LECTURE 8: Schrodinger's Equation

Goal of the lecture: introduce and derive Schrodinger's equation

What I expect you to learn: understand this derivation of Schrodinger's equation

Corresponds to sections 2.3 and 3.1 of textbook, see also French and Taylor

Schrödiger's equation (in 1 dimension):

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

- What is $\Psi(x,t)$?
- How was this partial differential equation derived?

→ we won't follow Schrödinger's derivation. We'll take a simpler, more direct path...

LET'S START SLOW...

we want to study non-relativistic particles.

so: $E = \frac{1}{2} m v^2 + V = \frac{p^2}{2m} + V$ (1)

from de Broglie's hypothesis we have

$\lambda = h/p$ or $p = \frac{h}{\lambda}$ $\rightarrow$ $k = \frac{2\pi}{\lambda}$

↳ wave number

$\Rightarrow \boxed{k = \frac{2\pi p}{h}}$ → notice $\boxed{k \propto p}$

we also have: $E = h\nu$, $\omega = 2\pi\nu$

$\Rightarrow \boxed{\omega = \frac{2\pi E}{h}}$ → $\boxed{\omega \propto E}$ → remember This

We have wave-related quantities (k, ω) associated with E and p

So: $p = k\hbar$ (2) $\quad \hbar = \frac{h}{2\pi}$

$E = \hbar\omega$ (3)

We insert (2) and (3) in (1) to get:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V \quad \Rightarrow \quad E = \frac{p^2}{2m} + V = \frac{mv^2}{2} + V$$

with $V = 0$ (free particle)

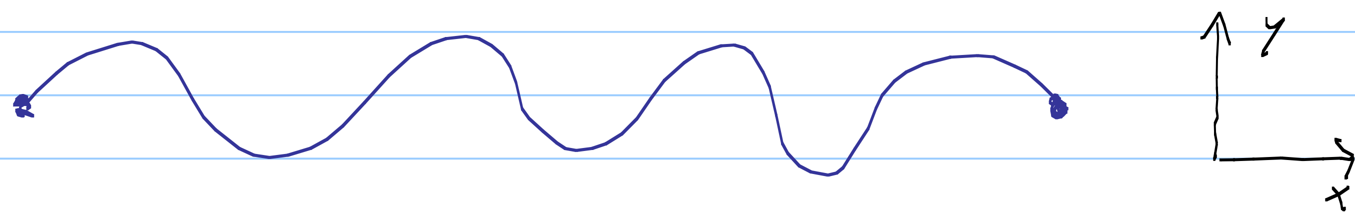
$$\boxed{\omega = \frac{\hbar k^2}{2m}} \quad (4)$$

We want wave equation that obeys (4)

i.e. $\omega \propto k^2$

LET'S LOOK AT A WAVE EQUATION FOR A SYSTEM WE KNOW AND SEE IF IT WILL WORK FOR QM:

WAVE EQUATION FOR IDEAL STRING CAN BE OBTAINED USING NEWTON'S 2^{nd} LAW



$$\frac{\partial^2 y}{\partial x^2} = \frac{\rho}{T}\frac{\partial^2 y}{\partial t^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} \qquad (5)$$

ρ: density per unit length
T: tension
v = velocity $= \sqrt{\frac{T}{\rho}}$

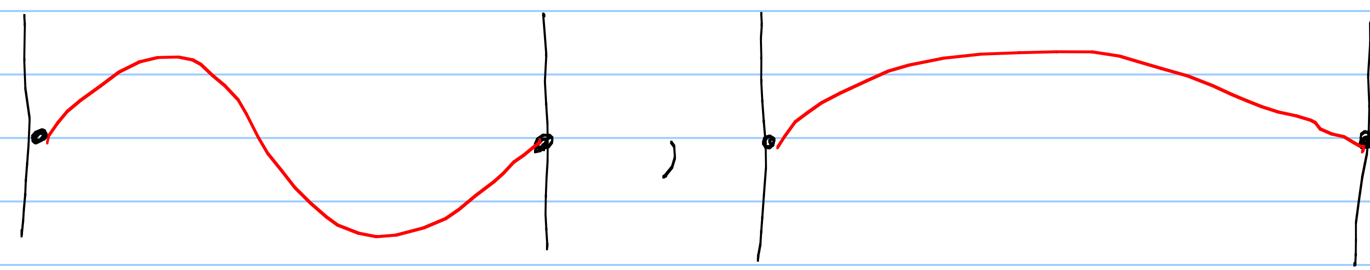
A solution of (5) is: $\boxed{y(x,t) = A \sin \frac{2\pi}{\lambda}(x - vt)}$ (6)

