Lecture #4: The Classical Wave Equation and Separation of Variables

Last time:

Two-slit experiment

* 2 paths to same point on screen
* 2 paths differ by $n\lambda$: constructive interference
* *1 photon interferes with itself*
* get 1 dot on screen: collapse of "state of system" to a single dot
* to determine the state of the system, need many experiments, many dots.

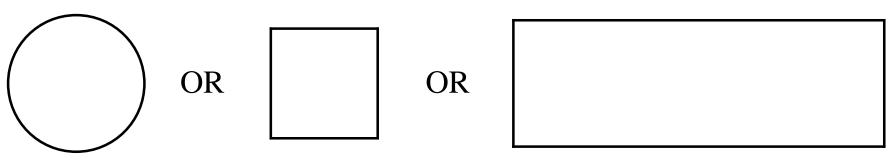
Joint uncertainty of z and p_z

Probability amplitude distribution (encodes 10, 01, or 11 where 1 = open, 0 = closed) collapses to single dot due to the act of detection of a photon. Destructive measurement.

Quantum Mechanics: information about the experimental setup (i.e. "the system") is "encoded" in results of a sequence of independent experiments. Seems mysterious.

Musicians know that the sound produced by an instrument reveals:

* detailed physical structure of the instrument
  e.g. drum head shaped as



* technique of musician

Same as for Quantum Mechanics.

Today: philosophy
wave equation
separation of variables
boundary conditions → normal modes
superposition of normal modes: "the pluck"
cartoons of motion

What do we know so far?

weirdness
wave-particle duality
interference
experiment samples probability *amplitude* (i.e. + or –) distribution
we can't see inside microscopic systems
we do experiments that *indirectly (and destructively) reveal* structure and mechanism
patterns- e.g. interference structure – reveal *structure* and *mechanism*
spectrum contains patterns

1st 1/2 of 5.61 deals with four exactly solved problems

Particle in a Box
Harmonic Oscillator
Rigid Rotor
Hydrogen Atom

These problems are templates for our Quantum Mechanical understanding of reality
Perturbation Theory will show us how to use the patterns associated with these simple problems to represent, decode, and understand reality.

I have been told many times that 5.61 is very difficult because it is very mathematical.

This lecture might be the most mathematical of the entire 5.61 course.

The goal is insight. For chemists, this is usually pictorial and qualitative.

I intend to show the pictures and insights behind the equations.

What are you expected to do when faced with one of the many differential equations in Quantum Mechanics?

1. Know where the differential equation comes from (not derive it)

2. Know standard methods used (by others) to solve it.

   * An example of an extremely common "second order" Ordinary Differential Equation:
   $$\frac{d^2 f}{dx^2} = kf \ .$$
   There are always 2 linearly independent general solutions for a 2^{nd}-order equation.
   * find a way to rewrite your equation as one of the well-known solved equations
   * separation of variables

What are we looking for?

* general solutions
- nodes (adjacent node spacing is $\lambda/2$)
- envelope (related to probability)
- phase velocity

* specific physical system, specific solution
- Boundary conditions
- usually get some sort of quantization from the 2nd boundary condition
- "normal modes"
- qualitative sketch: nodes, envelope, frequency of each normal mode

* initial condition: the **"**pluck**"**
- superposition of normal modes
- localization, motion, dephasing, rephasing

Combine all of this into a description of the physical system.

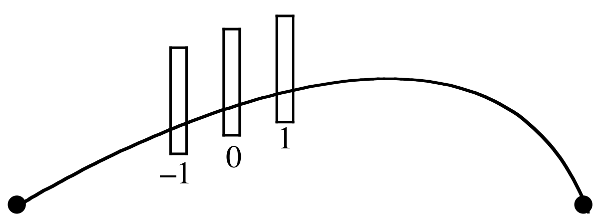
Wave Equation: where does it come from?

Hooke's Law (for a spring)

$$F = -kx$$

displacement

force constant



chop string into small segments, located at positions $\{x_i\}$ along the string

segment –1 pulls segment 0 down by force
$-k\,[u(x_0) - u(x_{-1})]$ **where** ($u(x_i)$ is the displacement of the segment at x_i.)

segment +1 pulls segment 0 up by force
$-k\;[u(x_0) - u(x_{+1})]$

The net force is

$$-k\underbrace{\left[\Delta u_{10} - \Delta u_{0-1}\right]}_{\text{This is } \frac{d^2u}{dx^2}} \text{ a difference of displacments.}$$

$$\frac{\partial^2 u}{\partial x^2} \qquad \frac{\partial^2 u}{\partial t^2}$$

F = ma (units conversion: **"m"** contains **information about** tension and mass of string)

wave equation is $\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$

u is displacement
v is a constant needed for consistency of units, which turns out to be velocity (as you will discover later)

How do we solve this second-order, linear, partial differential equation?

