \sqrt{\langle (x-x_0)\rangle^2} = \sqrt{2Dt}$

Note $\sqrt{t}$ dependence
In homework you will derive this in 2-D, 3-D

* This problem can be solved in a variety of ways. Fourier transform is appropriate because there are no constraints in x $(-\infty < x < \infty)$. If there are boundary conditions, other approaches may be more appropriate

Compare diffusion vs. kinematics

In kinematics : $x = vt \sim t$ mean position changes

Diffusion : $\Delta x_{rms} = \sqrt{2Dt} \sim t^{1/2}$ mean position unchanged

Ex: a small protein in the cell has $D \sim 10^{-6}\ cm^2/s$

$\therefore$ a pulse of protein will diffuse through:

a bacterium ($1\mu m = 10^{-4}$ cm) in $t = \frac{x^2}{2D} = \frac{10^{-8}}{2\cdot 10^{-6}} = 5$ ms

a human cell ($10\mu m = 10^{-3}$ cm) in $t = \frac{10^{-6}}{2\cdot 10^{-6}} = 0.5$ s

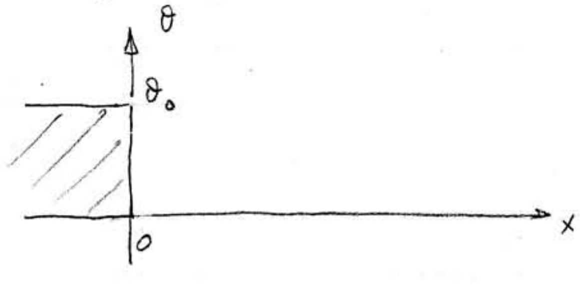
longest axon ($1m = 10^2$ cm) in $t = \frac{10^4}{2\cdot 10^{-6}} = 5\times 10^9 s$!

$= 150$ yrs !

Clearly, diffusion does not work for transporting molecules over long distances

Ex: <u>diffusion with fixed boundary</u> (1-D)

Now let's impose boundary condition at $x=0$ such that $\theta = \theta_0$ at $t=0$

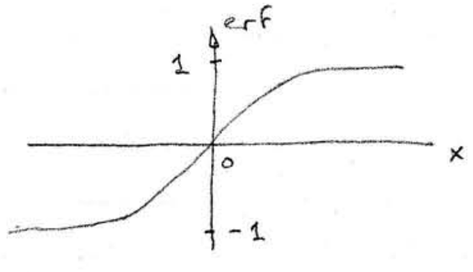


This could be diffusion of heat or particles from an infinite surface at $x=0$

If $\theta(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-(x-x_0)^2/4Dt}$ is a sol'n, then any

sum or integral of $\theta(x,t)$ will <u>also</u> be a sol'n

Consider error f'n $\text{erf} \equiv \frac{2}{\sqrt{\pi}} \int_0^x du\, e^{-u^2}$



$\mathrm{erf}(0) = 0$

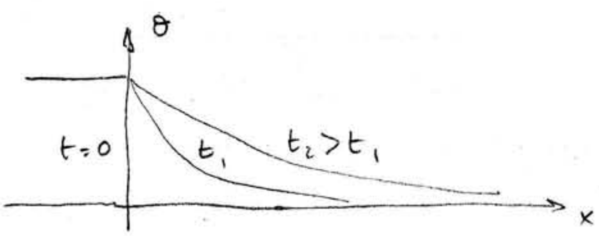
$\mathrm{erf}(\infty) = 1 \qquad \mathrm{erf}(-\infty) = -1$

Note that initial condition is a step function with
$\vartheta = \vartheta_0$ for $x \leq 0$, $\theta = 0$ for $x > 0$

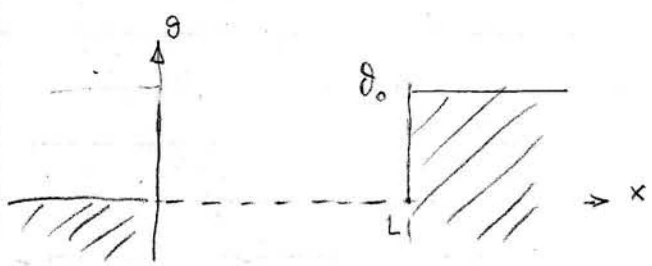
Since $\theta(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-x^2/4Dt} = \delta(x)$ for $t = 0$

Its integral will be a step f'n

Sol'n is $\boxed{\vartheta(x,t) = \theta_0 \left(1 - \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right)}$



Ex: <u>diffusion with two fixed boundaries</u>
Now let's impose boundary conditions such that
$\vartheta = 0$ at $x = 0$, $\vartheta = \vartheta_0$ at $x = L$



This could be system between two reservoirs at different temperatures or chemical potential

We saw last time that steady-state sol'n $\left(\frac{\partial\theta}{\partial t} = 0\right)$

$\theta_{s.s.} = \vartheta_0 \frac{x}{L}$ varies linearly from 0 to ϑ_0

Assume initial condition is $\theta = 0$
Now see how it evolves to $\theta_{ss.}$ sol'n.

Because range of x is finite $(0 \le x \le L)$ appropriate sol'ns are Fourier series in $\sin kx$ or $\cos kx$ with $k = \frac{n\pi}{L}$

Plugging into diffusion eq'n, sol'ns are of the form

$$\theta(x,t) \sim e^{-k^2 D t} \sin kx \quad \text{or} \quad e^{-k^2 D t} \cos kx \qquad k = \frac{n\pi}{L}$$

Note that steady state occurs when $t \to \infty$, so these sol'ns $\to 0$
To get $\theta_{s.s.} = \theta_0 \frac{x}{L}$ we have to add it to the other sol'ns
To satify boundary conditions, only $\sin kx$ works

$$\therefore \boxed{\theta(x,t) = \theta_0 \frac{x}{L} + \sum_{n=1}^{\infty} A_n e^{-\left(\frac{n\pi}{L}\right)^2 D t} \sin \frac{n\pi}{L} x}$$

Has the right behavior at $t \to \infty$, $x = 0, L$ at all t

To get A_n, we need to satisfy initial condition $\theta(x,0) = 0$

$$-\frac{\theta_0}{L} x = \sum_{n=1}^{\infty} A_n \sin \frac{n\pi}{L} x$$

From theory of Fourier series

$$A_n = \frac{2}{L} \int_0^L dx \left(-\frac{\theta_0 x}{L}\right) \sin \frac{n\pi}{L} x = \frac{(-1)^n}{n} \frac{2\theta_0}{\pi}$$