

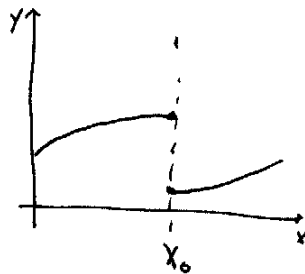
# Physics 2D Homework Solutions - Ch. 5

#1.) Of the functions graphed in Figure P5.1, which are candidates for the Schrödinger wavefunction of an actual physical system? For those that are not, state why they fail to qualify.

There's only a few absolute requirements for a wavefunction:

1.)  $\Psi$  represents a probability for locating a particle at a point, and should therefore be single-valued for any given  $x$ . It doesn't make any sense for there to be different values of the probability located at the same point.

2.) This implies that  $\Psi$  should also be continuous; no big ugly jumps. Something discontinuous, like



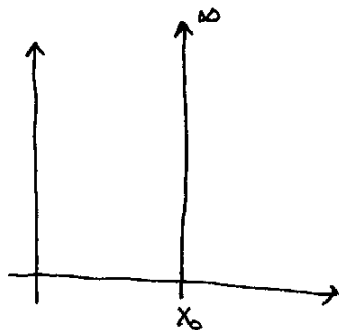
Is double valued at  $x_0$ , if we examine

$$\lim_{x \rightarrow x_0^+} \Psi \neq \lim_{x \rightarrow x_0^-} \Psi$$

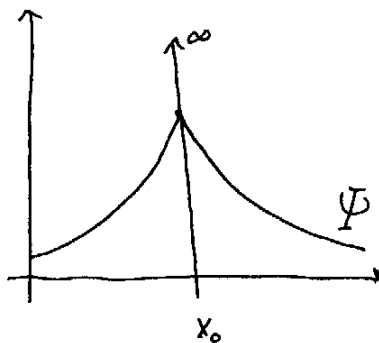
3.) Most of the time, we will also require  $\Psi$  to be smooth, that is, require  $\frac{d\Psi}{dx}$  to be continuous.

#1.) continued

This can be violated, though, for example near infinite potentials.  
For example, something called a "delta function potential" looks like a single infinite spike at some point  $x_0$ .

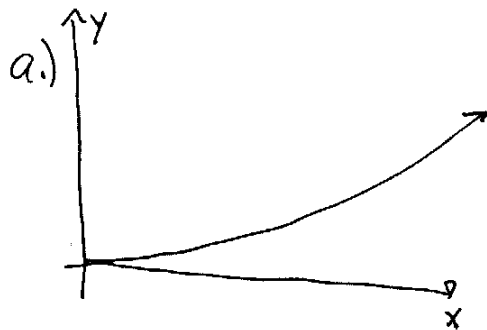


At  $x_0$ ,  $\Psi$  won't be smooth, but it will be continuous and single valued:



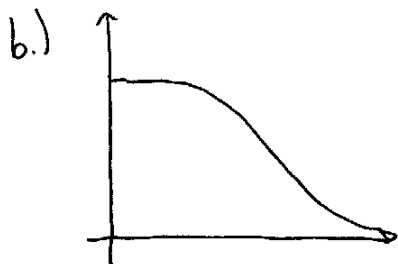
4.) Last, we require  $\Psi$  to be finite for all values of  $x$  (even  $x \rightarrow \pm\infty$ ). No infinite probabilities!

Down to business

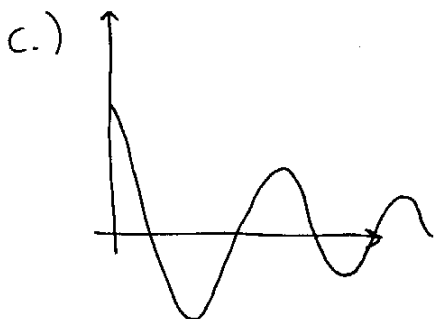


No good! As  $x \rightarrow \infty$   
 $\Psi \rightarrow \infty$ , so it violates  
Kuhlman golden rule #4.

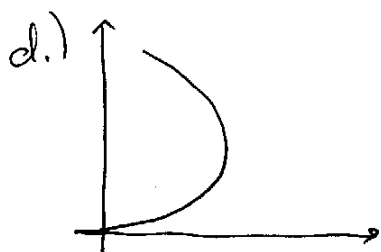
#1.) continued



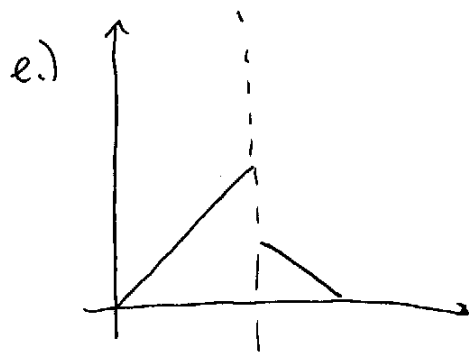
Nice, smooth, finite, and continuous.  
Looks good!



Even looks wavy! What more  
could you ask for?



Stinky! Double valued for some  $x$ .  
No go.



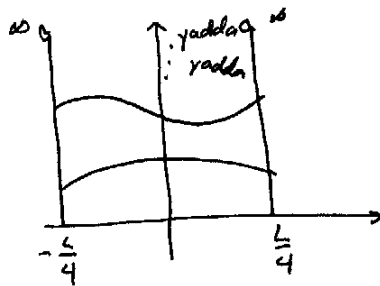
Even worse! At least d.) was continuous.  
Letter e.), you suck.

#2.) A particle is described by the wavefunction

$$\psi(x) = \begin{cases} A \cos\left(\frac{2\pi x}{L}\right) & -\frac{L}{4} \leq x \leq \frac{L}{4} \\ 0 & \text{otherwise} \end{cases}$$

a.) Determine the normalization constant  $A$ .

First of all, this is our old friend particle in a box, where the box is length  $\frac{L}{2}$



So we could just cheat and say "We found that in section 5.4. Let's use that and let  $L \rightarrow \frac{L}{2}$ !"

This way is for wussies! Let's tough it out  
Some can look ourselves in the mirror.

