Lectures 15&16: The Diffusion Equation

References: Course Pack p.64-69, 102-107.

In classical physics, almost all time dependent phenomena may be described by the wave equation or the diffusion equation. At the micro and nanometer scale, diffusion is often the dominant phenomenon.

The 1D diffusion equation has the form $\dfrac{\partial^2 F(x,t)}{\partial x^2} = \dfrac{1}{D}\dfrac{\partial F(x,t)}{\partial t}$.

F is the quantity that diffuses. It is usually a concentration, for example the concentration of a chemical diffusing through a region, the concentration of particles in a liquid, the concentration of defects in a solid, concentration of spin densities, etc.
D is the diffusion constant. *D* has dimensions $[\text{length}]^2/[\text{time}]$, i.e. units m^2s^{-1}.

Heat conduction also obeys this situation. *F* is then temperature, *T*. And many books write $D = h^2 = \dfrac{K}{\rho C}$
where h^2 is the thermal diffusivity of the material, which depends on *K* the thermal conductivity, ρ the density and *C* the specific heat of the material. (For metal, typically $h^2 \sim 1\times10^{-4}\, m^2s^{-1}$.)

So we have the heat flow equation $\dfrac{\partial^2 T(x,t)}{\partial x^2} = \dfrac{1}{h^2}\dfrac{\partial T(x,t)}{\partial t}$.

We will study heat flow because it is a concept familiar from daily life but the same mathematics can be applied to many other diffusion situations.

Thermal Relaxation of a rod with ends held at 0°C

Consider a perfectly insulated rod of length *L*. Both ends are held at temperature 0ºC at all times.
At time $t = 0$, the temperature distribution along the rod has a given function $T(x, 0)= f(x)$.

Step 1 Our differential equation is $\dfrac{\partial^2 T(x,t)}{\partial x^2} = \dfrac{1}{h^2}\dfrac{\partial T(x,t)}{\partial t}$.

Look for solutions of the form $T(x,t) = X(x)\,\theta(t)$.

Substituting this into the PDE gives $\dfrac{d^2X(x)}{dx^2}\theta(t) = \dfrac{1}{h^2}X(x)\dfrac{d\theta(t)}{dt}$.

Multiply both sides by $\dfrac{1}{X(x)\,\theta(t)}$: $\dfrac{1}{X(x)}\dfrac{d^2X(x)}{dx^2} = \dfrac{1}{h^2}\dfrac{1}{\theta(t)}\dfrac{d\theta(t)}{dt}$.

To be true at all *x, t*, both sides of the above equation must be equal to a constant.

Step 2 Since we are told in the boundary conditions that both ends of the rod are held at 0°C at all times we choose a negative constant, $-k^2$, to give LHO type solutions, and rearrange to get two ODEs:

$$\frac{d^2X(x)}{dx^2} = -k^2X \qquad \text{which has general solution} \quad X(x) = A\cos kx + B\sin kx$$

$$\frac{d\theta(t)}{dt} = -k^2h^2\theta(t) \qquad \text{which has general solution} \quad \theta(t) = Ce^{-k^2h^2t}$$

We have $T(0, t) = T(L, t) = 0$, so $X(0) = X(L) = 0$, so (similar to previous problems) $A = 0$, $B = n\pi/L$.

So we have special solutions $T_n(x,t) = X(x)\theta(t) = B_n \sin\dfrac{n\pi x}{L}e^{-\frac{t}{\tau_n}}$, where $\tau_n = \dfrac{1}{h^2k^2} = \left(\dfrac{L}{n\pi h}\right)^2$.

Step 3 The general solution therefore is $T(x,t) = \sum_n T_n(x,t) = \sum_n B_n \sin\dfrac{n\pi x}{L}e^{-\frac{t}{\tau_n}}$.

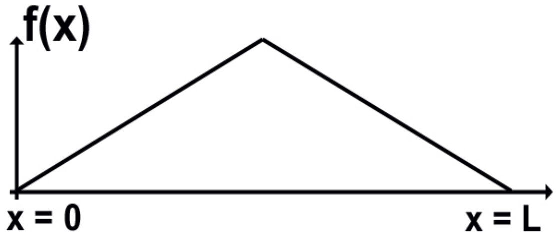
Step 4 At time t = 0, the temperature distribution is $T(x, 0)= f(x)$, so $T(x,0) = \sum_n B_n \sin\frac{n\pi x}{L} = f(x)$.

Thus the coefficients B_n are the coefficients of the half-range Fourier sine series of the function $f(x)$.

Let's say that the temperature distribution along the rod at t = 0 is triangular.

