LECTURE 16: General Solution to the Infinite Well (adding time dependence)

Goals of the 1-d lectures: learn how to solve Schrodinger's equation for some simple problems

What I expect you to learn:

- How to solve the time depenedent infinite well problem the free particle wave-function

- Develop your understanding of how quantum systems evolve with time

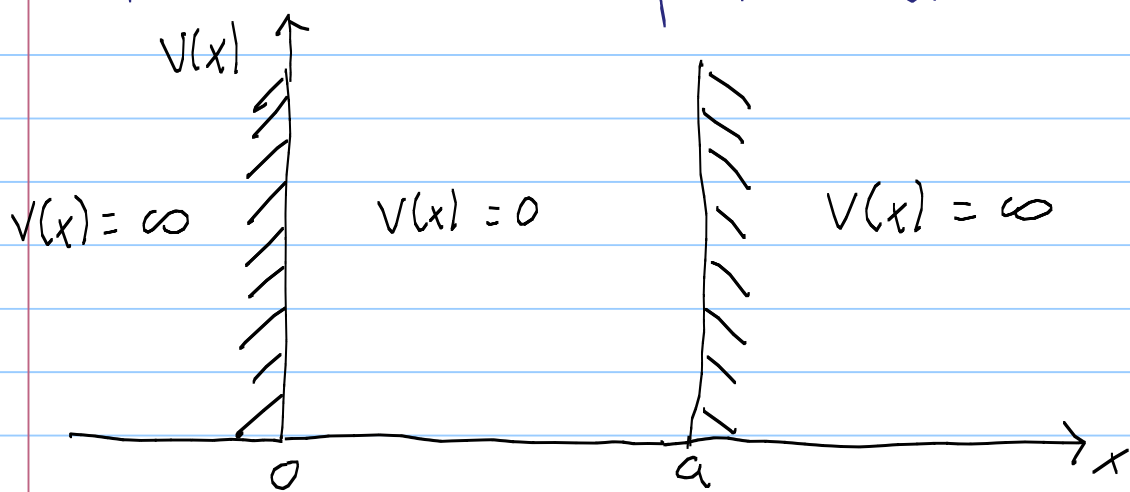
(Roughly corresponds to sections 3.5-4.5 of textbook)

Midterm: Wednesday Oct 25th at 11:00 IN CLASS

INFINITE WELL RECAP:

The infinite potential well:

$$\boxed{\begin{array}{lll} V(x) & = \infty & x < 0 \\ & = 0 & 0 < x < a \\ & = \infty & a < x \end{array}}$$



- We found that the solutions yielded quantised values:

$$\Rightarrow K_n = \frac{n\pi}{a} \quad \Rightarrow \quad p_n = \frac{n\pi\hbar}{a} \quad \Rightarrow \quad \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

- Solutions could be written as: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$
- The general solution could be written as:

$$\psi(x) = \sum_{n=1}^{\infty} A_n \psi_n(x), \quad \text{with} \quad A_m = \int_0^a dx\, \psi_m^*(x)\, \psi(x)$$

INFINITE WELL RECAP:

WE SAW THAT $\langle H \rangle = \sum_{n=1}^{\infty} E_n |A_n|^2$

with $\int_0^a \psi(x)^* \psi(x)\, dx = 1$, $\psi(x) = \sum_{n=1}^{\infty} A_n \psi_n(x)$, we have

$$1 = \int_0^a dx\, \psi^*(x) \sum_n A_n \psi_n(x) = \sum_n A_n A_n^* = \sum_n |A_n|^2 = \sum_n p_n$$

$\Rightarrow$ p_n : probability of finding particle with energy E_n

$$\langle H \rangle = \sum_n E_n p_n$$

We postulated that a measurement of the energy of the particle in the infinite well would yield an energy eigenvalue and would leave the wave function in an energy eigenstate (eigenfunction).