(6) $= A\sin(kx - \omega t)$

(6') and $A\sin(kx + \omega t)$ is also a solution

Let's start again with the string but try a different approach: "reverse engineering"

If I look at a string, I observe the solutions:



etc.

$\boxed{\text{Given the solution, can I find the equation?}}$

(7) $\longrightarrow$ $\frac{\partial y}{dx} = kA\cos(kx - \omega t)$ (used (6))

(8) $\longrightarrow$ $\frac{\partial y}{dt} = -\omega A\cos(kx - \omega t)$

So from 7 and 8, I have

$$\frac{\partial y}{\partial x} = -\frac{K}{w}\frac{\partial y}{\partial t} = -\frac{1}{v}\frac{\partial y}{\partial t} \qquad (9)$$

v = velocity of wave

9 looks okay but has a major flaw:

it only describes waves going in one direction

Had we started with 6: $A \sin(Kx + wt)$, the equation would have been: $\frac{\partial y}{\partial x} = \frac{K}{w}\frac{\partial y}{\partial t}$

this problem is solved if I use second derivatives

We found an equation for the string

Now we start trying to derive Schrödinger's equation.

Let's suppose $\boxed{\Psi(x,t) = A\sin(kx - \omega t)}$ is a solution to our wave equation. Then: $(y = \Psi(x,t))$

↳ **(worth a shot, it worked for the string...)**

(10) $\dfrac{\partial y}{\partial x} = Ak\cos(kx - \omega t)$, $\dfrac{\partial^2 y}{\partial x^2} = -Ak^2\sin(kx - \omega t)$ (11)

(12) $\dfrac{\partial y}{\partial t} = -A\omega\cos(kx - \omega t)$, $\dfrac{\partial^2 y}{\partial t^2} = -A\omega^2\sin(kx - \omega t)$ (13)

We need our equation to obey $\omega \propto k^2$

→ we get a k^2 from (11)

→ we get a ω from (12)

$\boxed{\text{But } \cos \neq \sin}$

Perhaps we started with the wrong solution

Let's try a complex solution

$$\psi(x,t) = A\, e^{i(kx-\omega t)}$$

$$\frac{\partial \psi}{\partial x} = iAk\, e^{i(kx-\omega t)} \quad (13) \qquad \frac{\partial^2 \psi}{\partial x^2} = -Ak^2 e^{i(kx-\omega t)} \quad (14)$$

$$\frac{\partial \psi}{\partial t} = -i\omega A\, e^{i(kx-\omega t)} \quad (15)$$

This looks good... : $\omega \propto k^2$

so

$$(14) = \frac{\partial^2 \psi}{\partial x^2} = -Ak^2 e^{i(kx-\omega t)} = -\frac{p^2}{\hbar^2}\psi$$

$$(15) = \frac{\partial \psi}{\partial t} = -i\omega A e^{i(kx-\omega t)} = -\frac{iE}{\hbar}\psi$$

Note: amplitude A is arbitrary.

So with $p^2 = 2mE$, we have:

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi = \frac{-i}{\hbar} 2m \frac{\partial \psi}{\partial t}$$ (look at 14 and 15 again)

with a potential: $p^2 = 2m(E-V) = \hbar^2 k^2$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2}(E-V)\psi = -i\frac{2m}{\hbar}\frac{\partial \psi}{\partial t} + \frac{2m}{\hbar^2}V\psi$$

which we can write in two forms

(16) $$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi}$$ time-independent

or

(17) $$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t}}$$ time dependent

So we found an equation starting from this solution : $\psi(x,t) = A e^{i(kx - \omega t)}$

Note that we could have found other differential equations that obeyed our constraint. But this one is simple, can be tested and shown to describe 'physical' reality.