$f(x) = x \quad$ for $0 < x < L/2$

$f(x) = -x + L \quad$ for $L/2 < x < L$



i.e. temperature midway in °C is equal to half distance in m.

Half-range sine series expression: $\quad f(x) = \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{d}$, $\quad$ where $\quad b_n = \frac{2}{d}\int_0^d f(x)\sin\frac{n\pi x}{d}\,dx$.

Here d = L,

So $\quad b_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx = \frac{2}{L}\int_0^{L/2} x\sin\frac{n\pi x}{L}dx + \frac{2}{L}\int_{L/2}^{L}(L-x)\sin\frac{n\pi x}{L}dx$

$\int x\sin\frac{n\pi x}{L}dx$ is found by parts $\quad set\ u = x\ so\ du = dx \quad set\ dv = \sin\frac{n\pi x}{L}dx\ so\ v = -\frac{L}{n\pi}\cos\frac{n\pi x}{L}$

So $\quad \int x\sin\frac{n\pi x}{L}dx = -\frac{Lx}{n\pi}\cos\frac{n\pi x}{L} + \int\frac{L}{n\pi}\cos\frac{n\pi x}{L}dx = -\frac{Lx}{n\pi}\cos\frac{n\pi x}{L} + \frac{L^2}{n^2\pi^2}\sin\frac{n\pi x}{L}$

So $b_n = \frac{2}{L}\left[-\frac{Lx}{n\pi}\cos\frac{n\pi x}{L} + \frac{L^2}{n^2\pi^2}\sin\frac{n\pi x}{L}\right]_0^{L/2} + \frac{2}{L}\int_{L/2}^{L} L\sin\frac{n\pi x}{L}dx + \frac{2}{L}\left[\frac{Lx}{n\pi}\cos\frac{n\pi x}{L} - \frac{L^2}{n^2\pi^2}\sin\frac{n\pi x}{L}\right]_{L/2}^{L}$

$$b_n = \frac{2}{L}\left[-\frac{L^2}{2n\pi}\cos\frac{n\pi}{2} + \frac{L^2}{n^2\pi^2}\sin\frac{n\pi}{2}\right] - 2\left[\frac{L}{n\pi}\cos\frac{n\pi x}{L}\right]_{L/2}^{L} + \frac{2}{L}\left[\frac{L^2}{n\pi}\cos n\pi - \frac{L^2}{2n\pi}\cos\frac{n\pi}{2} + \frac{L^2}{n^2\pi^2}\sin\frac{n\pi}{2}\right]$$

$$b_n = \left[-\frac{L}{n\pi}\cos\frac{n\pi}{2} + \frac{2L}{n^2\pi^2}\sin\frac{n\pi}{2}\right] - 2\left[\frac{L}{n\pi}\cos n\pi - \frac{L}{n\pi}\cos\frac{n\pi}{2}\right] + \left[\frac{2L}{n\pi}\cos n\pi - \frac{L}{n\pi}\cos\frac{n\pi}{2} + \frac{2L}{n^2\pi^2}\sin\frac{n\pi}{2}\right]$$

$$b_n = \frac{4L}{n^2\pi^2}\sin\frac{n\pi}{2}$$

n = 1, $b_1 = \frac{4L}{\pi^2}$	n = 2, $b_2 = 0$	n = 3, $b_3 = -\frac{4L}{3^2\pi^2} = -\frac{4L}{9\pi^2}$	n = 4, $b_4 = 0$

So $\quad b_n = \frac{4L}{n^2\pi^2} \quad for\ n = 1, 5, 9 \quad$ and $\quad b_n = -\frac{4L}{n^2\pi^2} \quad for\ n = 3, 7, 11$

Half-range sine series is written: $f(x) = \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{d}$, so here $f(x) = \sum_{n=1}^{\infty} \frac{4L}{n^2\pi^2} \sin\frac{n\pi}{2} \sin\frac{n\pi x}{L}$

Step 5 At time t = 0, the temperature distribution is $T(x, 0) = f(x)$, so $T(x,0) = \sum_{n=1} B_n \sin\frac{n\pi x}{L} = f(x)$

