LECTURE 15: The Time-Independent Schrodinger Equation, Stationary States, and the Infinite Well.

Goals of the lecture: Solve our first one-dimensional problem: the infinite potential well

What I expect you to learn:

- How to obtain and when to use the time-indep. Schrodinger equation
- How to solve the infinite potential well problem
- What is the expansion postulate and its physical interpretation

(Roughly corresponds to sections 3.5 and 4.5 of textbook)

The Time-Indepedent Schrodinger Equation

Recall the time dependent Schrodinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(r,t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \right] \psi(r,t) \qquad (1)$$

For the case where the potential V does not depend on t, we can use the method of separation of variables to split the wave function into a postition-dependent part and a time dependent part:

$$\psi(r,t) = \psi(r) \cdot F(t) \qquad (2).$$

Substitute (2) into (1):

$$i\hbar\, \psi(r) \frac{\partial F(t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r)\psi(r) \right] F(t)$$

divide both sides by: $\psi(r) F(t)$:

$$\underbrace{i\hbar \frac{1}{F(t)} \frac{\partial F(t)}{\partial t}}_{(3)\ \text{Time dep. only}} = \underbrace{\frac{1}{\psi(r)} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r)\psi(r) \right]}_{(4)\ \text{position dep. only}}$$

$\Rightarrow$ both sides must be equal to a constant

The Time-Indepedent Schrodinger Equation

LET'S START WITH EQUATION (3): $i\hbar \frac{1}{F(t)} \frac{\partial F(t)}{\partial t} = E \qquad (5)$

dimension of E

MATH BREAK (you should learn (6) and (7))

MOUSE PROBLEM IN MY HOUSE, STARTS IN THE FALL. LET N_0 be number of mice who got in. Now, the mice start to reproduce... How does N change with time? Let α be related to the number of females and how often they give birth. then:

$$\frac{dN}{dt} = \alpha N \qquad (6)$$

the solution to (6) is: $N = N_0 e^{\alpha t} \qquad (7)$

α is positive in my house. I've neglected the death rate for now (until I buy traps...)

The Time-Indepedent Schrodinger Equation

So the solution to 5 is then:

$$F(t) = C \exp\left(\frac{-iEt}{\hbar}\right) \quad (8)$$

we can set $C = 1$ and let $\psi(r)$ carry the required normalization:

$$\boxed{\psi(r,t) = \psi(r) \exp\left(\frac{-iEt}{\hbar}\right) \quad (9)}$$

We can write equation 4 as

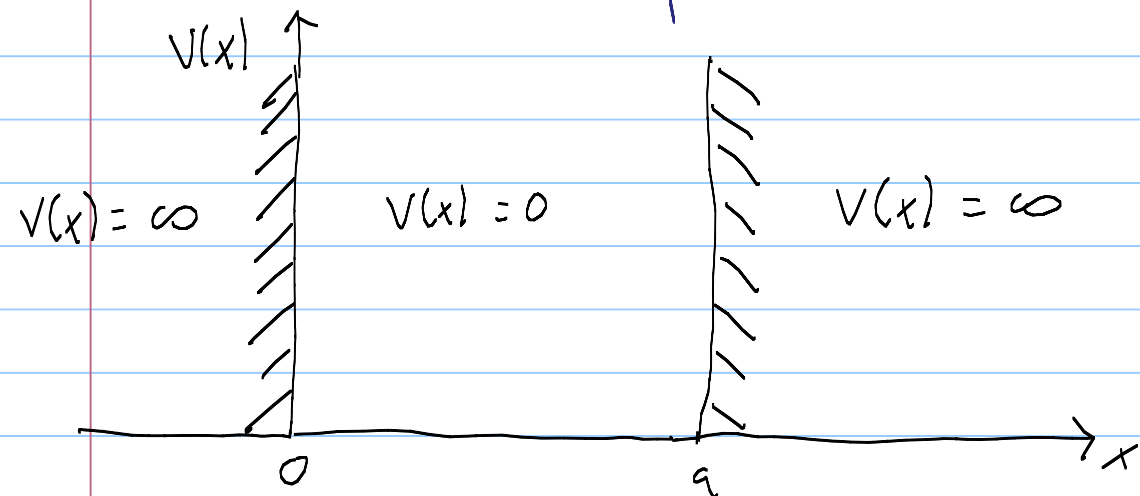
$$\boxed{\underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\,\psi(r)}_{\text{Time-independent Schrodinger equation, which is an eigenvalue equation}} \quad (10)}$$