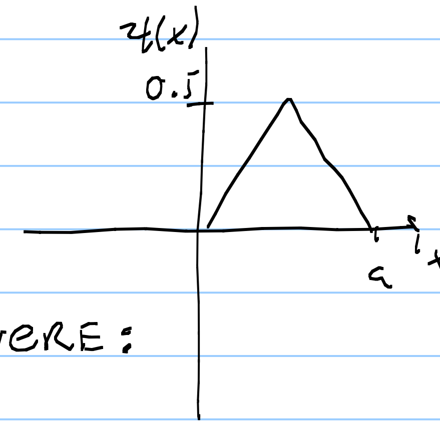
To answer the question: what is the probablility of measuring a given energy eigenvalue (En) , I need to calculate the amplitude (An)

INFINITE WELL RECAP:

We saw the following example

CONSIDER A PARTICLE IN AN INFINITE WELL WITH THE FOLLOWING WAVE FUNCTION:

$$\psi(x) = A(x/a) \;, \quad 0 < x < a/2$$
$$= A(1 - x/a) \;, \quad a/2 < x < a$$



THE SOLUTIONS WE FOUND FOR THE A_n WERE:

$$\Rightarrow |A_n|^2 = \frac{96}{\pi^4 n^4} \quad \text{for odd } n,$$
$$= 0 \quad \text{for even } n$$

$P_1 = 98.6\%$
$P_3 = 1.2\%$
$P_2 = 0 = P_4$ etc.

GENERAL SOLUTION FOR A TIME INDEP. POTENTIAL

WE SAW THAT WE COULD EXPRESS $\Psi(x,t) = \psi(x) F(t)$

WHERE $F(t) = C \exp\left(-iEt/\hbar\right)$ or $C(T_0) \exp\left[\frac{-iE}{\hbar}(t - T_0)\right]$

WE HAVE $\psi(x) = \sum_n A_n \psi_n(x)$

$$\Rightarrow \Psi(x,t) = \sum_n A_n \psi_n(x)\, C(T_0) \exp\left[\frac{-iE_n}{\hbar}(t - T_0)\right]$$

we could rewrite $\Psi(x,t) = \sum_n A_n \psi_n(x) \exp\left(-iEt/\hbar\right)$

with $A_n = C_n(T_0) \exp\left(iE_n T_0/\hbar\right)$

IF WE KNOW THE WAVE FUNCTION Ψ AT A PARTICULAR TIME T_0, we can DETERMINE Ψ FOR ALL VALUES OF T:

$$A_n = \exp\left(iET_0/\hbar\right) \int \psi_n^*(x)\, \Psi(x, T_0)\, dx$$

$$\Psi(x,t) = \sum_n \left[\int \psi_n^*(x')\, \Psi(x', T_0)\, dx'\right] \psi_n(x) \exp\left[\frac{-iE}{\hbar}(t - T_0)\right]$$

GENERAL SOLUTION FOR A TIME INDEP. POTENTIAL

So we have: $\Psi(x,t) = \sum_n A_n \psi_n(x) \exp(-iEt/\hbar)$

$P(x,t) = \Psi^*(x,t)\,\Psi(x,t)$

$$= \sum_n \sum_m A_m^* A_n \exp\left[-i(E_n - E_m)t/\hbar\right] \psi_m^*(x)\,\psi_n(x)$$

$$= \sum_n |A_n|^2 |\psi_n|^2 + \sum_n \sum_{\substack{m \\ n \neq m}} A_m^* A_n \exp\left[\frac{-it}{\hbar}(E_n - E_m)\right] \psi_m^*(x)\,\psi_n(x)$$

→ Pure eigenstates have no time dep.

→ the larger the ΔE, the faster the probability evolves versus time

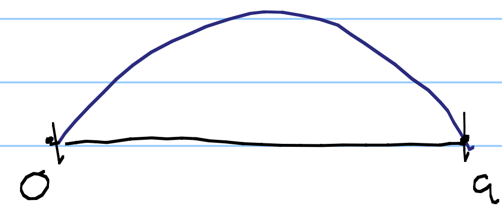
→ $P(x,t)$ is time dependent, physical quantities will in general depend on time. Show however that $\langle H \rangle$ does not depend on time (exercise).