$|\psi(x)|^2$  is the probability amplitude, and to find the probability to find a particle in the region  $a \leq x \leq b$ ,

$$P = \int_a^b |\psi(x)|^2 dx$$

Now, our particle is inside this box, so we know

$$P = \int_{-\frac{L}{4}}^{\frac{L}{4}} |\psi(x)|^2 dx$$

#2.) continued

It HAS to be in the box somewhere! So the probability to locate it in there is 100%

$$\begin{aligned} P &= \int_{-\frac{L}{4}}^{\frac{L}{4}} |\psi(x)|^2 dx = 1 \\ &= \int_{-\frac{L}{4}}^{\frac{L}{4}} A^2 \cos^2\left(\frac{2\pi x}{L}\right) dx \\ &= A^2 \int_{-\frac{L}{4}}^{\frac{L}{4}} \cos^2\left(\frac{2\pi x}{L}\right) dx \end{aligned}$$

$$\text{Let } u = \frac{2\pi x}{L} \quad \text{when } x = -\frac{L}{4}, u = -\frac{\pi}{2}$$

$$du = \frac{2\pi}{L} dx \quad x = \frac{L}{4}, u = \frac{\pi}{2}$$

$$\Rightarrow dx = \frac{L}{2\pi} du$$

$$= \frac{A^2 L}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos^2 u du$$

Remember how to do this one?

$$= \frac{A^2 L}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{2} (1 + \cos 2u) du$$

$$= \frac{A^2 L}{2\pi} \left[ \frac{u}{2} + \frac{\sin 2u}{4} \right]_{-\frac{\pi}{2}}^{\frac{\pi}{2}} = \frac{A^2 L}{4}$$

#2.) continued

And so we know

$$\frac{A^2 L}{4} = 1$$

$$\therefore A = \sqrt{\frac{4}{L}}$$

b) What is the probability that the particle will be found between  $x=0$  and  $x = \frac{L}{8}$  if a measurement of its position is made?

Just do

$$P = \int_0^{\frac{L}{8}} |\psi(x)|^2 dx$$

$$= \frac{4}{L} \int_0^{\frac{L}{8}} \cos^2\left(\frac{2\pi x}{L}\right) dx$$

Do this the same way as part a.)

$$= \frac{2}{\pi} \int_0^{\frac{\pi}{4}} \cos^2 u \, du$$

$$= \frac{2}{\pi} \left[ \frac{u}{2} + \frac{\sin 2u}{4} \right] \Big|_0^{\frac{\pi}{4}}$$

$$P = \frac{2}{\pi} \left( \frac{\pi}{8} + \frac{1}{4} \right)$$

#3.) A free electron has a wavefunction

$$\psi(x) = A \sin(5 \times 10^{10} x)$$

where  $x$  is measured in meters (That means  $5 \times 10^{10}$  has units  $\text{m}^{-1}$ !) Find

a.) the electron's de Broglie wavelength

For a free particle, the wavefunction always has the form

$$\psi(x) = A \sin(kx + \phi)$$

So we know that in our case,  $\phi = 0$  and

$$k = 5 \times 10^{10} \equiv \frac{2\pi}{\lambda}$$

$$\therefore \lambda = \frac{2\pi}{5 \times 10^{10}} = 0.126 \text{ nm}$$

b.) the electron's momentum

Well, you should remember

$$\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda} = 5.26 \times 10^{-24} \frac{\text{kg m}}{\text{s}} = 32.8 \frac{\mu\text{eV}}{c}$$

That's a little sissy momentum. Using  $p = mv$  gives you  $v = 0.01 c$ , so we're non relativistic

# 3.) continued

c.) the electron's energy in electron volts

$$K = \frac{p^2}{2m} = 15.1 \times 10^{-18} \text{ J} \\ = 94 \text{ eV}$$

#5.) In a region of space, a particle with zero energy has a wave function

$$\psi(x) = A x e^{-x^2/L^2}$$

a.) Find the potential energy  $U$  as a function of  $x$ .

The Schrödinger equation has the form

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

For our particle,  $E=0$ , so

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = U(x)\psi(x)$$

$$\Rightarrow U(x) = \frac{1}{\psi(x)} \frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2}$$

Right? Plug in our wavefunction.

#5.) continued

$$U(x) = \frac{1}{A x e^{-x^2/L^2}} \frac{\hbar^2}{2m} \frac{d^2}{dx^2} (A x e^{-x^2/L^2})$$

Take Those derivatives! (Don't forget chain + product rule!)

$$\frac{d^2}{dx^2} (A x e^{-x^2/L^2}) = \frac{d}{dx} \left( A e^{-x^2/L^2} - \frac{2A}{L^2} x^2 e^{-x^2/L^2} \right)$$

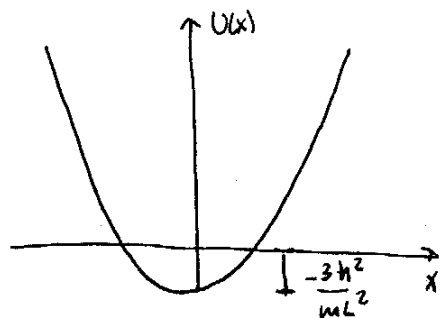
$$= -\frac{2Ax}{L^2} e^{-x^2/L^2} - \frac{4Ax}{L^2} e^{-x^2/L^2} + \frac{4Ax^3}{L^4} e^{-x^2/L^2}$$

$$= \frac{2Ax(2x^2 - 3L^2)}{L^4} e^{-x^2/L^2}$$

So 
$$U(x) = \frac{\hbar^2}{2mL^2} \left( \frac{4}{L^2} x^2 - 6 \right)$$

b.) Make a sketch of  $U(x)$  versus  $x$

Parabola centered at  $x=0$  with  $U(0) = -\frac{3\hbar^2}{mL^2}$



#6.) continued

So that

$$\hat{H}\psi_n = \frac{\hbar^2 k^2}{2m} \psi(x)$$

(note that this is  $\frac{p^2}{2m}$  for  $p = \hbar k$ )

That constant multiplying  $\psi(x)$  is the energy

$$\hat{H}\psi(x) = E\psi(x)$$

$$\therefore E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

#7.) Show that allowing the state  $n=0$  for a particle in a one dimensional box violates the uncertainty principle,  $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$

The particle is somewhere inside the box, right?

$$\text{So } \Delta x = L \quad (L = \text{box length})$$

For a particle in a box,

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (\text{Eq. 5.17})$$

for  $n=0$

$$E_n = 0$$

#7.) Inside the box, all energy is kinetic

$$E = K = \frac{\langle p^2 \rangle}{2m} = 0$$

$$\therefore \langle p^2 \rangle = 0$$

Now,

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

So that

$$\begin{aligned} \langle p \rangle &= \int_0^L \psi^*(x) \hat{p} \psi(x) dx \\ &= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \left(-i\hbar \frac{d}{dx}\right) \sin\left(\frac{n\pi x}{L}\right) dx \\ &= -i\hbar \left(\frac{2n\pi}{L^2}\right) \int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi x}{L}\right) dx \\ &= 0 \end{aligned}$$

So that

$$\begin{aligned} \Delta p &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \quad \text{Eq. 5.34} \\ &= 0 \end{aligned}$$

$$\therefore \boxed{\Delta x \Delta p = 0}$$

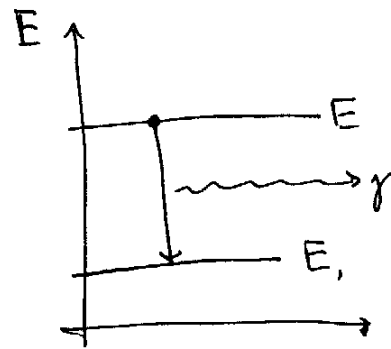
#9.) The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by a square well. Imagine a proton confined in an infinitesquare well of length  $10^{-5}$  nm, a typical nuclear diameter. Calculate the wavelength and energy associated with the photon that is emitted when the proton undergoes a transition from the first excited state ( $n=2$ ) to the ground state ( $n=1$ ). In what region of the electromagnetic spectrum does this wavelength belong?