Time-independent Schrodinger equation, which is an eigenvalue equation

The Time-Indepedent Schrodinger Equation

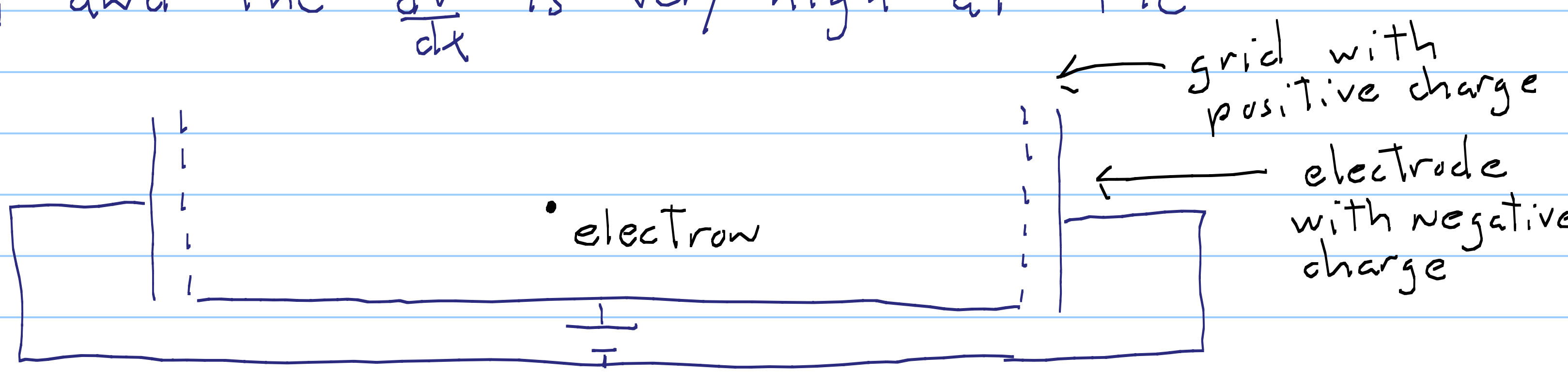
The infinite potential well:

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



This is an idealized case which should be a good approximation for cases where the potential well is deep wrt the particle's energy, and the $\frac{dV}{dx}$ is very high at the walls

e.g.



THE INFINITE WELL

FROM 10, WE MUST HAVE:

$$\psi(x) = 0 \quad x < 0$$
$$\psi(x) = 0 \quad x > a$$

INSIDE THE BOX, $V(x) = 0$ SO WE CAN WRITE 10

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\,\psi(r)$$

AS:

$$\boxed{\frac{d^2 \psi(x)}{dx^2} + \frac{2mE}{\hbar^2} \psi(x) = 0} \qquad (11)$$

IF $E < 0$, THEN 11 TAKES THE FORM

$$\frac{d^2 y}{dx^2} - k^2 y = 0$$ whose solution gives a linear combination of the form:

$$A e^{kx} + B e^{-kx}$$ → not acceptable. Why?

THE INFINITE WELL (cont.)

So $E<0$ does not work so we try $E>0$

(11) takes the form: $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad (12)$$

the most general solution to (12) is a linear combination of the form

$$A\sin kx + B\cos kx$$

we need $\psi(0) = 0 \Rightarrow B = 0$

$$\psi(x) = A\sin kx \qquad \text{with } k^2 = \frac{2mE}{\hbar^2}$$

we also need $\psi(a) = 0 \Rightarrow ka = n\pi$

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

THE INFINITE WELL (CONT.)

So WE HAVE:

$$\psi(x) = A \sin Kx \quad , \quad K = \frac{n\pi}{a} \quad \Rightarrow \quad \boxed{\psi(x) = A \sin\left(\frac{n\pi x}{a}\right)}$$

What is A? $\rightarrow$ Need To normalize:

$$\int_0^a |\psi(x)|^2 \, dx = 1 = \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx$$

note: $\displaystyle\int \sin^2 \alpha x \, dx = \frac{x}{2} - \frac{\sin 2\cancel{\alpha} x}{4a}$

$$\Rightarrow \quad A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = A^2 \left(\frac{x}{2} - \frac{a}{4n\pi} \sin\left(\frac{2n\pi x}{a}\right) \Big|_0^a \right)$$

$$\Rightarrow A^2 \frac{a}{2} = 1 \quad \Rightarrow \quad \boxed{A = \sqrt{\frac{2}{a}}}$$

INFINITE WELL (CONT)

