Physics 2D, Winter 2005 Quiz 6 Key

1. Designer Wavefunctions (6 points)

(a) You are given that ψ_1 and ψ_2 are two solutions of the TISE with the same energy, E. What does that mean, mathematically? It means

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_1 + U(x)\,\psi_1 = E\,\psi_1 \qquad (1)$$

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_2 + U(x)\,\psi_2 = E\,\psi_2 \qquad (2)$$

The question is, mathematically, does

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 (A\,\psi_1 + B\,\psi_2) + U(x)\,(A\,\psi_1 + B\,\psi_2) = E\,(A\,\psi_1 + B\,\psi_2) \ ?$$

To answer the question, we must expand $\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 (A\,\psi_1 + B\,\psi_2)$.

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 (A\,\psi_1 + B\,\psi_2) = A\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_1 + B\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_2$$

I just distributed the derivative. I don't have to apply any derivatives. Then, expanding the rest of the equation in question gives

$$A\,\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_1 + B\,\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_2 + A\,U(x)\,\psi_1 + B\,U(x)\,\psi_2 = A\,E\,\psi_1 + B\,E\,\psi_2$$

Next, collecting the A and B yields

$$A\left(\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_1 + U(x)\,\psi_1\right) + B\left(\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_2 + U(x)\,\psi_2\right) = A\,E\,\psi_1 + B\,E\,\psi_2$$

If I use the given relationships above, (1) and (2), then I find

$$A\,(E\,\psi_1) + B(E\,\psi_2) = A\,E\,\psi_1 + B\,E\,\psi_2$$

This is true, so yes, the linear combination of two wave functions which are solutions *with the same energy* is a solution, with that energy.

(b) Now, we have a linear combination of wave functions with different energies.

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_1 + U(x)\,\psi_1 = E_1\,\psi_1 \qquad (1)$$

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_2 + U(x)\,\psi_2 = E_2\,\psi_2 \qquad (2)$$

The question is, mathematically, does

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 (A\,\psi_1 + B\,\psi_2) + U(x)\,(A\,\psi_1 + B\,\psi_2) = E_3\,(A\,\psi_1 + B\,\psi_2) \ ?$$

I have introduced a new energy E_3 for the superposition since there is no reason to expect that the energy for

the superposition is E_1 or E_2. Expanding as above gives

$$A \frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^2 \psi_1 + B \frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^2 \psi_2 + A\, U(x)\, \psi_1 + B\, U(x)\, \psi_2 = A\, E_3\, \psi_1 + B\, E_3\, \psi_2$$

Collecting the A and B then yields

$$A\left(\frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^2 \psi_1 + U(x)\, \psi_1\right) + B\left(\frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^2 \psi_2 + U(x)\, \psi_2\right) = A\, E_3\, \psi_1 + B\, E_3\, \psi_2$$

Finally, using equations (1) and (2) gives

$$A\,(E_1\, \psi_1) + B\,(E_2\, \psi_2) = A\, E_3\, \psi_1 + B\, E_3\, \psi_2 \qquad (3)$$

Now, for this equation to be true, it must be true no matter what ψ_1 or ψ_2 are. This is a tremendously important mathematical principle. Particularly, the equation must be true if even ψ_1 is zero everywhere. I.e.,

$$B\, E_2\, \psi_2 = B\, E_3\, \psi_2 \qquad (4a)$$

This is true, if $E_3 = E_2$. However, the equation (3) must also be true if ψ_1 is nonzero and ψ_2 is zero every where, then we need

$$A\, E_1\, \psi_1 = A\, E_3\, \psi_1. \qquad (4b)$$

This is true only if $E_3 = E_1$. Since $E_1 \neq E_2$, we cannot satisfy both of these requirements (4a) and (4b) for one value of E_3. Thus Equation (3) is not true in general. A linear combo of two wavefunctions that solve the TISE, *but have different energies,* is *not* a solution of the TISE.