This is easier than it sounds. We are describing the situation as a particle in a box, so we know the energy states are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m_p L^2}$$

$$\text{So } E_2 = \frac{4 \pi^2 \hbar^2}{2m_p L^2}$$

$$E_1 = \frac{\pi^2 \hbar^2}{2m_p L^2}$$



The emitted photon has the difference in energy between these two states

#9) continued

$$\Delta E = \frac{3\pi^2 \hbar^2}{2m_p L^2} = 6.14 \text{ MeV}$$

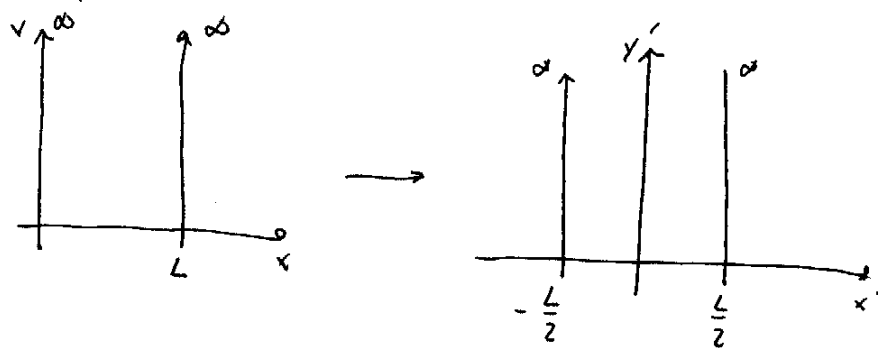
$$\Delta E = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{\Delta E} = 2.02 \times 10^{-4} \text{ nm}$$

That's in the gamma ray region

#11.) Consider a particle moving in a one dimensional box with walls at  $x = -\frac{L}{2}$  and  $x = \frac{L}{2}$ .

a.) Write the wavefunctions and probability densities for the states  $n=1$ ,  $n=2$ , and  $n=3$

This is just like the box with ends at  $x=0$  and  $x=L$ , except shifted to the left:



It's the exact same problem, so the wavefunctions should be the same, except with

$$x = x' + \frac{L}{2}$$

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We know that  $E = \sqrt{p^2 c^2 + m^2 c^4}$

So using  $p = \frac{n \hbar \pi}{L}$ , we get

$$E = \sqrt{\frac{n^2 \hbar^2 \pi^2 c^2}{L^2} + m^2 c^4}$$

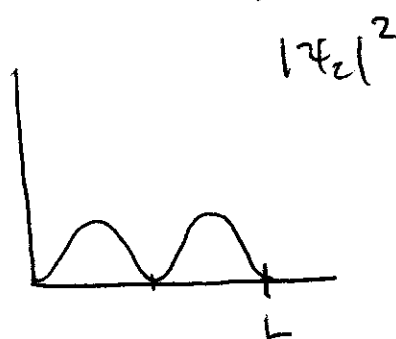
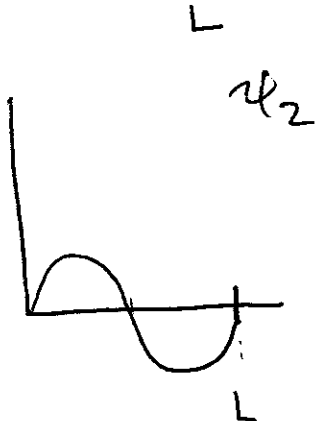
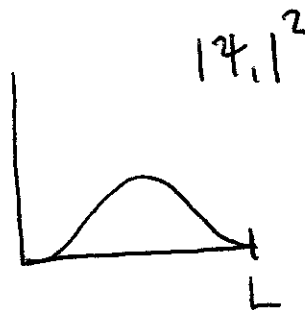
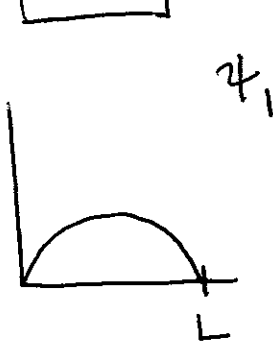
Ground state:  $n=1$ , so  $E = \sqrt{\frac{\hbar^2 \pi^2 c^2}{L^2} + m^2 c^4}$

Using  $L = 10^{-12} \text{ m}$ ,  $m = m_e$ , we get  $E = 804 \text{ keV}$

$$\text{Thus } KE = E - mc^2 = \boxed{293 \text{ keV}}$$

The non-rel. answer is  $KE = \frac{\pi^2 \hbar^2}{2mL^2} = 377 \text{ keV}$ , off by almost  $\boxed{30\%}$ !

17 a



b) Prob of finding electron bet.  $x=a$  and  $x=b$  is

$$\int_a^b |\psi(x)|^2 dx = \int_a^b |\psi_1(x)|^2 dx$$

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right), \text{ so}$$

$$\text{Prob} = \frac{2}{L} \int_a^b \sin^2\left(\frac{\pi x}{L}\right) dx$$

Can do the integral by using  $u = \frac{\pi x}{L}$

$$\rightarrow \frac{2}{L} \int_{\frac{\pi a}{L}}^{\frac{\pi b}{L}} \sin^2 u \cdot \frac{L}{\pi} du = \frac{2}{\pi} \int_{\frac{\pi a}{L}}^{\frac{\pi b}{L}} \sin^2 u du$$

$$= \frac{2}{\pi} \left[ \frac{u}{2} - \frac{\sin 2u}{4} \right]_{\frac{\pi a}{L}}^{\frac{\pi b}{L}}$$

$$= \frac{2}{\pi} \cdot \frac{1}{2} \left( \frac{\pi b}{L} - \frac{\pi a}{L} \right) + \frac{2}{\pi} \frac{1}{4} \left( \sin\left(\frac{2\pi b}{L}\right) - \sin\left(\frac{2\pi a}{L}\right) \right)$$

