E. F. Deveney / BSC Physics: PH 402 Quantum

Note Title

Schrödinger 4.2 = ∞ Square well

time-indep-shro

2 Bound System ⇒ 1) ∞ Square well
2) Harmonic Oscillator

1) ∞ Square well.

We've used this case already as launching pad for really the entire "computing" aspects of the Q.M. formalism, --- i.e. "shut up & calculate" to get observables $\langle x \rangle \pm \Delta x$ for example

to do that, we just used the soln to the ∞ well

$$\hat{H}\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

$$\Psi(x,t) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) e^{\frac{-i\hbar \pi^2 t}{2ma^2}} & 0 \leq x \leq a \\ 0 & \text{, otherwise.} \end{cases}$$

Now we will get this solns explicity

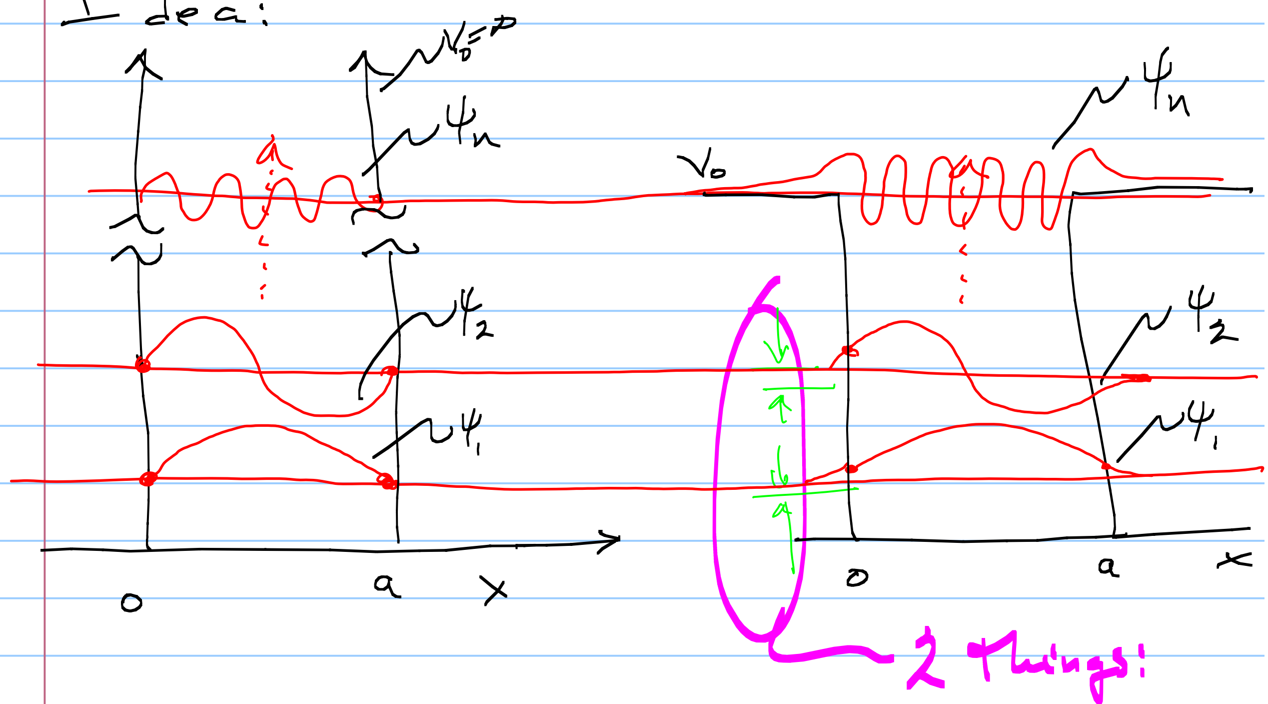
by Solving for $\Psi(x,t) = \psi(x)\, e^{-i\frac{E_T}{\hbar}t}$

from $\hat{H}\psi(x) = E_T(x)$

So again we will find energy eigenstates!

recall ∞-square well = ideal case.... but we will use it for $\cong$ Quantitative results and for Qualitative feel of real problems.