2. Think *inside* the box

(a) As we know, we need the wave function to be zero outside of the box, including the edges of the box. I.e.,

$$\psi(x = -L/4) = 0 \quad \text{and} \quad \psi(x = +L/4) = 0$$

Also, inside the box, the potential is zero, so the functions must be solutions to the TISE, with zero potential:

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi(x) = E\,\psi(x)$$

i.e.,

$$\psi''(x) = -\frac{2mE}{\hbar^2}\,\psi(x)$$

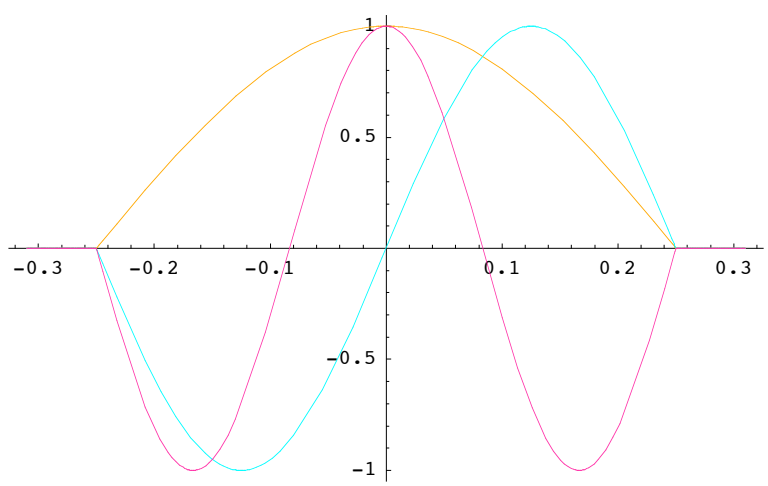
Now, there is no potential energy, so $E = p^2/2m$, and $2mE/\hbar^2 = p^2/\hbar^2$, so the above equation can be written

$$\psi''(x) = -(p/\hbar)^2\,\psi(x)$$

The solutions to this differential equation, as we have seen are

$$\psi(x) = A\sin(p\,x/\hbar) + B\cos(p\,x/\hbar)$$

Now, our plots for $n = 1, 2, 3$ are sinusoidal curves that are zero at the ends of the box and have either 1, 2, or 3 extrema (humps). The $n = 1, 2, 3$ plots are shown here in orange, blue, and pink, respectively.



In order to meet the boundary conditions, we need

either 1) $A = 0$ and $\cos(p\,[L/4]/\hbar) = \cos(p\,[-L/4]/\hbar) = 0$
or 2) $B = 0$ and $\sin(p\,[L/4]/\hbar) = -\sin(p[-L/4]/\hbar) = 0$

That is, some of the solutions are sines ($B = 0$) and others are cosines ($A = 0$). There is no mixing. For the cosines, $\cos(p\,L/4\,\hbar) = 0$ means that we require

for cosines, $p\,L/4\,\hbar = (n - 1/2)\,\pi$ $\quad n = 1, 2, 3, \ldots$
$p = (n - 1/2)\,\frac{4\,\pi\,\hbar}{L}$

For the sines, $\sin(p\,L/4\,\hbar) = 0$ means that we require

for sines, $p\,L/4\,\hbar = n\,\pi$ $\quad n = 1, 2, 3, \ldots$
$p = n\,\frac{4\,\pi\,\hbar}{L}$

Note that this has the proper units for momentum.
So, at last, as you might have guessed from the plots, our first three wave functions are

$$\psi_1 = A_1 \cos(\tfrac{1}{2}\,\tfrac{4\pi}{L}\,x)$$
$$\psi_2 = B_1 \sin(1 \cdot \tfrac{4\pi}{L}\,x)$$
$$\psi_3 = A_2 \cos(\tfrac{3}{2}\,\tfrac{4\pi}{L}\,x)$$