BACK TO THE INFINITE WELL

CONSIDER THE FOLLOWING WAVE FUNCTION (at $T=0$)

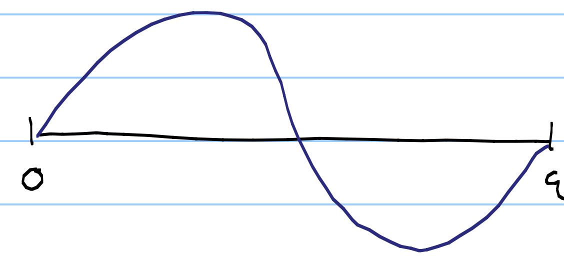
$$\psi(x) = A\sin\left(\frac{\pi x}{a}\right) + A\sin\left(\frac{2\pi x}{a}\right)$$

$\psi(x) =$



$n=1$

$+$



$n=2$

$$\psi(x,t) = \underbrace{A\sin\left(\frac{\pi x}{a}\right)}_{F_1} e^{\frac{-iE_1}{\hbar}T} + \underbrace{A\sin\left(\frac{2\pi x}{a}\right)}_{F_2} e^{\frac{-iE_2}{\hbar}T}$$

$$\psi(x,t) = F_1\, e^{-iE_1T/\hbar} + F_2\, e^{-iE_2t/\hbar}$$

$$P(x,t) = \left(F_1\, e^{iE_1T/\hbar} + F_2\, e^{iE_2T/\hbar}\right)\left(F_1\, e^{-iE_1T/\hbar} + F_2\, e^{-iE_2T/\hbar}\right)$$

$$= F_1^2 + F_2^2 + F_1F_2\left[e^{i(E_1-E_2)T/\hbar} + e^{-i(E_1-E_2)t/\hbar}\right]$$

$$= F_1^2 + F_2^2 + 2F_1F_2\cos\left(\frac{T}{\hbar}(E_1-E_2)\right)$$

THE INFINITE WELL (cont.)

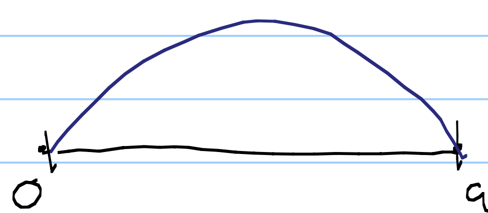
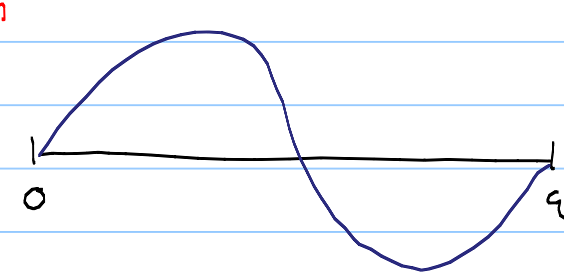
$$P(x,t) = F_1^2 + F_2^2 + 2F_1F_2 \cos\left(\frac{t}{\hbar}(E_1 - E_2)\right)$$

oscillates between $(F_1+F_2)^2$ and $(F_1-F_2)^2$

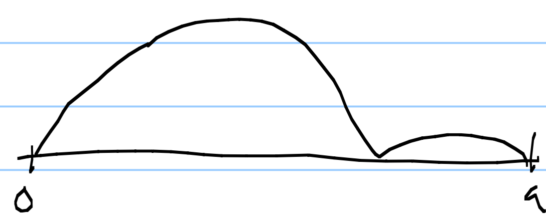
we have $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$, $E_2 = \frac{4\hbar^2\pi^2}{2ma^2}$, $E_1 - E_2 = -3E_1$

$\Rightarrow \frac{3E_1}{\hbar} T = \pi, 3\pi, 5\pi, \ldots$

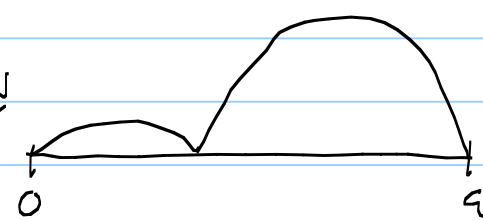
$\rightarrow$ obtain same config. when $\frac{3E_1}{\hbar} T = 2\pi, 4\pi, \ldots$

$\psi(x) =$  + 

$T = \frac{\hbar\pi}{3E_1}$

$P(x,0) =$ 

$P(x,t)$



THE INFINITE WELL (CONT.)

