Problem Set 4 8.04 Spring 2013 Solutions March 05, 2013

Problem 1. (10 points) Simultaneous Eigenstates

We do *not* in fact know the state's momentum precisely. As an example, consider the ground state of a particle in a box of width L:

$$\phi_0(x) = \begin{cases} 0 & \text{for } x < 0\\ \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) & \text{for } 0 < x < L\\ 0 & \text{for } x > 0 \end{cases}$$
(1)

Our friend's claim that this state has a definite momentum is equivalent to claiming that this state is a momentum eigenstate. If that were so, it would satisfy the momentum eigenvalue equation:

$$\hat{p}\phi_E = p\phi_E \quad \Rightarrow \quad \frac{\hbar}{i} \frac{d\phi_E}{dx} = p\,\phi_E(x).$$
(2)

Considering the region 0 < x < L, we have

$$\frac{\hbar}{i}\frac{d\phi_0}{dx} = \frac{\hbar}{i}\frac{d}{dx}\left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right) = \frac{\pi\hbar}{iL}\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right),\tag{3}$$

which cannot be expressed as a multiple of  $\phi_0$ . The state is therefore *not* a momentum eigenstate.

To really drive the point home, we can compute the momentum space wavefunction  $\psi(k)$ :

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{0}^{L} \left( \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right) e^{-ikx} dx = \frac{\sqrt{\pi L} (1 + e^{-ikL})}{\pi^2 - k^2 L^2}.$$
 (4)

The momentum space probability density is given by  $|\tilde{\psi}(k)|^2$ :

$$|\tilde{\psi}(k)|^2 = \frac{2\pi L (1 + \cos kL)}{(\pi^2 - k^2 L^2)^2},\tag{5}$$

which is plotted in the graph on the next page, where the x-axis is in units of 1/L and the y-axis is in units of L. The momentum space probability density clearly has a finite width to it, which means that there is some uncertainty in the wavefunction's momentum. The wavefunction is not a momentum eigenstate.

Our friend's mistake was in assuming that since V(x) = 0 inside the box, the particle is just like a free particle, and that knowing the energy precisely implies knowing the momentum precisely. The particle is, however, definitely *not* a free particle, because the potential goes from 0 to  $\infty$  at x = 0 and x = L. Even though we only have to solve the energy eigenvalue



equation in the region 0 < x < L (because we know a priori that  $\phi_E(x) = 0$  outside the box), it is important to remember that the wavefunction formally extends over all space, even if it happens to be zero in some regions. Put another way, the particle "feels" the potential from  $x = -\infty$  to  $\infty$ , even if it is confined to a finite region. In fact, it is more correct to say that the particle is confined only because it feels the potential everywhere.

Suppose your friend now comes back to you, having read the previous paragraph, and says "fine, let's just have V(x) = 0 everywhere then". In *that* case, wavefunctions of the form  $Ae^{ikx}$  become energy eigenstates, and they *are* in fact also momentum eigenstates (try it!). However, the momentum eigenstate  $Ae^{ikx}$  is in no way localized, so we have simply traded uncertainty in momentum for uncertainty in position, consistent with the uncertainty principle. Note that, also in this case where V = 0 everywhere, not all energy eigenstates are also momentum eigenstates, e.g.  $\sin(kx) = \frac{1}{2}(e^{ikx} - e^{-ikx})$ , which has precisely energy  $E = \frac{\hbar^2 k^2}{2m}$  but average momentum  $\langle p \rangle = 0$ .

Here's a tip for life: don't fight the uncertainty principle. You will always lose. Even if your name is Einstein<sup>1</sup>.

<sup>&</sup>lt;sup>1</sup>Take a look at this if you're interested: http://en.wikipedia.org/wiki/Bohr-Einstein\_debates.

Problem 2. (10 points) Formal Properties of Energy Eigenstates

(a) (3 points) If  $\phi_E(x)$  is an energy eigenstate, then it satisfies the energy eigenvalue equation:

$$\hat{E}\phi_E = E\phi_E \quad \text{or} \quad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\phi_E = E\phi_E.$$
 (6)

Taking the complex conjugate of both sides gives

$$\hat{E}\phi_E^* = E\phi_E^*$$
 or  $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\phi_E^* = E\phi_E^*,$  (7)

where E is unaffected by the complex conjugation (as can be seen by its explicit form<sup>2</sup>), and the same is true for E, because the eigenvalues of observables had better be real. Equation 7 takes the form of an energy eigenvalue equation for  $\phi_E^*$ , which is another way of saying that if  $\phi_E$  is an eigenstate with eigenvalue E, then so is  $\phi_E^*$ . Now suppose we add Equations 6 and 7 together:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\phi_E + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\phi_E^* = E\phi_E + E\phi_E^* \tag{8a}$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\left[\phi_E + \phi_E^*\right] = E[\phi_E + \phi_E^*].$$
(8b)