Plugging in  $L=1\text{nm}$ ,  $a=.15\text{nm}$ ,  $b=.35\text{nm}$  gives

$$\text{Prob} = (.35 - .15) + \frac{1}{2\pi} (\sin(.3\pi) - \sin(.7\pi)) = \boxed{\frac{2}{10}}$$

$$c] \text{ Now Prob} = \int_a^b |\psi_n(x)|^2 dx = \frac{2}{L} \int_a^b \sin^2\left(\frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{\pi} \int_{\frac{2\pi a}{L}}^{\frac{2\pi b}{L}} \sin^2 u du$$

$$= \frac{1}{2\pi} \left( \frac{2\pi b}{L} - \frac{2\pi a}{L} \right) + \frac{1}{\pi 4} \left( \sin\left(\frac{4\pi a}{L}\right) - \sin\left(\frac{4\pi b}{L}\right) \right)$$

$$= \left( \frac{b}{L} - \frac{a}{L} \right) + \frac{1}{4\pi} \left( \sin\left(\frac{4\pi a}{L}\right) - \sin\left(\frac{4\pi b}{L}\right) \right)$$

which here = 0.35

$$d] E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} = \frac{n^2 \pi^2 (hc)^2}{2mc^2 L^2}$$

Using  $(hc)^2 = 197.3 \text{ eV} \cdot \text{nm}$ , we get

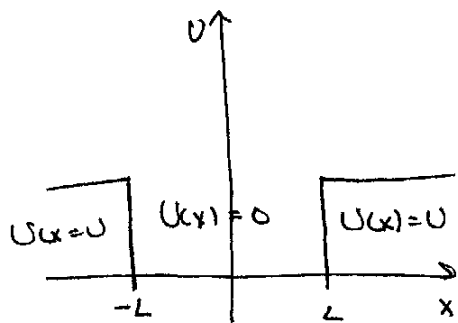
$$\boxed{E_1 = 0.376 \text{ eV}} \quad , \quad \boxed{E_2 = 4E_1 = 1.5 \text{ eV}}$$

## Physics 2D Homework - Ch. 5 Set 2

#20) Consider a particle with energy  $E$  bound to a finite square well of height  $U$  and width  $2L$  situated on  $-L \leq x \leq L$ . Because the potential energy is symmetric about the midpoint of the well, the stationary state waves will be either symmetric (cosine solutions) or antisymmetric (sine solutions) about this point.

a.) Show that for  $E < U$ , the conditions for smooth joining of the interior and exterior waves lead to the following equation for the allowed energies of the symmetric waves.

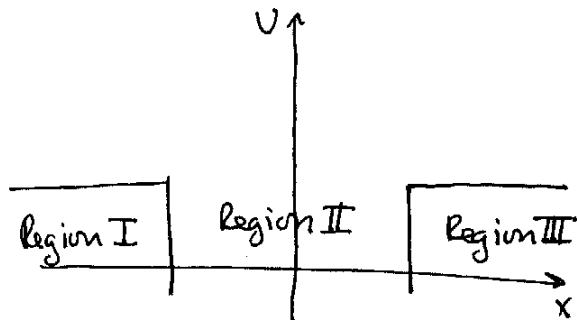
Let me start out by solving the finite square well problem for  $\psi$ . Our box now looks like:



Since the potential is finite, there is some probability to find the particle in those regions. To find out how much, whip out the Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x) \psi(x) = E \psi(x)$$

We need to divide up our problem into three regions:



In Region I, the potential  $U(x)$  is  $U(x)=U$ , so the Schrödinger Eq. is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi \quad \text{Region I}$$

In Region II, the potential is zero, so we get

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \text{Region II}$$

Region III is the same as I:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi \quad \text{Region III}$$

The solution to region II is easiest, cuz that's what you guys did last week:

$$\text{Region II: } \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 = \frac{d^2\psi}{dx^2} + k^2\psi \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow \psi = A \sin(kx) + B \cos(kx)$$

The solutions to Regions I and III are just a little more complicated

$$\text{Region I III: } -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-U)}{\hbar^2} \psi = 0$$

$$\frac{d^2\psi}{dx^2} + k'^2 \psi = 0 \quad k'^2 = \frac{2m(E-U)}{\hbar^2}$$

# 20.) continued

So far, it's exactly the same as Region II, except with the  $U$  thrown in. However, there's a little complication. We're told  $E < U$ , so that means  $k'^2$  is negative. We can make it explicit by saying

$$k'^2 = \frac{2m(E-U)}{\hbar^2} = - \frac{2m(U-E)}{\hbar^2}$$

That means  $k'$  has to be imaginary!

$$k' = i \sqrt{\frac{2m(U-E)}{\hbar^2}} = i\alpha \quad ; \quad \alpha^2 = \frac{2m(U-E)}{\hbar^2}$$

So we have

$$\frac{d^2\psi}{dx^2} + k'^2\psi = 0$$

$$\Rightarrow \psi = C e^{ik'x} + D e^{-ik'x}$$

$$= C e^{-\alpha x} + D e^{\alpha x} \quad (\text{could also be } C \sinh(\alpha x) + D \cosh(\alpha x) \text{ if you're into hyperbolic functions})$$

So let's list our solutions:

$$\text{Region I: } \psi(x) = A e^{\alpha x} + B e^{-\alpha x} \quad \alpha^2 = \frac{2m(U-E)}{\hbar^2}$$

$$\text{Region II: } \psi(x) = C \sin(kx) + D \cos(kx) \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\text{Region III: } \psi(x) = E e^{\alpha x} + F e^{-\alpha x}$$

We can simplify some stuff by demand  $\psi$  be finite.

In region I, as  $x \rightarrow \infty$ , we want  $\psi$  to be finite (go to zero)

#20.) continued

So

$$\text{Region I: } \psi(x \rightarrow -\infty) = \lim_{x \rightarrow -\infty} (Ae^{\alpha x} + Be^{-\alpha x}) = 0$$

$$\lim_{x \rightarrow -\infty} e^{\alpha x} = 0$$

$$\lim_{x \rightarrow -\infty} e^{-\alpha x} = \infty$$

So to keep  $\psi$  finite,

$$B = 0$$

$\therefore$  In region I,

$$\psi(x) = Ae^{\alpha x}$$

Similarly, to keep region III finite as  $x \rightarrow +\infty$ ,

$$\text{Region III: } \psi(x \rightarrow \infty) = \lim_{x \rightarrow +\infty} (Ee^{\alpha x} + Fe^{-\alpha x}) = 0$$

$$\lim_{x \rightarrow +\infty} e^{\alpha x} = \infty$$

$$\lim_{x \rightarrow +\infty} e^{-\alpha x} = 0$$

$$\therefore E = 0$$

So in region III,

$$\psi(x) = Fe^{-\alpha x}$$

#20.) continued

Plus, in this problem, we're only worried about the symmetric (cosine) states. So now we're left with

$$\text{Region I: } \psi(x) = Ae^{\alpha x}$$

$$\text{Region II: } \psi(x) = D\cos(kx)$$

$$\text{Region III: } \psi(x) = Fe^{-\alpha x}$$

At the boundaries, we want to force  $\psi$  to be continuous, i.e.,

at  $x = -L$

$$Ae^{-\alpha L} = D\cos(kL) \quad (1)$$

at  $x = +L$

$$Fe^{-\alpha L} = D\cos(kL) \quad (2)$$

We also want  $\psi$  to be smooth at the boundaries (smooth =  $\frac{d\psi}{dx}$  is continuous)

at  $x = -L$

$$\frac{d\psi}{dx}_{\text{Region I}} = \frac{d\psi}{dx}_{\text{Region II}}$$

$$\begin{aligned} \Rightarrow A\alpha e^{-\alpha L} &= -Dk\sin(-kL) \\ &= Dk\sin(kL) \end{aligned} \quad (3)$$