WAVE FUNCTION REGENERATION:

AN INFINITE WELL WAVE FUNCTION WILL RECOVER IT'S ORIGINAL SHAPE AFTER A CERTAIN TIME $= \frac{2\pi\hbar}{E_1} = T_R$

First note that $E_n = n^2 E_1$

we write $\Psi(x, T_r) = \sum_{n=1}^{\infty} A_n \Psi_n(x) \exp\left[-i n^2 E_1 \frac{2\pi}{E_1}\right]$

$$= \sum_{n=1}^{\infty} A_n \Psi_n(x) \exp(-i n^2 \cdot 2\pi)$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$\rightarrow \sum_{n=1}^{\infty} A_n \Psi_n(x) \left(\cos(-n^2 \cdot 2\pi) + i\sin(-n^2 \cdot 2\pi)\right)$$

$\Rightarrow$ Wave function is regenerated at times $mT_R = \frac{m2\pi\hbar}{E_1}$

THE INFINITE WELL (cont.)

For the rest of the lecture we'll take a look at the solution to our last infinite well example and visualise other infinite well examples.

Here's some homework to improve your intuition: play with the infinite well simulation at:

www.flastad.com/qm1d/

-take a look at various eigenstates and superpositions of eigenstates
-Use a superposition of 2 eigenstates. Does the system evolve more quickly if the energy difference is greater?
-Measure the energy: what happens to the wave function?
-what happens when you change the particle's mass
-what happens when you change the well's width
-can you observe wave function regeneration for a complicated superposition of eigenstates
-etc.

$\boxed{\text{Example}}$ Infinite well Problem with Time dep.

A PARTICLE OF MASS m IS TRAPPED IN AN INFINITE WELL OF LENGTH a. THE WAVE FUNCTION AT $T=0$ IS:

$$\psi(x,0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)$$

where A is a REAL CONSTANT

1- FIND A
2- IF ENERGY IS MEASURED WHAT ARE THE POSSIBLE VALUES AND THEIR PROBABILITIES
3- WHAT IS THE AVERAGE ENERGY
4- FIND $\psi(x,t)$
5- WHAT IS THE PROBABILITY OF FINDING THE SYSTEM IN THE STATE $\varphi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{5\pi x}{a}\right)$
6- WRITE THE PROBABILITY DENSITY $P(x,t)$

1- LET'S REWRITE THE WAVE FUNCTION $\psi(x)$ IN TERMS OF THE EIGEN FUNCTIONS $\psi_n(x)$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\Rightarrow \psi(x) = \frac{A}{\sqrt{2}} \psi_1(x) + \sqrt{\frac{3}{10}} \psi_3(x) + \sqrt{\frac{1}{10}} \psi_5(x)$$