Normalization, not required for quiz:
We have to find the coefficients A_1, B_1, and A_2 by normalizing the wavefunctions, i.e. making sure that the probability that the particle is in the box is 1, which means that the particle really is in the box. The probability density (ProbDens) is the square of the wavefunction:

$$ProbDens_1(x) = \psi_1{}^2 = A_1{}^2\, cos^2(2\,\pi\,x/L)$$

Then, we integrate this over the width of the box, using the fact that the integral of $cos^2\,\theta$ over one half of a period is just one half the interval of the integral

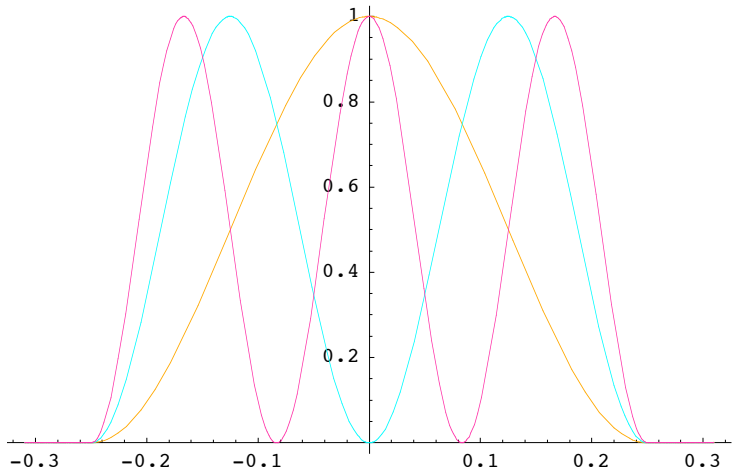
$$\int_{-L/4}^{L/4} Prob_1(x)\,dx = A_1{}^2 \int_{-L/4}^{L/4} cos^2(2\,\pi\,x/L)\,dx = A_1{}^2 \cdot \tfrac{1}{2}\,\tfrac{L}{2} = A_1{}^2 \cdot \tfrac{L}{4}$$

In order to have this equal one, we need $A_1 = \frac{2}{\sqrt{L}}$.
Doing the same thing for ψ_2 and ψ_3 gives the same normalization factor, i.e.,

$$\psi_1 = \tfrac{2}{\sqrt{L}}\, cos(\tfrac{2\pi}{L}\,x)$$
$$\psi_2 = \tfrac{2}{\sqrt{L}}\, sin(\tfrac{4\pi}{L}\,x)$$
$$\psi_3 = \tfrac{2}{\sqrt{L}}\, cos(\tfrac{6\pi}{L}\,x)$$

Well, that was long, but the rest is easy as pie.

(b) The probability density is just the square of the wavefunction. The sketches, which you can do without finding the wavefunctions in detail are here.



The equations are

$$\text{ProbDens}_1(x) = \frac{4}{L}\cos^2\left(\frac{2\pi}{L}x\right)$$
$$\text{ProbDens}_2(x) = \frac{4}{L}\sin^2\left(\frac{4\pi}{L}x\right)$$
$$\text{ProbDens}_3(x) = \frac{4}{L}\cos^2\left(\frac{6\pi}{L}x\right)$$

(c) The energies as mentioned above are given by $E_n = \frac{1}{2m}{p_n}^2$. We found above that for the ground state, $p = \frac{1}{2}\frac{4\pi\hbar}{L}$ from $n = 1$ in the cosine solution, and for the first excited state, $n = 1$ for the sine solution, $p = \frac{4\pi\hbar}{L}$. So the energies are

$$E_1 = \frac{1}{2m}\left(\frac{2\pi\hbar}{L}\right)^2$$

$$E_2 = \frac{1}{2m}\left(\frac{4\pi\hbar}{L}\right)^2$$

Note (if you didn't already) that these agree with the general formula, $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ except that the length of the above box is $L/2$.

(Wave function plotting)