#20.) continued

at  $x=L$

$$\frac{d\psi}{dx} \text{ Region III} = \frac{d\psi}{dx} \text{ Region II}$$

$$\Rightarrow -F\alpha e^{-\alpha L} = -D \sin(kL) \quad (4)$$

Divide eq. (3) by (1) and (4) by (2) to get

$$\alpha = k \frac{\sin(kL)}{\cos(kL)}$$

$$\therefore \boxed{k \tan(kL) = \alpha} \quad \blacksquare$$

b.) Show that the energy condition in a.) can be written as

$$k \sec(kL) = \sqrt{\frac{2mU}{\hbar^2}}$$

$$\text{Since } \alpha^2 = \frac{2mU}{\hbar^2} - \frac{2mE}{\hbar^2}$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\alpha^2 + k^2 = \frac{2mU}{\hbar^2}$$

$$\therefore \alpha = \sqrt{\frac{2mU}{\hbar^2} - k^2}$$

#20.) continued

$$\therefore k \tan(kL) = \sqrt{\frac{2mU}{\hbar^2} - k^2}$$

$$k^2 \tan^2(kL) = \frac{2mU}{\hbar^2} - k^2$$

$$k^2 (\tan^2(kL) + 1) = \frac{2mU}{\hbar^2}$$

Use the trig identity

$$\tan^2 \theta + 1 = \sec^2 \theta$$

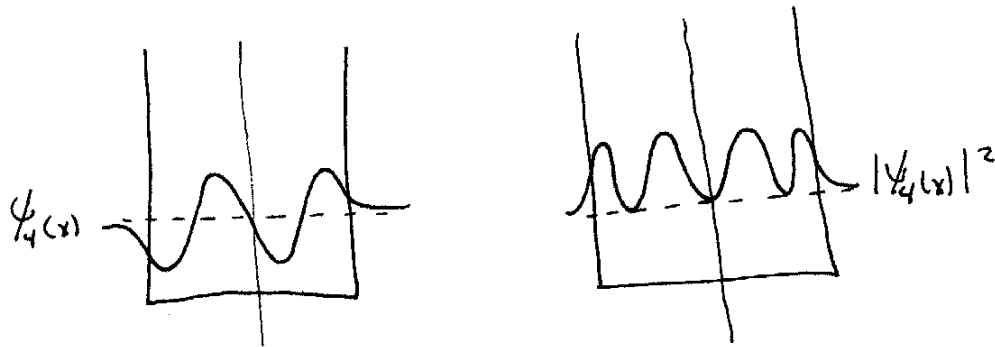
$$\therefore \boxed{k \sec(kL) = \sqrt{\frac{2mU}{\hbar^2}}}$$

Apply the result in this form to an electron trapped at a defect site in a crystal, modeling the defect as a square well of height 5 eV and width 0.2 nm. Write a simple computer program to find the ground state energy for the electron. Give your answer accurate to  $\pm 0.001$  eV.

You can do this using Excel like I did on that one problem way back when if you want, but it won't teach you anything other than how to work a computer. So I'll pass.

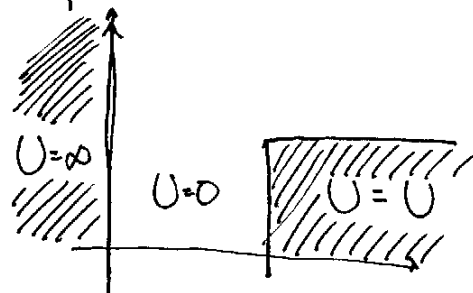
#21.) Sketch the wavefunction  $\psi(x)$  and the probability density  $|\psi(x)|^2$  for the  $n=4$  state of a particle in a finite potential well

That will just be the next highest wave in figure 5.13, p. 202:



#23.) Consider a square well having an infinite wall at  $x=0$  and a wall of height  $U$  at  $x=L$ . For the case of  $E < U$ , obtain solutions to the Schrödinger equation inside the well ( $0 \leq x \leq L$ ) and in the region beyond ( $x > L$ ) that satisfy the appropriate boundary conditions at  $x=0$  and  $x=\infty$ . Enforce the proper matching conditions at  $x=L$  to find the allowed energies of this system. Are there conditions for which no solution is possible? Explain.

Ok, here's our box



#25.) The wave function

$$\psi(x) = C x e^{-\alpha x^2}$$

also describes a state of the quantum oscillator, provided the constant  $\alpha$  is chosen properly.

a.) Using Schrödinger's equation, obtain an expression for  $\alpha$  in terms of the oscillator mass  $m$  and the classical frequency of vibration  $\omega$ . What is the energy of this state?

Schrödinger's equation for a quantum oscillator is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \quad (\text{eq. 5.25})$$

Take derivatives:

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= \frac{d^2}{dx^2} (C x e^{-\alpha x^2}) = \frac{d}{dx} (C e^{-\alpha x^2} - 2C x \alpha e^{-\alpha x^2}) \\ &= -2C \alpha x e^{-\alpha x^2} - 4C x \alpha e^{-\alpha x^2} + 4C x^3 \alpha^2 e^{-\alpha x^2} \\ &= 4C \alpha^2 x^3 e^{-\alpha x^2} - 6C \alpha x e^{-\alpha x^2} \end{aligned}$$

So Erwin's equation up there looks like

$$\begin{aligned} -\frac{\hbar^2}{2m} (4C \alpha^2 x^3 - 6C \alpha x) e^{-\alpha x^2} + \frac{1}{2} m \omega^2 (C x^3 e^{-\alpha x^2}) \\ = E C x e^{-\alpha x^2} \end{aligned}$$

#25.) continued

All those terms have  $C$ 's and  $e^{-\alpha x^2}$ 's in 'em so cancel those out and rearrange to get

$$4\alpha^2 x^2 - 6\alpha = \left(\frac{m\omega}{\hbar}\right)^2 x^2 - \frac{2mE}{\hbar^2}$$