Idea:



1) real, true energies might be shifted slightly

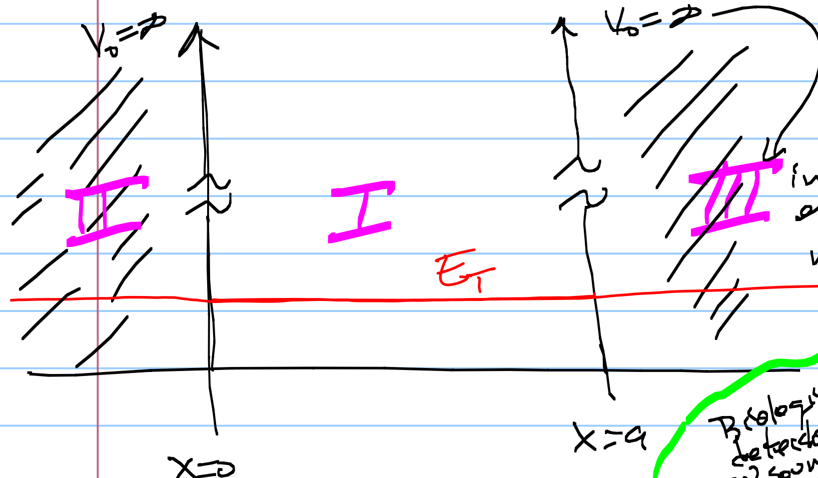
2) ψ does leak a bit in real case

Also can expect that $\cong$ to real is not as good when $E_T \cong V_0$

ψ_n as n gets Big!

1-D

so ∞ square well = Bound ie by (in) potential on 2 sides



$= e^-$ sandwiched in thin layer between semi-conductors

IS sandwich in all 3 directions ψ_{e^-} = Quantum "dot" very hot thing these days

Biological detectors, new source of inexpensive lights, lasers & more

$$\hat{H}\psi = E_T\psi \Rightarrow \psi'' + A\psi = 0 \;;\; A = \frac{2m}{\hbar^2}(E_T - V)$$

3-regions

II & III

$E_{TOT} < V$

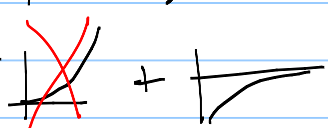
solns

I

$E_T > V$

$$\psi(x) = C_1 e^{\sqrt{A}x} + C_2 e^{-\sqrt{A}x}$$

II & III =



Blows up, can't normalize ψ so

$$\psi(x) = C_2 e^{-\sqrt{A}x}$$

$$\sqrt{A} = \sqrt{\frac{2m}{\hbar^2}(E_T - \infty)} = \infty$$

$$\psi_{II \,\&\, III} = C_2 e^{-\infty} = 0$$

No Penetration into ∞ potent well!

tunneling → 0

I guess we should reserve tunneling for "thru" a potential & this should be no penetration

Region I $\quad E > V \quad (V=0) \therefore \sqrt{A} = \frac{\sqrt{2mE_I}}{\hbar}$

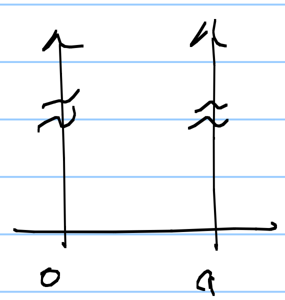
So
$$\psi_I(x) = C_1 e^{i\sqrt{A}x} + C_2 e^{-i\sqrt{A}x}$$

OR

$$\Rightarrow \quad \psi_I = C_1 \cos(\sqrt{A}\,x) + C_2 \sin(\sqrt{A}\,x)$$

easier to use this equivalent soln!

So



$$\psi_I(x) = C_1 \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) + C_2 \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$

Now all we have to do is make sure that ψ meets the BC's.

* Note ψ & $\frac{d\psi}{dx}$ do not have to be smooth from $\pm$ & about $x=0$ & $x=a$. Outside of these regions $\psi = 0 \Rightarrow$ period.