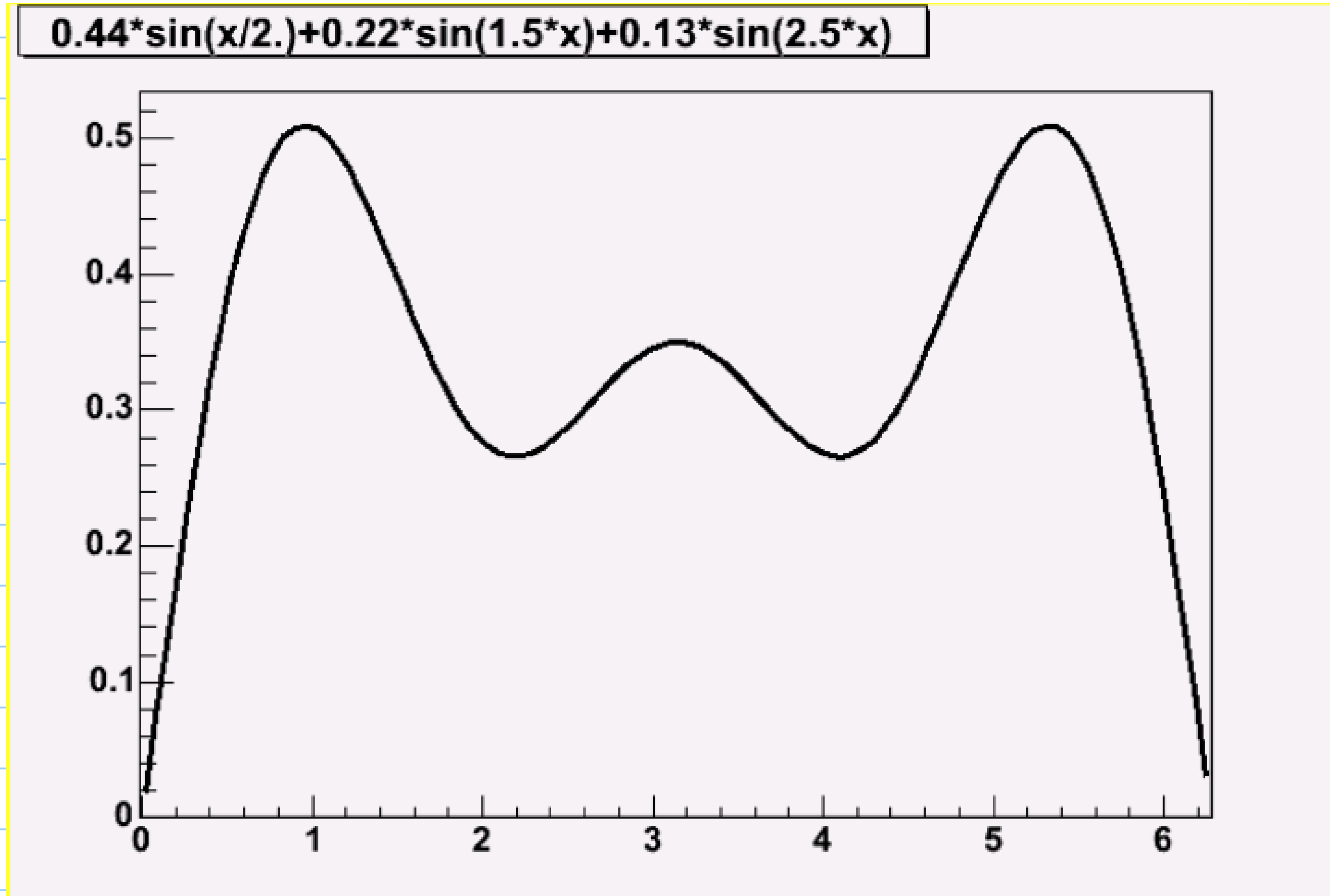
$$\int_{-\infty}^{\infty} \psi_n(x)^* \psi_m(x)\, dx = \delta_{nm} \Rightarrow \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} = 1$$

$$\frac{5A^2}{10} + \frac{4}{10} = \frac{10}{10}$$

$$A^2 = \frac{6}{5} \Rightarrow A = \sqrt{\frac{6}{5}}$$

or $$\psi(x) = \sqrt{\frac{3}{5}} \psi_1(x) + \sqrt{\frac{3}{10}} \psi_3(x) + \sqrt{\frac{1}{10}} \psi_5(x)$$

$$\psi(x) = \sqrt{\frac{3}{5}}\,\psi_1(x) + \sqrt{\frac{3}{10}}\,\psi_3(x) + \sqrt{\frac{1}{10}}\,\psi_5(x)$$ 13



2- $\psi(x)$ is composed of 3 eigenstates $\Rightarrow$ there 3 possible values for the energy measurement

$$E_1 = \pi^2\hbar/2ma^2$$
$$E_3 \quad 9\pi^2\hbar/2ma^2$$
$$E_5 \quad 25\pi^2\hbar/2ma^2$$