Equate coefficients of like powers of  $x$ :

$$4\alpha^2 = \left(\frac{m\omega}{\hbar}\right)^2$$

$$\Rightarrow \boxed{\alpha = \frac{m\omega}{2\hbar}}$$

and

$$6\alpha = \frac{2mE}{\hbar^2}$$

$$\therefore \boxed{E = \frac{3\alpha \hbar^2}{m} = \frac{3}{2} \hbar \omega}$$

b.) Normalize this wave

Okay dorky. The thing can be anywhere between  $-\infty < x < \infty$ ,

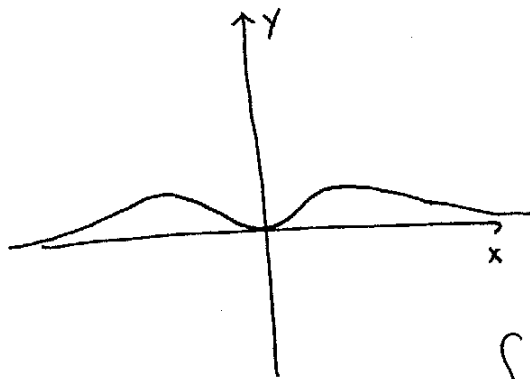
So

$$P = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$= C^2 \int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx$$

#25.) continued

To do this, we can use a keen little math trick. Note that the integrand is symmetric under  $x \rightarrow -x$ . If you plot it, it looks like:



See? It's symmetric about the y-axis. Now, an integral gives you the area under the curve, but since the area from  $-\infty$  to zero is the same as from zero to  $\infty$ , we can write

$$\begin{aligned}\int_{-\infty}^{\infty} f(x) dx &= \int_{-\infty}^0 f(x) dx + \int_0^{\infty} f(x) dx \\ &= \int_0^{\infty} f(x) dx + \int_0^{\infty} f(x) dx\end{aligned}$$

$$\therefore \int_{-\infty}^{\infty} f(x) dx = 2 \int_0^{\infty} f(x) dx \quad \text{if } f(x) = f(-x)$$

Sneaky! So now we can say

$$P = 2C^2 \int_0^{\infty} x^2 e^{-2\alpha x^2} dx$$

Still pretty hairy. The easiest thing to do is look it up, but you masochists out there can try to integrate by parts. Pain hurts me, though, so I'll look it up and say

$$P = 2C^2 \int_0^{\infty} x^2 e^{-2\alpha x^2} dx = 2C^2 \left( \frac{1}{8\alpha} \sqrt{\frac{\pi}{2\alpha}} \right) = 1$$

#25.) continued

So,

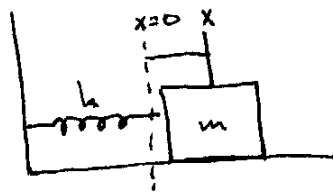
$$C = \left( \frac{32\alpha^3}{\pi} \right)^{1/4}$$

Sweet merciful god in heaven above!

#26.) Show that the oscillator energies in equation 5.29 correspond to the classical amplitudes

$$A_n = \sqrt{\frac{(2n+1)\hbar}{m\omega}}$$

Huh? Well, what they mean by that is that to solve the Quantum harmonic oscillator, we're using the potential  $U = \frac{1}{2}m\omega^2 x^2$ . That's the same potential that you get when you do the ol' block on a spring problem! That problem looks like



The energy of this thing is its kinetic:

$$K = \frac{1}{2}mv^2$$

Plus its potential stored in the spring

$$U = \frac{1}{2}m\omega^2 x^2$$

#29.) continued

$\langle x \rangle$  is the same classically and quantum mechanically.

$\langle x^2 \rangle$  differs by that factor of  $\frac{L^2}{2\pi^2}$ , but for general

$n$ , you get

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2(n\pi)^2}$$

So for large  $n$ , we can drop it and recover the classical result.

#30.) An electron is described by the wave function

$$\psi(x) = \begin{cases} 0 & x < 0 \\ Ce^{-x}(1-e^{-x}) & x > 0 \end{cases}$$

where  $x$  is in nanometers and  $C$  is a constant.

a.) Find the value of  $C$  that normalizes  $\psi$

$$\begin{aligned} P &= \int_0^{\infty} C^2 e^{-2x}(1-e^{-x})^2 dx \\ &= C^2 \int_0^{\infty} (e^{-2x} - 2e^{-3x} + e^{-4x}) dx \\ &= C^2 \left[ -\frac{e^{-2x}}{2} + \frac{2e^{-3x}}{3} - \frac{e^{-4x}}{4} \right] \Big|_0^{\infty} \\ &= C^2 \left[ \frac{1}{2} - \frac{2}{3} + \frac{1}{4} \right] = \frac{C^2}{12} = 1 \end{aligned}$$

$$\therefore C = \sqrt{12}$$

#30.) continued

b.) Where is the electron most likely to be found? That is, for what value of  $x$  is the probability of finding the electron largest?

The probability density is

$$|\psi(x)|^2 = 12(e^{-2x} - 2e^{-3x} + e^{-4x})$$

Maximize!

$$\frac{d|\psi(x)|^2}{dx} = 12(-2e^{-2x} + 6e^{-3x} - 4e^{-4x}) = 0$$

$$\Rightarrow -1 + 3e^{-x} - 2e^{-2x} = 0$$

$$\text{let } u = e^{-x}$$

$$= 2u^2 - 3u + 1 = 0$$

$$\Rightarrow u = \frac{3 \pm \sqrt{9-8}}{4} = \frac{3 \pm 1}{4} = 1, \frac{1}{2}$$

$$u = e^{-x} = 1$$

$$\Rightarrow x = 0 \quad \text{min}$$

$$u = e^{-x} = \frac{1}{2}$$

$$\Rightarrow \boxed{x = \ln 2 \quad \text{max}}$$

#30.) continued

c.) calculate  $\langle x \rangle$  for this electron and compare your results with its most likely position. Comment on any differences you find.

$$\langle x \rangle = \int_0^{\infty} \psi^*_x \psi dx = C^2 \int_0^{\infty} x(e^{-2x} - 2e^{-3x} + e^{-4x}) dx$$

We need to know how to do an integral of the form

$$\int x e^{-ax} dx$$

When in doubt, there's no reason to be subtle. . Integrate it by parts:

$$\begin{aligned} \text{let } u &= x & dv &= e^{-ax} dx \\ dx &= du & v &= -\frac{e^{-ax}}{a} \end{aligned}$$

$$\begin{aligned} \Rightarrow \int x e^{-ax} dx &= -\frac{x e^{-ax}}{a} + \frac{1}{a} \int e^{-ax} dx \\ &= -\frac{x e^{-ax}}{a} - \frac{e^{-ax}}{a^2} \end{aligned}$$

$$\begin{aligned} \therefore \int_0^{\infty} x e^{-ax} dx &= -\frac{x e^{-ax}}{a} \Big|_0^{\infty} - \frac{e^{-ax}}{a^2} \Big|_0^{\infty} \\ &= \frac{1}{a^2} \end{aligned}$$