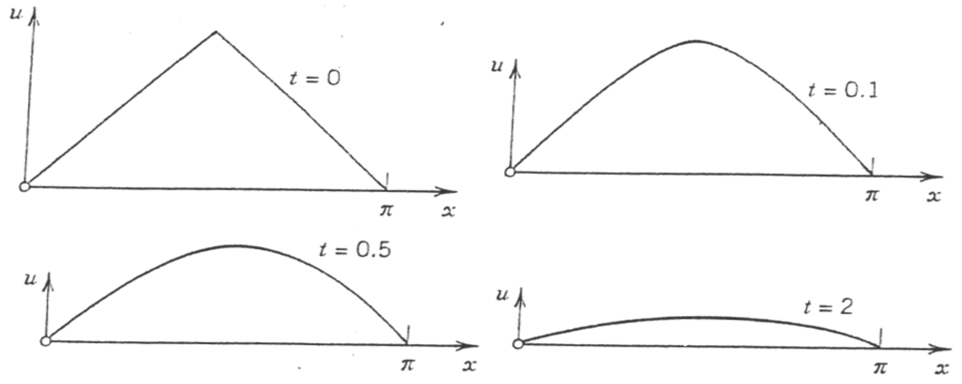
Therefore comparing terms $B_n = \frac{4L}{n^2\pi^2} \sin\frac{n\pi}{2}$.

Step 6 The full solution for the rod is therefore: $T(x,t) = \sum_n B_n \sin\frac{n\pi x}{L} e^{-\frac{t}{\tau_n}} = \sum_{n=1}^{\infty} \frac{4L}{n^2\pi^2} \sin\frac{n\pi}{2} \sin\frac{n\pi x}{L} e^{-\frac{t}{\tau_n}}$

where $\tau_n = \frac{1}{h^2 k^2} = \left(\frac{L}{n\pi h}\right)^2$

$$T(x,t) = \frac{4L}{\pi^2}\left[\frac{1}{1}\sin\frac{\pi x}{L} e^{-\frac{\pi^2 h^2 t}{L^2}} - \frac{1}{9}\sin\frac{3\pi x}{L} e^{-\frac{9\pi^2 h^2 t}{L^2}} + \frac{1}{25}\sin\frac{5\pi x}{L} e^{-\frac{25\pi^2 h^2 t}{L^2}} - .....\right]$$

Now we have all the boundary conditions, we can stick in appropriate values of h and find how the temperature profile drops over time. It can be shown that T(x,t) with increasing time looks like this:



Notice how the fundamental frequency lasts the longest.

Thermal relaxation of an isolated body

In the last example the ends of rod were immersed in a massive reservoir at 0°C so that heat was able to continually flow out of the rod. Now imagine that the ends are insulated just like the rest of the rod. Imagine we start at time = 0 with the same triangular temperature distribution as before. With time, the temperature distribution will become uniform. The temperature of the body will then be at some non zero temperature.

The rate of heat flow is known to be proportional to the temperature gradient $\frac{\partial T(x,t)}{\partial x}$.

The body being isolated means there is no heat flow out of the ends so at x = 0 and $x = L$,

$\frac{\partial T(x,t)}{\partial x}|_{x=0} = \frac{\partial T(x,t)}{\partial x}|_{x=L} = 0$. Applying these boundary solutions to the general solution for $X(x)$ we find

that since, $X(x) = A\cos kx + B\sin kx$ then $\left.\frac{dT(x,t)}{dx}\right|_{x=0} = \left.\frac{dX(x,t)}{dx}\right|_{x=0} = -Ak\sin kx + Bk\cos kx$.

Therefore $0 = -Ak\sin k0 + Bk\cos k0$ and so $0 = B$

and $\quad 0 = -Ak\sin kL + Bk\cos kL \quad$ and so $\quad 0 = -Ak\sin kL$ and therefore $\quad kL = n\pi \quad or \quad k = \frac{n\pi}{L}$

Putting this back into expression for *X(x)* we find $X(x) = A\cos kx = A_n \cos\frac{n\pi x}{L}$

Therefore following the same steps as above we find the special solutions and the corresponding general solution have the respective forms:

$$T_n(x,t) = A_n\cos(n\pi x/L)e^{-t/\tau_n} \qquad \text{and} \qquad T(x,t) = \sum_n T_n(x,t) = \sum_n A_n \cos\frac{n\pi x}{L}e^{-\frac{t}{\tau_n}}$$

We are therefore left with the cosine rather than the sine terms in the expression and so we must solve the Half range COSINE series for the temperature function *f(x)*.

Half-range cosine series: $f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L}$, where $a_n = \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx$.

This can be shown to give coefficients: $a_0 = \frac{L}{2}$ and $a_n = \frac{2L}{n^2\pi^2}\left(2\cos\frac{n\pi}{2} - \cos n\pi - 1\right)$

Giving $\quad f(x) = \frac{L}{4} + \sum_{n=1}^{\infty}\frac{2L}{n^2\pi^2}\left(2\cos\frac{n\pi}{2} - \cos n\pi - 1\right)\cos\frac{n\pi x}{L}$

n = 1, $a_1 = 0$	n = 2, $a_2 = \frac{2L}{2^2\pi^2}(-4) = \frac{-8L}{2^2\pi^2}$	n = 3, $a_3 = 0$	n = 4 $a_4 = 0$	n = 5, $a_5 = 0$

n = 6, $a_6 = \frac{2L}{6^2\pi^2}(2\cos 3\pi - \cos 6\pi - 1) = \frac{2L}{6^2\pi^2}(-4) = \frac{-8L}{6^2\pi^2}$

Comparison with the general solution at time = 0 i.e. $T(x,0) = \sum_n T_n(x,0) = \sum_n A_n\cos\frac{n\pi x}{L}$ allows the coefficients A_n to be determined.