THE PROBABILITY OF MEASURING E_n CAN BE OBTAINED BY:

with $\int_0^a \psi(x)^* \psi(x)\, dx = 1$, $\psi(x) = \sum_{n=1}^{\infty} A_n \psi_n(x)$, we have

$$1 = \int_0^a dx\, \psi^*(x) \sum_n A_n \psi_n(x) = \sum_n A_n A_n^* = \sum_n |A_n|^2 = \sum_n P_n$$

$$\rightarrow P_1 = |A_1|^2 = \left|\sqrt{\tfrac{3}{5}}\right|^2 = \frac{3}{5}$$

$$P_3 = 3/10$$

$$P_5 = 1/10$$

THE AVERAGE ENERGY IS GIVEN BY:

$$\langle H\rangle = \sum_n E_n p_n \quad , \quad E_n = n^2 E_1$$

$$= \frac{3}{5}\cdot E_1 + \frac{3}{10}\cdot 9E_1 + \frac{1}{10}\cdot 25 E_1 = \frac{58}{10} E_1$$

$$= \frac{58}{10}\cdot\frac{\pi^2\hbar^2}{2ma^2} = \frac{29}{10}\,\frac{\pi^2\hbar^2}{2ma^2}$$

$$\Psi(x,t) = \sqrt{\frac{3}{5}}\,\psi_1(x)\,e^{-iE_1t/\hbar} + \sqrt{\frac{3}{10}}\,\psi_3(x)\,e^{-iE_3t/\hbar} + \sqrt{\frac{1}{10}}\,\psi_5(x)\,e^{-iE_5t/\hbar}$$

THE AMPLITUDE FOR FINDING THE SYSTEM IN STATE:

$\varphi(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{5\pi x}{a}\right) e^{-iE_5t/\hbar}$ WILL BE GIVEN BY

$$A_n = \int_0^a \psi_n^*(x)\,\varphi(x)\,dx = \sqrt{\frac{1}{10}}\int_0^a \psi_n^*(x)\,e^{-iE_5t/\hbar}\,\psi_5(x)\,dx$$

$$A_5 = \sqrt{\frac{1}{10}}\,e^{-iE_5t/\hbar} \quad , \quad P_5 = |A_5|^2 = \frac{1}{10}.$$

6- Probability density

WE HAVE:

$$\Psi(x,t) = \underbrace{\sqrt{\frac{3}{5}}\,\psi_1(x)}_{a(x)}\, e^{-iE_1 t/\hbar} + \underbrace{\sqrt{\frac{3}{10}}\,\psi_3(x)}_{b(x)}\, e^{-iE_3 t/\hbar} + \underbrace{\sqrt{\frac{1}{10}}\,\psi_5(x)}_{c(x)}\, e^{-iE_5 t/\hbar}$$

$E_3 = 9E_1$, $E_5 = 25E_1$, let $\varepsilon = \frac{E_1}{\hbar}$

$$P(x,t) = \Psi^*(x,t)\,\Psi(x,t)$$

$$= \left(a(x)\,e^{i\varepsilon t} + b(x)\,e^{i9\varepsilon t} + c(x)\,e^{i25\varepsilon t}\right) \times$$
$$\left(a(x)\,e^{-i\varepsilon t} + b(x)\,e^{-i9\varepsilon t} + c(x)\,e^{-i25\varepsilon t}\right)$$

$$= a^2(x) + b^2(x) + c^2(x) + a(x)b(x)\,e^{-i8\varepsilon t} + a(x)c(x)\,e^{-i24\varepsilon t}$$
$$+ b(x)a(x)\,e^{i8\varepsilon t} + b(x)c(x)\,e^{-i16\varepsilon t} + c(x)a(x)\,e^{+i24\varepsilon t} + c(x)b(x)\,e^{i16\varepsilon t}$$

$$= a^2(x) + b^2(x) + c^2(x) + 2a(x)b(x)\cos(8\varepsilon t) + 2a(x)c(x)\cos(24\varepsilon t) +$$
$$2b(x)c(x)\cos(16\varepsilon t)$$