#30.) continued

So,

$$\langle x \rangle = C^2 \left( \frac{1}{4} - \frac{2}{9} + \frac{1}{16} \right) = \frac{13}{12}$$

$$\boxed{\langle x \rangle = 1.083 \text{ nm}}$$

#31.) For any eigenfunction  $\psi_n$  of the infinite square well, show that  $\langle x \rangle = \frac{L}{2}$  and that

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2(n\pi)^2}$$

where  $L$  is the well dimension

For the infinite square well,

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

So

$$\langle x \rangle = \frac{2}{L} \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$= \frac{2}{L} \int_0^L x \left[ \frac{1}{2} (1 - \cos\left(\frac{2n\pi x}{L}\right)) \right] dx$$

$$= \frac{1}{L} \int_0^L \left[ x - x \cos\left(\frac{2n\pi x}{L}\right) \right] dx$$

#32.) continued

Now we have to find the probability to locate the particle between  $\langle x \rangle - \Delta x$  and  $\langle x \rangle + \Delta x$ :

$$P = \int_{\langle x \rangle - \Delta x}^{\langle x \rangle + \Delta x} |\psi(x)|^2 dx = \int_{-\frac{x_0}{\sqrt{2}}}^{\frac{x_0}{\sqrt{2}}} C^2 e^{-2|x|/x_0} dx$$

$$= 2C^2 \int_0^{\frac{x_0}{\sqrt{2}}} e^{-2x/x_0} dx$$

$$= \frac{2C^2}{-2/x_0} e^{-2x/x_0} \Big|_0^{\frac{x_0}{\sqrt{2}}}$$

$$\boxed{P = 1 - e^{-\sqrt{2}} = 0.757}$$

which is independent of  $x_0$

#33.) Calculate  $\langle x \rangle$ ,  $\langle x^2 \rangle$ , and  $\Delta x$  for a quantum oscillator in its ground state.

The ground state wavefunction of the quantum oscillator is:

$$\psi(x) = \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \exp\left[ -\frac{m\omega}{2\hbar} x^2 \right]$$

So

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi dx = \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \int_{-\infty}^{\infty} x e^{-\frac{m\omega}{\hbar} x^2} dx$$

#3.) continued

Again, the integrand is odd, and the interval is symmetric

$$\therefore \langle x \rangle = 0$$

$$\langle x^2 \rangle = \left( \frac{m\omega}{\hbar} \right)^{1/2} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} dx$$

Now the integrand is even, so

$$= 2 \left( \frac{m\omega}{\hbar} \right)^{1/2} \int_0^{\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} dx$$

Now let's use their hint:

$$\int_0^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$

with  $a = \frac{m\omega}{\hbar}$

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega}$$

$$\Delta X = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \left( \frac{\hbar}{2m\omega} \right)^{1/2}$$

34 a) We expect  $\langle p_x \rangle = 0$ , since the particle is oscillating - just moves back and forth.

b) We know  $E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ .

$$\text{So } \langle E \rangle = \frac{\langle p^2 \rangle}{2m} + \frac{1}{2}m\omega^2 \langle x^2 \rangle$$

Since  $\langle E \rangle = \frac{1}{2}\hbar\omega$  for the ground state,

$$\frac{1}{2}\hbar\omega = \frac{\langle p^2 \rangle}{2m} + \frac{1}{2}m\omega^2 \langle x^2 \rangle$$

$$\Rightarrow \langle p^2 \rangle = 2m \left[ \frac{1}{2}\hbar\omega - \frac{1}{2}m\omega^2 \langle x^2 \rangle \right]$$

$$= m\hbar\omega - m^2\omega^2 \langle x^2 \rangle.$$

We know  $\langle x^2 \rangle = \frac{\hbar}{2m\omega}$ , so  $\langle p^2 \rangle = \frac{\hbar m \omega}{2}$

$$\text{c) } \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \left( \frac{\hbar m \omega}{2} \right)^{1/2}$$

Notice:  $\Delta p \Delta x = \left( \frac{\hbar m \omega}{2} \right)^{1/2} \left( \frac{\hbar}{2m\omega} \right)^{1/2} = \frac{\hbar}{2}$  (The minimum uncertainty!)

#39.) Nonstationary states. Consider a particle in an infinite square well described initially by a wave that is a superposition of the ground and first excited states of the well

$$\Psi(x,0) = C [\psi_1(x) + \psi_2(x)]$$

a) Show that the value  $C = \frac{1}{\sqrt{2}}$  normalizes this wave, assuming  $\psi_1$  and  $\psi_2$  are themselves normalized

First of all, you need to know that the  $\psi_n(x)$ 's of the square well are what's called orthogonal. That is,

$$\int_0^L \psi_n^*(x) \psi_m(x) dx = \begin{cases} 0 & \text{if } n \neq m \\ 1 & \text{if } n = m \end{cases}$$

You can show this using

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

But I'm not going to. Take my word for it. You might want to try proving it, though.

So let's normalize  $\Psi(x,0)$

$$P = \int_0^L \Psi^* \Psi dx = \int_0^L C^2 [\psi_1^*(x) + \psi_2^*(x)] [\psi_1(x) + \psi_2(x)] dx$$

#39.) continued

$$= C^2 \int_0^L [\psi_1^* \psi_1 + \psi_2^* \psi_2 + \psi_1^* \psi_2 + \psi_2^* \psi_1] dx$$

Since the  $\psi_n$ 's are orthogonal, the last two terms vanish

$$= C^2 \int_0^L [\psi_1^* \psi_1 + \psi_2^* \psi_2] dx$$

$\psi_1$  and  $\psi_2$  are themselves normalized, so this is

$$= C^2 (1+1) = 2C^2 = 1$$

$$\therefore \boxed{C = \frac{1}{\sqrt{2}}}$$

b.) Find  $\Psi(x,t)$  at any later time  $t$ .

Remember that to get the time dependent solution, you just multiply by

$$\phi_n(t) = e^{-i \frac{E_n}{\hbar} t}$$

$$\Psi(x,t) = C [\psi_1(x,t) + \psi_2(x,t)]$$

$$\boxed{\Psi(x,t) = C [\psi_1(x) e^{-i \frac{E_1}{\hbar} t} + \psi_2(x) e^{-i \frac{E_2}{\hbar} t}]}$$

#39) continued

c.) Show that the superposition is not a stationary state, but that the average energy in this state is the arithmetic mean  $(E_1 + E_2)/2$  of the ground and first excited state energies  $E_1$  and  $E_2$ .