* look for a similar, exactly solved problem
* employ bag of tricks

most important trick is **separation of variables**

try $u(x,t) = X(x)\,T(t)$

does it work? If it does not, we will get $u(x,t) = 0$ (the "trivial solution")

$$\frac{\partial^2}{\partial x^2}\left[X(x)T(t)\right] = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\left[X(x)T(t)\right]$$

not operated on by $\frac{\partial}{\partial x}$

not operated on by $\frac{\partial}{\partial t}$

Multiply both sides of the equation on the left by $\frac{1}{X(x)T(t)}$. $T(t)$ cancels on LHS, $X(x)$ cancels on RHS.

Get

$$\underbrace{\frac{1}{X(x)}\frac{\partial^2 X}{\partial x^2}}_{\text{only } x} = \frac{1}{v^2}\underbrace{\frac{1}{T(t)}\frac{\partial^2 T}{\partial t^2}}_{\text{only } t}$$

x and t are independent variables. This equation can only be satisfied if both sides are equal to a constant. Called the *separation constant*.

$$\frac{1}{X}\frac{d^2X}{dx^2} = K \qquad \frac{1}{v^2}\frac{1}{T}\frac{d^2T}{dt^2} = K$$

Note: we now have *total* not *partial* derivatives: linear, 2nd-order, and ordinary differential equations.

general solutions for *X(x)* have the form

K > 0	e^{+kx}, e^{-kx}	let $K = k^2$
OR		
K < 0	sin kx, cos kx	let $K = -k^2$

(always have 2 linearly independent solutions for 2nd-order equation)

K > 0	general solution	$X(x) = Ae^{kx} + Be^{-kx}$
K < 0	general solution	$X(x) = C \sin kx + D \cos kx$

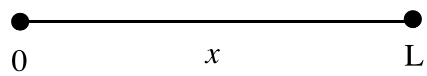
also for *T(t)* equation

$$\frac{d^2T}{dt^2} = v^2 KT$$

K > 0 $T(t) = Ee^{vkt} + Fe^{-vkt}$

K < 0 $T(t) = G \sin vkt + H \cos vkt$.

Now look at Boundary Conditions



$$\left.\begin{array}{l} u(0,t)=0 \\ u(L,t)=0 \end{array}\right\} \text{ ends of string are tied down.}$$

For <u>K > 0</u>, try to satisfy boundary conditions

$$X(0)=Ae^{0}+Be^{-0}=0$$

$$A+B=0 \qquad \therefore A=-B$$

$$X(L)=0=Ae^{kL}+Be^{-kL}=A\left(e^{kL}-e^{-kL}\right)$$

$e^{kL}-e^{-kL}$ can never be 0

$A=0 \qquad u(x,t)=0 \qquad$ a trivial solution.

looks bad. What about <u>K < 0</u> solutions?