So we have: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

THESE SOLUTIONS HAVE AN INTERESTING PROPERTY:

$$\int_0^a dx\, \psi_n^*(x)\,\psi_m(x) = \frac{2}{a}\int_0^a dx \sin\frac{n\pi x}{a}\sin\frac{m\pi x}{a}$$

$$= \frac{1}{a}\int dx \left(\cos\frac{(n-m)}{a}\pi x - \cos\frac{(n+m)}{a}\pi x \right)$$

$$= \frac{\sin[(n-m)\pi]}{(n-m)\pi} - \frac{\sin[(n+m)\pi]}{(n+m)\pi}$$

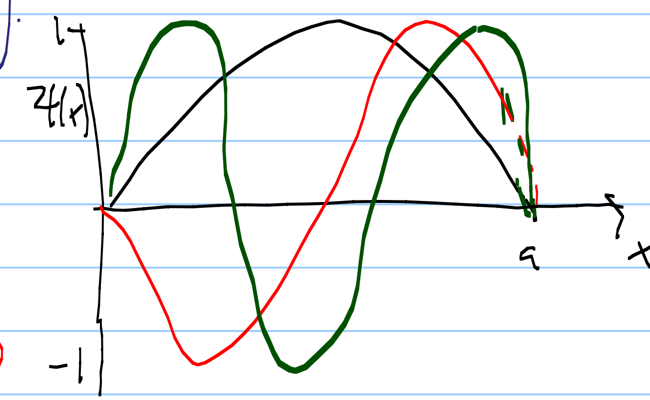
$= 0$ if $n \neq m$

$= 1$ if $n = m$ (L'Hospital's rule)

INFINITE WELL

SOME REMARKS ON THE PHYSICS OF THE INFINITE WELL:

1 - THE STATE OF LOWEST ENERGY (aka "THE GROUND STATE") is GIVEN BY: $\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$.



The lowest energy: $E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$

Classically, the lowest energy would be?

2 - $\langle p \rangle = \int_0^a \psi_n^*(x)\left(-i\hbar \frac{d}{dx}\right)\psi_n(x)\,dx = \int_0^a dx \frac{d}{dx}\left(\frac{\psi_n(x)^2}{2}\right)$

because $\psi(x)$ is real, $\psi(x) = \psi(x)^*$

$= \frac{-i\hbar}{2}\left(\psi_n^2(a) - \psi_n^2(0)\right) = \boxed{0}$

but $\langle p^2 \rangle = 2mE_n = \boxed{\frac{\hbar^2 \pi^2 n^2}{a^2}}$

3 - THE LARGER THE NUMBER OF NODES FOR THE SOLUTION THE HIGHER THE ENERGY:

$$\langle T \rangle = \frac{\langle p^2 \rangle}{2m} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx\, \psi^*(x) \frac{d^2}{dx} \psi(x)$$

$$= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left\{ \frac{d}{dx} \left(\psi^*(x) \frac{d\psi(x)}{dx} \right) - \frac{d\psi^*(x)}{dx} \frac{d\psi(x)}{dx} \right\}$$

$$= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left| \frac{d\psi(x)}{dx} \right|^2$$

The more $\psi(x)$ changes quickly (wrt x), the more $\langle T \rangle$ will be large.

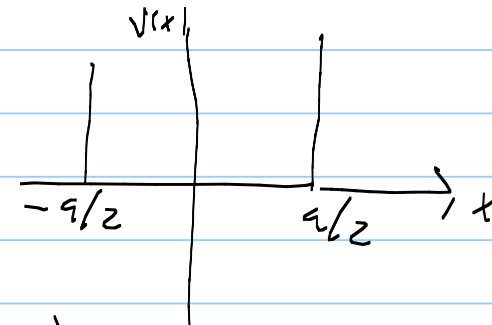
4 - FOR $n > 1$, THERE ARE REGIONS IN THE WELL WHERE THE PARTICLE CANNOT BE FOUND.

INFINITE WELL (CONT.)

5- THERE ARE TWO KINDS OF SOLUTION: THOSE THAT ARE SYMMETRIC WITH RESPECT TO $\frac{a}{2}$ AND THOSE THAT ARE NOT.

