Lecture 14: The Schrödinger & 2D Laplace Equations

The procedure used in the previous lecture to solve the wave equation can be applied to other PDEs. In this lecture we demonstrate its application to the Schrödinger equation and 2D Laplace equation.

The Schrödinger Equation

Consider the time dependent Schrödinger equation in 1 dimensional space:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}.$$

In a region of zero potential, $V(x,t) = 0$, this simplifies to:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}=i\hbar\frac{\partial\Psi(x,t)}{\partial t}.$$

Let us solve this subject to boundary conditions $\Psi(0, t) = \Psi(L, t) = 0$ (as for the *infinite potential well*).

Step 1: Separation of the Variables
Our boundary conditions are true at special values of x, for *all* values of time, so we look for solutions of the form $\Psi(x, t) = X(x)T(t)$. Substitute this into the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2X(x)}{dx^2}T(t)=i\hbar\, X(x)\frac{dT(t)}{dt}$$

Multiply both sides by $1/X(x)T(t)$: $$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2}=\frac{i\hbar}{T}\frac{dT}{dt}$$

Now we have separated the variables. The above equation can only be true for all x, t if both sides are equal to a constant. It is conventional (for good reasons – see below and PHY202!) to call the constant E.

So we have	$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2}=E$	which rearranges to	$\frac{d^2X}{dx^2}=-\frac{2mE}{\hbar^2}X$.	(i)
And	$\frac{i\hbar}{T}\frac{dT}{dt}=E$	which rearranges to	$\frac{dT}{dt}=-\frac{iE}{\hbar}T$.	(ii)

Step 2: Satisfying the Boundary Conditions

For X(x)
Our boundary conditions are $\Psi(0, t) = \Psi(L, t) = 0$, which means $X(0) = X(L) = 0$.
So clearly we need $E > 0$, so that equation (i) has the form of the harmonic oscillator equation.

It is simpler to rewrite (i) as $\frac{d^2X}{dx^2}=-k^2X$ where $k^2=\frac{2mE}{\hbar^2}$, i.e. $E=\frac{\hbar^2k^2}{2m}$.

Then the general solution for $X(x)$ is $X(x)=A\cos kx+B\sin kx$.

Apply the boundary conditions: $X(0) = 0$ gives $A = 0$; we must have $B \neq 0$ so $X(L) = 0$ requires

$\sin kL=0$, i.e. $k_n = n\pi/L$, so $X_n(x)=B_n\sin\frac{n\pi x}{L}$ for $n = 1, 2, 3, \ldots$.

For T(t)
Equation (ii) has solution $T=T_0e^{-iEt/\hbar}$ (See lecture 3 first order ODEs).

So we have special solutions: $\Psi_n(x,t)=X_n(x)T_n(t)=B_n\sin\frac{n\pi x}{L}\,e^{-iE_nt/\hbar}$ where $E_n=\frac{\hbar^2k_n^{\,2}}{2m}=\frac{n^2\hbar^2\pi^2}{2mL^2}$.

(These are the *energy eigenstates* of the system.)

Step 3: Constructing the General Solution

Hence the general solution is $\Psi(x,t)=\sum_{n=1}^{\infty}\Psi_n(x,t)=\sum_{n=1}^{\infty}B_n\sin\frac{n\pi x}{L}\exp(-iE_nt/\hbar)$.

(In general therefore a particle will be in a *superposition* of eigenstates.)

Step 4: Solution of Complete Problem using Fourier Series

If we know the state of the system at $t = 0$, we can find the state at any later time.

For example, suppose that $\Psi(x,0)=\sqrt{\frac{2}{L}}\left[\frac{1}{\sqrt{2}}\sin\frac{\pi x}{L}+\frac{1}{\sqrt{2}}\sin\frac{2\pi x}{L}\right]$. Then we can deduce that

$$\Psi(x,t)=\sqrt{\frac{2}{L}}\left[\frac{1}{\sqrt{2}}\sin\frac{\pi x}{L}\exp(-iE_1t/\hbar)+\frac{1}{\sqrt{2}}\sin\frac{2\pi x}{L}\exp(-iE_2t/\hbar)\right] \text{ where } E_1=\frac{\hbar^2\pi^2}{2mL^2},\ E_2=\frac{4\hbar^2\pi^2}{2mL^2}.$$

The Laplace Equation in 2D

In the next lecture we will start looking at the diffusion equation, $\nabla^2u=\frac{1}{h^2}\frac{\partial u}{\partial t}$. One physical phenomenon governed by this equation is heat flow. That is, in many situations, $T(x, y, z, t)$ satisfies $\nabla^2T=\frac{1}{h^2}\frac{\partial T}{\partial t}$.

In 'steady state' problems where nothing is changing with time, the equation simplifies to $\nabla^2T=0$, which is the Laplace equation. (This can be applied to electrostatics if the temperatures were replaced by potentials.) We will look at this equation in 2D by considering the following exercises

<u>Exercise 1</u>

Consider a rectangular metal plate 10 cm wide and very long. The two long sides and the far end are held at 0ºC and the base at 100ºC. Find the steady state temperature distribution inside the plate. NB. You will need to use the superposition principle at the end to satisfy the boundary conditions!!

Our PDE is $\nabla^2T=\frac{\partial^2T}{\partial x^2}+\frac{\partial^2T}{\partial y^2}=0$.