So all that we need to do is make sure $\psi(0) = \psi(a) = 0$

OK, lets do it

1) $\psi(0) = C_1 \cos(0) + C_2 \cancel{\sin(0)}^{\,0} = 0$

$C_1 = 0$ $\Big\}$ Done: $C_1 = 0$ already

$$\psi(x) = C_2 \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$ so far. Next

$$\psi(x=a) = C_2 \sin\left(\frac{\sqrt{2mE}}{\hbar} x\right) = 0$$

well $C_2 = 0$ is possibility but then

$\psi(x) = 0$ doesn't help so

for $C_2 \neq 0$

must be

$$\sin\left(\frac{\sqrt{2mE}}{\hbar} x\right) = 0$$

This is true for, if,

$$\frac{\sqrt{2mE_T}}{\hbar} x = 0, \pi, 2\pi, 3\pi \cdots = n\pi$$

$$\frac{\sqrt{2mE_T}}{\hbar} = n\pi, \quad n=0, 1, 2, 3 \cdots$$

$E = 0$ or $E_T = 0$

so $\underbrace{\psi(x) = C_2 \sin(0) = 0}$

doesn't help either to have $\psi(x)$ that vanishes every where!

so $$\frac{\sqrt{2mE_T}}{\hbar} = n\pi \quad \text{for } n = 1, 2, 3 \cdots$$

or $E_T = \frac{\hbar^2 \pi^2}{2ma^2} n^2$; $n = 1, 2, 3 \ldots$

call

$E_n \Rightarrow$'s E_{TOT} for state n $= \frac{\hbar^2 \pi^2}{2ma^2} n^2$

$n = 1, 2, 3 \ldots$

Lets think:

$n = 0$, no wave function, $\psi_0^* \psi = 0$ = no particle

$n = 1$

$E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$ = Lowest possible energy of the particle ≡ Zero pt energy of system: If it is there, can't be any less than this!

next possible ψ_n is ψ_2 w/

$E_2 = E_1 (2^2)$

Then

$E_3 = E_1 (3^2)$

$E_n = E_1 (n^2)$

QUANTUM Says: Particle energies are Quantized
exist only in discrete states
w/ energies that jump.

In between, for energies other than quantized in these steps,
The particle $\psi = 0$ & doesn't "Exist"

Cool..... but back to $\psi_{I}(x) = ?$

well so far

$$\psi_{I}(x) = C_2 \sin\left(\frac{\sqrt{2mE}}{\hbar} x\right)$$

but $E_I = E_n$ so must have distinct ψ_n for each ψ_n

$$\psi_n(x) = C_2 \sin\left(\frac{\sqrt{2mE_n}}{\hbar} x\right)$$

$$= C_2 \sin\left(\sqrt{\frac{\frac{\cancel{2m}\,\cancel{\hbar^2}\pi^2 n^2}{\cancel{2m}\, a^2}}{\cancel{\hbar^2}}}\; x\right)$$

$$\psi_n(x) = C_2 \sin\left(\frac{n\pi x}{a}\right)$$

What's left? Born's ... probabilistic requirement

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\, \psi_n(x)\, dx = 1$$; Let C_2 = norm constant

⋮

$$|C_2|^2 \int_0^{\infty} \sin^2 \frac{n\pi x}{a}\, dx = 1$$

note limits

we've done a million times now! * need $\cos(\alpha \pm \beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$