$\rightarrow$ THIS BECOMES MORE EXPLICIT IF WE MOVE THE WELL:

$$x \rightarrow x - a/2$$



$$\sin\left(\frac{n\pi x}{a}\right) \rightarrow \sin\left(\frac{n\pi x}{a} - \frac{n\pi}{2}\right) = \sin\frac{n\pi x}{a}\cos\frac{n\pi}{2} - \cos\frac{n\pi x}{a}\sin\frac{n\pi}{2}$$

$\rightarrow$ For $n = 1, 3, 5, \ldots$ $\quad \psi_n(x) = \sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a}$ $\quad$ odd

$\rightarrow$ For $n = 2, 4, 6, \ldots$ $\quad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$ $\quad$ even

6- THE MOST GENERAL FORM FOR $\psi(x)$ WILL BE GIVEN BY:

$$\psi(x) = \sum_{n=1}^{\infty} A_n \sin\frac{n\pi x}{a}, \quad \text{or} \quad \psi(x) = \sum_{n=1}^{\infty} A_n \psi_n(x)$$

How can we extract the A_n?

we have:

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

$$= \sum_{n=1}^{\infty} A_n \int_0^a dx\, \psi_m^*(x)\, \psi_n(x) = \sum_{n=1}^{\infty} A_n \delta_{mn} = A_m$$

$$\Rightarrow A_m = \int_0^a dx\, \psi_m^*(x)\, \psi(x)$$

INFINITE WELL (cont)

7- $$H\,\psi_n(x) = E_n\,\psi_n(x)$$

$$\langle H\rangle = \int_0^a dx\,\psi^*(x)\,H\,\psi(x) = \int_0^a dx\,\psi^*(x)\,H\sum_{n=1}^{\infty} A_n\psi_n$$

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

$$= \sum_{n=1}^{\infty} E_n\,|A_n|^2$$

with $\int_0^a dx\,\psi^*(x)\,\psi(x) = 1$, we have

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

WE POSTULATE THAT AN ENERGY MEASUREMENT WILL YIELD AN EIGENVALUE AND LEAVE THE PARTICLE IN THE STATE ψ_n

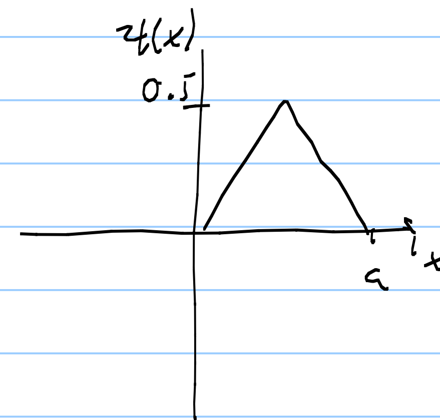
$\Rightarrow$ average energy $= \langle H\rangle = \sum_n E_n p_n$

p_n : probability of finding particle with energy E_n

EXAMPLE INFINITE WELL PROBLEM

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

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



a) calculate A
b) calculate the probability that a measurement of energy yields the eigenvalue E_n

a: $\psi(x)$ is symmetric and real so we can take

$$A^2\, 2 \cdot \int_0^{a/2} \frac{x^2}{a^2}\, dx = A^2 \cdot 2 \cdot \left.\frac{x^3}{3a^2}\right|_0^{a/2} = \frac{A^2 \cdot 2}{3a^2} \cdot \frac{a^3}{8} = \frac{A^2 a}{12}$$

$$\Rightarrow \frac{A^2 a}{12} = 1 \quad \Rightarrow A = \sqrt{\frac{12}{a}}$$

EXAMPLE INFINITE WELL PROBLEM (cont.)

b: we need to calculate the A_n:

$$A_n = \int_0^a dx\, \psi(x) \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$$

$$= \frac{\sqrt{24}}{a}\left[\int_0^{a/2} dx \left(\frac{x}{a}\right) \sin\frac{n\pi x}{a} + \int_{a/2}^{a} dx \left(1 - x/a\right) \sin\frac{n\pi x}{a}\right.$$

change variables: $\frac{\pi x}{a} = u$ in first integral

$\frac{\pi x}{a} = \pi - u$ in the second integral

we get: $A_n = \frac{\sqrt{24}}{\pi} \int_0^{\pi/2} du\, \frac{u}{\pi} \sin\left(nu\left(1-(-1)^n\right)\right)$

$\rightarrow$ only odd solutions

EXAMPLE INFINITE WELL PROBLEM (cont)

After integrating we get:

$$A_n = \frac{\sqrt{24}}{\pi} \cdot 2 \frac{1}{\pi n^2} (-1)^{n+1}$$

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

$$= 0 \quad \text{for even } n$$

Prob. of obtaining $E_1 = \frac{96}{\pi^4} = 98.6\%$

$E_2 = 0$

$E_3 = \frac{96}{\pi^4 \cdot 3^4} = 1.2\%$