What is meant by a stationary state is that the probability density does not change in time. So the way to show this is if something is a stationary state, then with respect to time the probability density is constant.

So

$$\frac{\partial |\Psi(x,t)|^2}{\partial t} = 0 \quad \text{if } \Psi(x,t) \text{ is a stationary state}$$

Let's try it with this one

$$\begin{aligned} |\Psi(x,t)|^2 &= C^2 \left[ \psi_1^*(x) e^{\frac{iE_1 t}{\hbar}} + \psi_2^*(x) e^{\frac{iE_2 t}{\hbar}} \right] \left[ \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right] \\ &= C^2 \left[ \psi_1^*(x) \psi_1(x) + \psi_2^*(x) \psi_2(x) + \psi_1^*(x) \psi_2(x) e^{-\frac{i(E_2 - E_1)t}{\hbar}} \right. \\ &\quad \left. + \psi_2^*(x) \psi_1(x) e^{\frac{i(E_2 - E_1)t}{\hbar}} \right] \end{aligned}$$

So

$$\boxed{\frac{\partial |\Psi(x,t)|^2}{\partial t} \neq 0!}$$

Not a stationary state!

#39.) continued

To get the average energy

$$\langle E \rangle = \int_0^L \Psi^*(x,t) \hat{E} \Psi(x,t) dx$$

Remember that

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

$$= C^2 \int_0^L [\psi_1^*(x) e^{\frac{iE_1 t}{\hbar}} + \psi_2^*(x) e^{\frac{iE_2 t}{\hbar}}] \left( i\hbar \frac{\partial}{\partial t} \right) [\psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x) e^{-\frac{iE_2 t}{\hbar}}] dx$$

$$= i\hbar C^2 \int_0^L [\psi_1^* e^{\frac{iE_1 t}{\hbar}} + \psi_2^* e^{\frac{iE_2 t}{\hbar}}] \left[ -i \frac{E_1}{\hbar} \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} - i \frac{E_2}{\hbar} \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right] dx$$

$$= C^2 \int_0^L [E_1 \psi_1^* \psi_1 + E_2 \psi_2^* \psi_2] dx$$

All the other terms go away thanks to orthogonality!

$$= C^2 (E_1 + E_2)$$

$$= \boxed{\frac{(E_1 + E_2)}{2} = \langle E \rangle}$$

Oh my god! Time for a Bud!

$$\langle x \rangle = \int \Psi^*(x, t) x \Psi(x, t)$$

$$= \int \left( \frac{1}{\sqrt{2}} (\psi_1^*(x) e^{+i\omega_1 t} + \psi_2^*(x) e^{+i\omega_2 t}) \right) x \left( \frac{1}{\sqrt{2}} (\psi_1(x) e^{-i\omega_1 t} + \psi_2(x) e^{-i\omega_2 t}) \right)$$

$$= \frac{1}{2} \left( \int x |\psi_1|^2 dx + \int x |\psi_2|^2 dx \right) + \frac{1}{2} \int (\psi_1 \psi_2^* e^{i(\omega_2 - \omega_1)t} + \psi_2 \psi_1^* e^{-i(\omega_2 - \omega_1)t}) dx$$

Now, since  $\psi_1$  &  $\psi_2$  are real,  $\psi_1 \psi_2^* = \psi_2 \psi_1^*$

and  $e^{i\theta} + e^{-i\theta} = 2 \cos \theta$ , so

$$\frac{1}{2} \int (\psi_1 \psi_2^* e^{i(\omega_2 - \omega_1)t} + \psi_2 \psi_1^* e^{-i(\omega_2 - \omega_1)t}) dx = \frac{1}{2} \int x \psi_1^* \psi_2 \cdot 2 \cos(\omega_2 - \omega_1)t dx$$

$$= \int x \psi_1^* \psi_2 \cos\left(\frac{E_2 - E_1}{\hbar} t\right)$$

Done!  $\langle x \rangle = \left[ \frac{1}{2} \left( \int x |\psi_1|^2 dx + \int x |\psi_2|^2 dx \right) \right] + \left[ \int x \psi_1^* \psi_2 dx \right] \cos\left(\frac{E_2 - E_1}{\hbar} t\right)$

For  $L = 1 \text{ nm}$ ,

$$x_0 = \frac{1}{2} [\langle x \rangle_1 + \langle x \rangle_2] = \frac{1}{2} \left[ \frac{L}{2} + \frac{L}{2} \right] = \boxed{\frac{L}{2}}$$

$$\begin{aligned} \text{and } A &= \int_0^L x \psi_1^* \psi_2 = \frac{2}{L} \int_0^L x \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx \\ &= \frac{1}{L} \int_0^L x \left[ \cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right) \right] dx \quad (\text{I used a trig identity}). \end{aligned}$$

Now integrate by parts:

$$\int x \cos(ax) dx = \frac{1}{a} x \sin(ax) - \int \frac{1}{a} \sin(ax) dx$$

$$\Rightarrow A = \frac{1}{L} \left[ \frac{L}{\pi} \int_0^L \sin\left(\frac{\pi x}{L}\right) + \frac{L}{3\pi} \int_0^L \sin\left(\frac{3\pi x}{L}\right) \right]$$

$$= + \left(\frac{L}{\pi}\right)^2 (-2) - \left(\frac{L}{3\pi}\right)^2 (-2)$$

$$= L^2 \left( \frac{2}{9\pi^2} - \frac{2}{\pi^2} \right) = \boxed{\frac{-16L}{9\pi^2}} = -0.18 \text{ nm for } L = 1 \text{ nm}.$$

$$\text{Time to shuttle back 'n' forth} = \text{Period} = \frac{1}{f} = \frac{2\pi}{\omega}$$

$$\text{Here, } \omega = \frac{E_2 - E_1}{\hbar} = \frac{3E_1}{\hbar} = \frac{3\pi^2 \hbar}{2mL^2}$$

$$\text{So } \frac{2\pi}{\omega} = \frac{4mL^2}{3\pi\hbar} = \boxed{3.67 \times 10^{-15} \text{ s}}$$

Classically, electron would have  $v = \left(\frac{2E}{m}\right)^{1/2} = \left(\frac{E_1 + E_2}{m}\right)^{1/2}$

$$E_1 + E_2 = \frac{5\pi^2 \hbar^2}{2mL^2}, \text{ so } v = \left(\frac{5\pi^2 \hbar^2}{2m^2 L^2}\right)^{1/2} = \sqrt{\frac{5}{2}} \frac{\pi \hbar}{mL} = \boxed{5.75 \times 10^5 \frac{\text{m}}{\text{s}}}$$

So it would take time  $2\left(\frac{L}{v}\right) = \boxed{3.47 \times 10^{-15} \text{ s}}$  classically!