Also, the solutions have some required properties:

- linearity: if A is a solution and B is a solution, $(A+B)$ is a solution

  → superposition principle

- allows ψ to be interpreted as a probability amplitude

  ↳ Probability has to be a real number

Another look at the solution:

$$\psi(x,t) = A\, e^{i(kx-\omega t)}$$

this describes an ordinary plane wave having wave number k and angular frequency ω

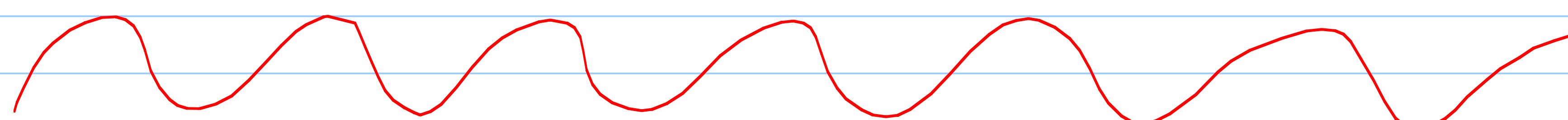
– remember that $p \propto k$

$p \to$ momentum

$k \to$ wave number

Why is this not a solution we would like to describe a particle in a certain region of space?

$\psi(x,t)$

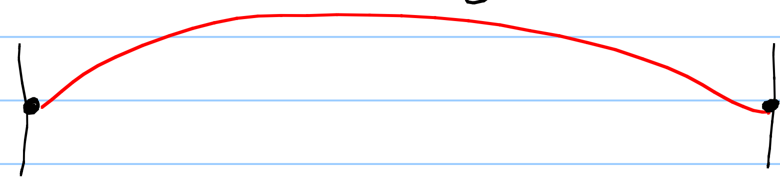


We'll need to add many plane waves to get a "good" solution...

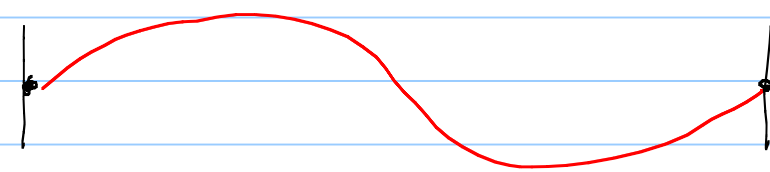
More on the solutions...

Let's go back to the string for now

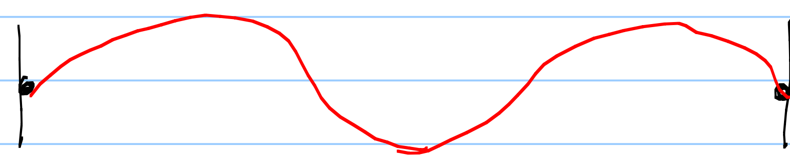
A



B



C



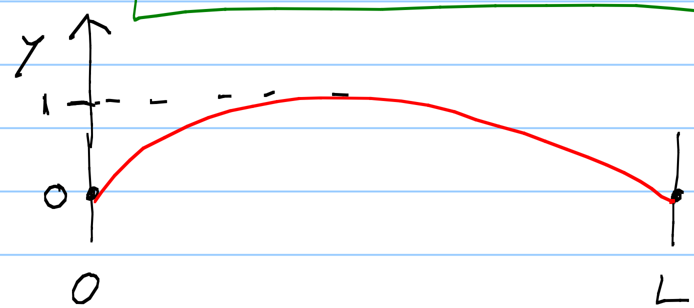
etc.

If you can get the string to vibrate as in A and also as in B, then you can get it to vibrate as the sum of A + B

So I could express a general solution as:

(18) $$y(x) = \boxed{\sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{L}} \longrightarrow \text{Fourier series}$$

Example:



$A_1 = 1$
$A_2 = 0$
$A_3 = 0$
...