The full solution then: $T(x,t) = \sum_n A_n\cos\frac{n\pi x}{L}e^{-\frac{t}{\tau_n}} = \frac{L}{4} - \frac{8L}{\pi^2}\left\{\frac{1}{2^2}\cos\frac{2\pi x}{L}e^{-\frac{2^2h^2\pi^2 t}{L^2}} + \frac{1}{6^2}\cos\frac{6\pi x}{L}e^{-\frac{6^2h^2\pi^2 t}{L^2}} + \right\}$

Notice how as t $\to$ 0 then $\left(e^{-\frac{n^2h^2\pi^2 t}{L^2}}\right) \to 0$ and so $T(x,\infty) = \frac{L}{4}$ This is the final uniform temperature of the rod.

Concluding Summary

1. Sinusoidal functions of *x* are solutions of the diffusion equation. Hence Fourier methods are again useful. (In fact Fourier actually invented them to solve heat flow problems.)
2. The temperature distribution decays exponentially with time.
3. The time constant of the decay is proportional to k^{-2}, i.e. to λ^2 and therefore also L^2. So the longest wavelengths (such as the fundamental) last longest.
4. Hence if we write an initial temperature distribution as a Fourier series, normally the first term is the most important in determining the behaviour at later times.

• Importance of $\tau \propto \lambda^2$

To see points 3&4 more clearly, we can rewrite $T(x,t) = \sum_n T_n(x,t) = \sum_n B_n \sin\frac{n\pi x}{L} \exp(-n^2 t/\tau_1)$

where τ_1 is the relaxation time of the 'fundamental' n = 1 term, $\tau_n = \left(\frac{L}{h\pi}\right)^2$.

After a time $t = \tau$, for example, the nth term has decayed by a factor $\exp(-n^2)$. Looking at values for this for *n = 1, 2, 3, …* below, we can see that the higher modes decay very fast indeed!

e^{-1}	0.37
e^{-4}	0.02

e^{-9}	1.2×10^{-4}
e^{-16}	1.1×10^{-7}

e^{-25}	1.4×10^{-11}
e^{-36}	2.3×10^{-16}

e^{-49}	5.3×10^{-22}

To know exactly how the temperature profile changes with time then we need all the terms. But usually a very good approximation can be obtained by considering just the first term.

• Importance of $\tau \propto L^2$

We are used to thinking of time scaling linearly with distance. For example, if it takes us 20 mins to walk a mile it takes 40 mins to walk 2 miles etc. But 'diffusion time' scales with the *square* of the length. Values of h^2 vary between $\sim 1\times10^{-4}\,\mathrm{m^2s^{-1}}$ for a metal and $\sim 1\times10^{-7}\,\mathrm{m^2s^{-1}}$ for cork.

So using $\tau_n = \left(\frac{L}{n\pi h}\right)^2$ from previous page in 1 second, heat travels a distance of very approximately $L \approx \pi h$, which is ~ *3* cm for a metal, ~ 1 mm for cork.

On an everyday scale. If food is cut up smaller it cooks faster! (Cookery books tell you the cooking time scales as the weight (= length^3), but actually it scales as the square of the thinnest dimension!)

On the large scale. Why don't we heat up because of the earth's core? The heat must travel through about 30 km of sand and gravel. Taking the diffusion constant for this material to be $h^2 \sim 1\times10^{-6}\,\mathrm{m^2s^{-1}}$, we have $\tau \sim L^2/\pi^2h^2 \sim 10^{14}$ seconds ~ 10^6 years.

On the small scale. Chemical diffusion constants for ions in water, D, are of the order of $D \sim 10^{-9}\mathrm{m^2s^{-1}}$ where $D = h^2$. Our bodies function because ions can diffuse in and out of our muscle cells, acting as switches. The time taken for ions to diffuse across a cell of width L= 10^{-6}m is $\tau \sim L^2/\pi^2 D \sim 10^{-4}$ seconds, which is suitably quick. Could humans be scaled up so our cells were 1 cm across and still function? No! because the time would then be $\tau \sim L^2/\pi^2 D \sim 10^4$ s which is too slow!