Step 1: Separation of the variables – look for solutions of the form *T(x, y) = X(x)Y(y)*.

So substituting gives $Y(y)\frac{\partial^2X(x)}{\partial x^2}+X(x)\frac{\partial^2Y(y)}{\partial y^2}=0$ and dividing through by *X(x)Y(y)* we get :

$$\frac{1}{X(x)}\frac{\partial^2X(x)}{\partial x^2}+\frac{1}{Y(y)}\frac{\partial^2Y(y)}{\partial y^2}=0 \quad\text{and so}\quad \frac{1}{X(x)}\frac{\partial^2X(x)}{\partial x^2}=-\frac{1}{Y(y)}\frac{\partial^2Y(y)}{\partial y^2}$$

Step 2: Satisfy the boundary conditions. Considering the BCs, choose an appropriate constant of separation. Find the general forms of *X(x)* and *Y(y)*. Apply relevant BCs. Find the special solutions.

Now we set both sides equal to a constant. When choosing the constant we must think carefully about the boundary conditions. We know that $X(0) = X(L) = 0$ and we know that in the Y direction up the page we expect an exponential drop or something similar from $T(x,0) = 100$ to $T(x,\infty) = 0$. Think back again to the LHO solution and the falling pencil solution in lecture 3 for 2nd order ODEs. It is clear now that for a solution in x such that $X(x) = 0$ more than once, the constant must be negative (like a LHO). For convenience we choose the constant as $-k^2$ so….

$$\frac{1}{X(x)}\frac{\partial^2X(x)}{\partial x^2}=-\frac{1}{Y(y)}\frac{\partial^2Y(y)}{\partial y^2}=-k^2$$

So $\frac{\partial^2 X(x)}{\partial x^2} = -k^2 X(x)$ and $\frac{\partial^2 Y(y)}{\partial y^2} = k^2 Y(y)$ with solutions of :-

$$X(x) = A\cos kx + B\sin kx \quad \text{and} \quad Y(y) = Ce^{-ky} + De^{ky}$$

Now we must again think of the boundary conditions and attempt to deduce *A,B,C*, and *D*. We know that *X(0) = X(L) = 0* and if this is true then *A = 0*. Also since *X(L) = 0 = B sin kx* then $kL = n\pi$ so we can say $X(x) = B\sin\frac{n\pi x}{L}$. Now looking at $Y(y) = Ce^{-ky} + De^{ky}$ and since we know that $T(x,y) \to 0$ as $y \to \infty$ then we can state that *D = 0* and $Y(y) = Ce^{-ky}$.

So special solution is $T(x,y) = Ce^{-ky} B\sin\frac{n\pi x}{L} = CBe^{\frac{-n\pi y}{L}} \sin\frac{n\pi x}{L} = \mathrm{Re}^{\frac{-n\pi y}{10}} \sin\frac{n\pi x}{10}$ if *P = CB* and *L=10.*

Step 3: Construct the general solution.

So the general solution can be written as $T(x,y) = \sum_{n=1}^{\infty} P_n e^{\frac{-n\pi y}{10}} \sin\frac{n\pi x}{10}$

This already satisfies the boundary conditions for *x,* namely that *T(0,y) = T(L,y) = 0*. All that remains is to calculate the required values of *P* such that the *T(x,0) =100* is satisfied.

Step 4: Use the remaining information to solve the complete problem. (Fourier series is useful.)

Since the temperature at *y = 0* is *100* then $T(x,0) = \sum_{n=1}^{\infty} P_n e^{\frac{-n\pi 0}{10}} \sin\frac{n\pi x}{10} = \sum_{n=1}^{\infty} P_n \sin\frac{n\pi x}{10} = 100$

Here is a lateral jump that isn't obvious!!!! Remember from lecture 5-8 that the Half-range sine series is a sum of sine terms that can represent things like plucked guitar strings. Look how similar this is to the expression for *T(x,0)* if we set *L = 10* and *f(x)=100.*

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

So all we have to do now is calculate the half-range sine series in the usual way.

$$P_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx = \frac{2}{10}\int_0^{10} 100\sin\frac{n\pi x}{10}dx = -20\left[\frac{10}{n\pi}\cos\frac{n\pi x}{10}\right]_0^{10} = \frac{-200}{n\pi}\left(\cos\frac{10n\pi}{10} - \cos 0\right)$$

$$P_n = \frac{-200}{n\pi}\left(\cos\frac{10n\pi}{10} - \cos 0\right) = \frac{-200}{n\pi}\left(\cos n\pi - 1\right)$$

So in order for the boundary conditions for *T(x,0) = 100* to be satisfied, we must take the following values of P_n in the sum.

n	P_n
1	$\frac{-200}{\pi}(-1-1) = \frac{400}{\pi}$
2	$\frac{-200}{2\pi}(1-1) = 0$
3	$\frac{-200}{3\pi}(-1-1) = \frac{400}{3\pi}$

Finally we can state the full solution:-

$$T(x,y) = \sum_{n=1}^{\infty} P_n e^{\frac{-n\pi y}{10}} \sin\frac{n\pi x}{10} = \sum_{n=1}^{n=\infty\ odd} \frac{400}{\pi n}\left(e^{\frac{-n\pi y}{10}} \sin\frac{n\pi x}{10}\right)$$