Other examples: www.falstad.com/fourier

FOURIER SERIES (quick overview)

A Fourier series is an expansion of a periodic function in of series sines and cosines:

$$F(x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \sin nx + \sum_{n=1}^{\infty} B_n \cos nx$$

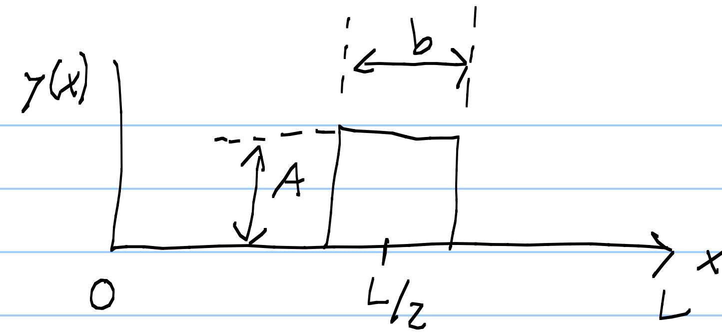
A_0, A_n, B_n are related to $F(x)$ through definite integrals.

$$\frac{dy}{dx} + p(x)y = 0$$

For solutions of linear homogeneous ordinary differential equation, the superposition principle holds: the solution to an arbitrary function is available if a sinusoid is a solution to the equation

→ some conditions apply: finite number of finite discontinuities etc.

Another example :



Our goal : To find what are the A_n ...

We will use the following relation :

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = 0 \quad \text{for } m \neq n$$

integers

multiply (18) on both sides by : $\sin\left(\frac{m\pi x}{L}\right)$

integrate to get :

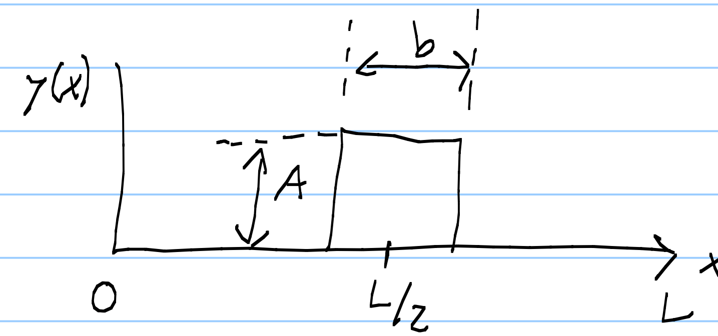
$$\int_0^L y(x) \sin\left(\frac{m\pi x}{L}\right) dx = \sum_{n=1}^{\infty} A_n \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right)$$

$$= A_n \int_0^L \sin^2\left(\frac{m\pi x}{L}\right) dx \qquad (19)$$

(19) $\rightarrow \int_0^L \sin^2\left(\frac{m\pi x}{L}\right) = \frac{L}{2}$ (for all values of m)

$$\Rightarrow A_n = \frac{2}{L}\int_0^L y(x)\,\sin\left(\frac{n\pi x}{L}\right)dx \qquad (20)$$

For our configuration we have:



$$A_n = \frac{2A}{L}\int_{(L-b)/2}^{(L+b)/2} \sin\left(\frac{n\pi x}{L}\right)dx$$

$$= \frac{2A}{n\pi}\left[\cos\frac{n\pi}{2L}(L-b) - \cos\frac{n\pi}{2L}(L+b)\right.$$

$$= \frac{4A}{n\pi}\sin\left(\frac{n\pi b}{2L}\right)\sin\left(\frac{n\pi}{2}\right)$$

$\rightarrow = 0$ if n is even

So, to recap:

- We tried to find a wave equation that obeyed the relation: $\boxed{\frac{\hbar k^2}{2m} \propto \omega}$

- We found a wave equation that could that but we had to change our solution!

- The solution to the wave equation that obeyed the relation above was complex

- The simplest solution, being a plane wave, does not represent a particle confined within a certain region of space

- Using Fourier Series, we saw how one could add plane waves to model arbitrary periodic functions.

- Next time, we'll introduce Fourier integral analysis and Fourier transforms to help us describe microsopic particles