Then $\sin^2\alpha + \cos^2\alpha = 1$

or

$$|C_2|^2 \frac{a}{2} = 1$$

$$C_2 = \pm\sqrt{\frac{2}{a}}$$

we know Q.M. $(-1) = e^{i\pi}$ = arbitrary phase, no effect on expectation

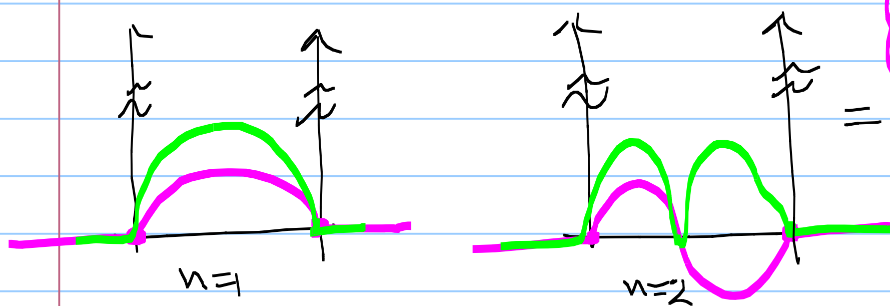
So chose $C_2 = +\sqrt{\frac{2}{a}}$

&

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) ; & 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}$$

where $E_{\text{tot}_n} = \frac{\hbar^2\pi^2}{2ma^2} n^2$; $n = 1, 2, 3 \dots \infty$

lets Look @ $\psi_n(x)$ & $\psi_n^* \psi_n$



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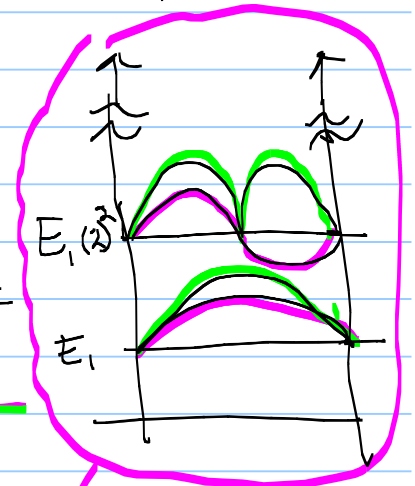
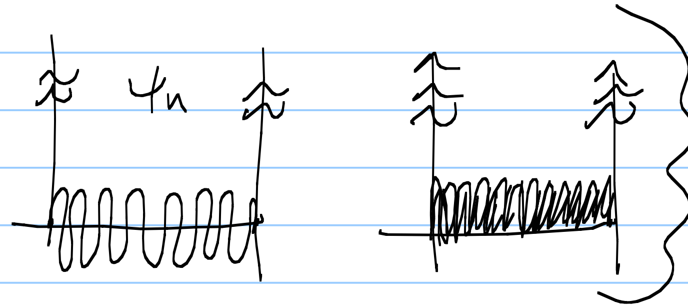


* recall idea of $n = \#$ of $\frac{1}{2}\lambda$ = standing wave condition.

This gives most info: $E_n, \psi_n, \psi_n^* \psi_n$

For $n \to$ Big, $E_n = E_1(n^2) =$ BIG

& ψ_n & $\psi_n^* \psi_n$

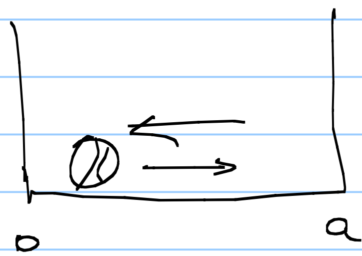


no longer acts very wave-like
Looks & Acts particle like!

and as a particle...

(1) Tennis ball $\rightarrow \Psi_{n\infty}$ $n \rightarrow \infty$

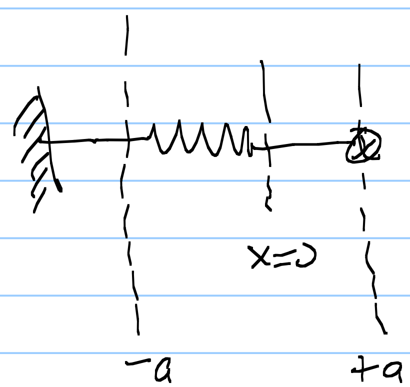
& see that $\Psi_n^* \Psi_n$ = Constant



equally likely to find classical Ball anywhere!

* Note: Ball does not speed up or slow down in collisions w/ wall ∴ does not spend more time there.

* Note: moving to Harmonic oscillation potential



$V(x) = \frac{1}{2}kx^2$

& clearly here ball does slow down @ ± a

So should have higher prob of being found here!