$$X(0)=C\sin 0+D\cos 0=0$$

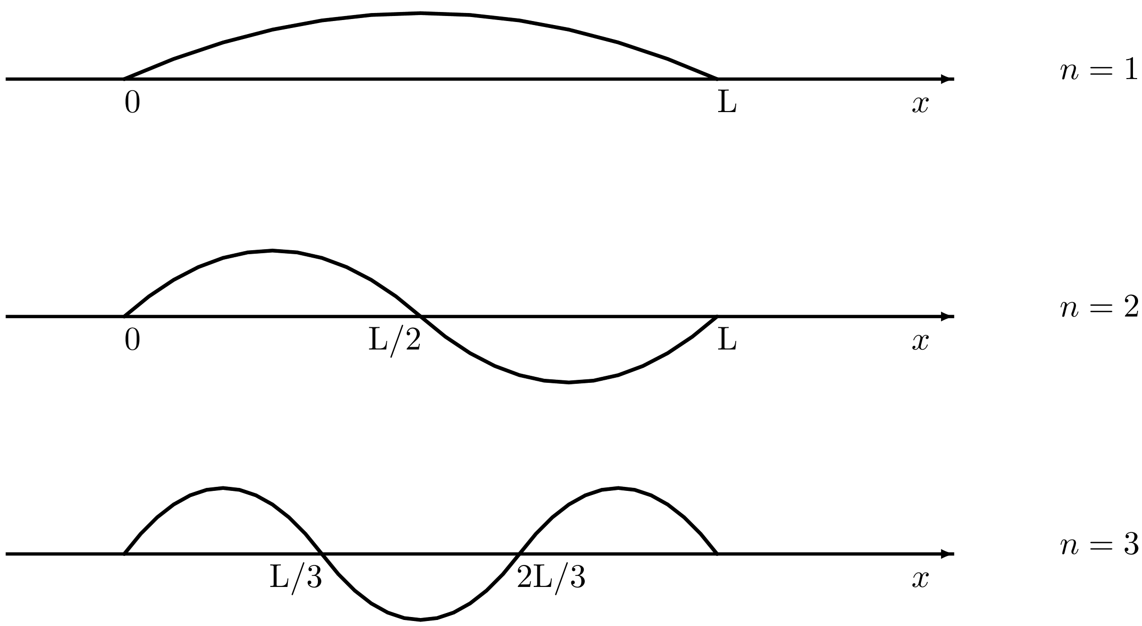
$$D=0$$

$$X(L)=C\sin kL+0=0$$

$$kL=n\pi \qquad n=0,1,2,\ldots$$

"quantization" $\qquad k_n=\dfrac{n\pi}{L} \qquad$ (without Quantum Mechanics)

Pictures are drawn without looking at $X(x)$ equation or using a computer to plot them.



Identical segments with alternating signs!

- # nodes is $n-1$
- nodes are equally spaced at $x = L/n$, $\lambda_n = 2(L/n)$.
- all lobes are the same, except for alternating sign of amplitude

Wonderful qualitative picture: cartoon = insight = memorable

Now look at $T(t)$ equation for $K < 0$.

$$T(t) = E\sin vk_n t + F\cos vk_n t$$

$$\omega_n \equiv vkn$$

$$T(t) = E_n \sin\omega_n t + F_n \cos\omega_n t$$

Normal modes, combining $X(x)$ and $T(t)$:

$$u_n(x,t) = \left(A_n \sin\frac{n\pi}{L}x\right)\left(E_n \sin n\omega t + F_n \cos n\omega t\right)$$

The two-term time-dependent factor of the n$^{\text{th}}$ normal mode can be rewritten in "frequency, phase" form as

$$E_n' \cos\left[n\omega t + \phi_n\right].$$

The next step is to consider the $t = 0$ pluck of the system. This pluck is always expressable as a linear combination of the normal modes.

$$u_{\text{pluck}}(x,t) = \sum_{n=1}^{\infty} \left(A_n E_n'\right) \sin\left(\frac{n\pi}{L} x\right) \cos\left(n\omega t + \phi_n\right).$$

There is a further simplification based on the trigonometric formula

$$\sin a \cos b = \frac{1}{2}\left[\sin(a+b) + \sin(a-b)\right]$$

which enables us to write u_{pluck} as

$$u_{\text{pluck}}(x,t) = \sum_{n=1}^{\infty} \left[\frac{A_n E_n'}{2}\right] \left\{\sin\left(\frac{n\pi}{L} x + n\omega t + \phi_n\right) + \sin\left(\frac{n\pi}{L} x - n\omega t - \phi_n\right)\right\}$$

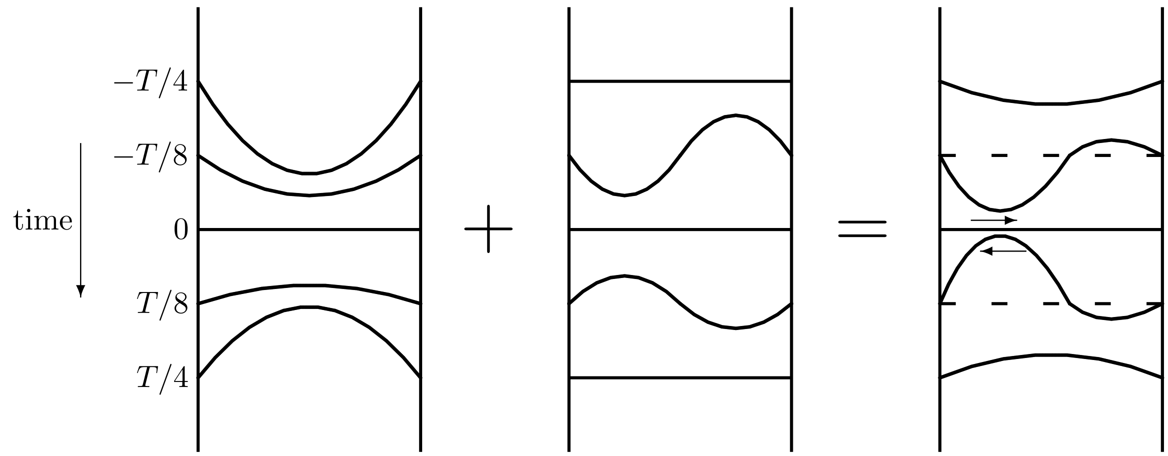
Something wonderful happens now:

* A single normal mode is a standing wave with no left-right motion, no "breathing".

* A superposition of 2 or more normal modes with different values of n gives more complicated motion. For two normal modes, where one is even-n and the other is odd-n, the time-evolving "wavepacket" will exhibit left-right motion. For two normal modes where both are odd or both even, the wavepacket motion will be "breathing" rather than left-right motion.

Here is a crude time lapse movie of a superposition of the $n = 1$ and $n = 2$ (fundamental and first overtone) modes.

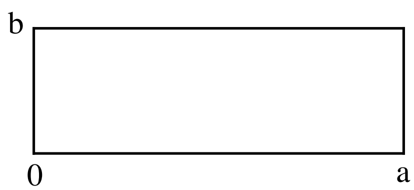
The period of the fundamental is $T = \frac{2\pi}{\omega}$. We are going to consider time-steps of T/8.



The time-lapse movie of the sum of two normal modes can be viewed as moving to left at $t = -T/4$, close to the left turning point at $t = -T/8$, at the left turning point but dephased at $t = 0$, moving to the right at $t = +T/8$. It will reach the right turning point but dephased at $t = T/2$. See McQuarrie, Figure 2.4.

In Quantum Mechanics you will see wavepackets that exhibit motion, breathing, dephasing, and rephasing. The "center of the wavepacket" will follow a trajectory that obeys Newton's laws of motion.

If we generalize from waves on a string to waves on a rectangular drum head,



the separable solution to the wave equation will have the form

$$u(x, y, t) = X(x)Y(y)T(t).$$

There will be two separation constants, and we will find that the normal mode frequencies are

$$\omega_{nm} = v\pi\left[\frac{n^2}{a^2} + \frac{m^2}{b^2}\right]^{1/2}$$

This is a more complicated quantization rule than for waves on a string, and it should be evident to an informed listener that these waves are on a rectangular drum head with edge lengths a and b. Why are real drum heads round?

NON-Lecture

There is an underlying unity of the e^{kx}, e^{-kx} and sin kx, cos kx solutions to

$$\frac{d^2y}{dx^2} = k^2 y.$$

Let's take a step back and look at the two simplest 2nd-order ordinary differential equations:

$$\frac{d^2y}{dx^2} = +k^2 y \rightarrow y(x) = Ae^{kx} + Be^{-kx} \qquad \textbf{(I)}$$

and

$$\frac{d^2y}{dx^2} = -k^2 y \rightarrow y(x) = C\sin kx + D\cos kx \qquad \textbf{(II)}$$

The solutions to these two equations are more similar than they look at first glance.

<u>Euler's formula</u> $(i \equiv (-1)^{1/2})$

$$e^{\pm i\theta} = \cos\theta \pm i\sin\theta \qquad \text{OR} \qquad \frac{1}{2}\left(e^{i\theta} + e^{-i\theta}\right) = \cos\theta$$

$$\frac{i}{2}\left(e^{-i\theta} - e^{i\theta}\right) = \sin\theta.$$

So we can express the solution of the second **(II)** differential equation in (complex) exponential form to bring out its similarity to the solution of the first **(I)** differential equation:

$$y(x) = C\sin kx + D\cos kx$$

$$= \frac{i}{2}C\left(e^{-ikx} - e^{ikx}\right) + \frac{1}{2}D\left(e^{ikx} + e^{-ikx}\right)$$

rearrange

$$= \frac{1}{2}(D - iC)e^{ikx} + \frac{1}{2}(D + iC)e^{-ikx}.$$

The (sin θ, cos θ) and $\left(e^{in}, e^{-in}\right)$ forms are two sides of the same coin. Insight. Convenience. What do we notice? *The general solutions to a 2^{nd}-order differential equation consist of the sum of two linearly independent functions, each multiplied by an unknown constant.*