This tells us that  $\phi_E + \phi_E^*$ , too, is an eigenstate with energy E. (Alternatively, we could've made the same point simply by invoking the principle of superposition, although this derivation makes it much more obvious that the new state also has eigenvalue E). Since  $\phi_E + \phi_E^*$  is real<sup>3</sup>, we see that the energy eigenfunctions can always be taken to be real by forming linear combinations (which the principle of superposition tells us we are allowed to do).

(b) (2 points) We once again begin with the eigenvalue equation:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\phi_E(x) = E\phi_E(x).$$
(9)

We now let  $x \to -x$ . There is nothing wrong with doing this — if you like, we're just expressing things in terms of a new variable  $y \equiv -x$ . Doing so gives

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2} + V(-x)\right)\phi_E(-x) = E\phi_E(-x)$$
(10a)

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\phi_E(-x) = E\phi_E(-x).$$
(10b)

<sup>&</sup>lt;sup>2</sup>There is also a deep reason for this. Stay tuned!

<sup>&</sup>lt;sup>3</sup>That's true for any complex number: if c = a + ib, then  $c + c^* = a + ib + a - ib = 2a$ , which is real.

To get to the second line, we used the fact that i) we're taking a *two* derivatives, so the two minus signs from each derivative cancel out, and ii) the evenness of V(x), *i.e.* V(x) = V(-x). Equation 10b tells us that if  $\phi_E(x)$  is an eigenstate, then so is  $\phi_E(-x)$ . Just like in the previous part of this problem, the principle of superposition allows us to form new eigenstates

$$\psi_{odd}(x) \equiv \frac{\phi_E(x) - \phi_E(-x)}{2} \quad \text{and} \quad \psi_{even}(x) \equiv \frac{\phi_E(x) + \phi_E(-x)}{2}. \tag{11}$$

One can check that these satisfy the conditions  $\psi_{odd}(-x) = -\psi_{odd}(x)$  and  $\psi_{even}(-x) = \psi_{even}(x)$  for odd and even functions respectively.

(c) (5 points) We start with the energy eigenvalue equation:

$$\hat{E}\psi = E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{12}$$

This can be rearranged to give

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2} [V(x) - E] \psi(x). \tag{13}$$

If  $E < V_{min}$ , then  $\psi$  and its second derivative always have the same sign. The easiest way to understand the implications of this is to imagine what would happen if we were asked to numerically integrate Equation 13 to find  $\psi(x)$  given initial conditions  $\psi(x_0)$  and  $\partial \psi / \partial x \big|_{x=x_0}$  at some point  $x = x_0$ . The simplest way to numerically integrate the equation would be to implement the following (very heuristic!) recipe:

- (a) Start with the value of  $\psi(x_n)$  at some point  $x_n$ .
- (b) Use the value of  $\partial \psi / \partial x$  at that point to get a linear estimate of the value of  $\psi$  at  $x_{n+1} \equiv x + \Delta x$  using

$$\psi(x_{n+1}) \approx \psi(x) + \frac{\partial \psi}{\partial x}\Big|_{x=x_n} \Delta x.$$
(14)

- (c) Use the value of  $\partial^2 \psi / \partial x^2$  at that point to get a linear estimate of the value of  $\partial \psi / \partial x$  at  $x_{n+1} \equiv x + \Delta x$ .
- (d) Repeat steps 1-3 for the point  $x_{n+1}$ .

Now consider several cases for the initial conditions:

•  $\psi(x_0) > 0$  and  $\partial \psi / \partial x \big|_{x=x_0} > 0$ . Since  $\psi(x_0) > 0$ , it follows from what we said above that  $\partial^2 \psi / \partial x^2 \big|_{x=x_0} > 0$ . This means that Step 3 of our algorithm makes  $\partial \psi / \partial x$  even more positive as we increase x by  $\Delta x$ . In turn, this makes  $\psi(x)$  also get more positive as we advance in x. Repeating this argument over and over again, we see that  $\psi(x)$  increases monotonically as we increase x, and so<sup>4</sup>  $\psi \to \infty$ as  $x \to \infty$ .

<sup>&</sup>lt;sup>4</sup>The rigorous amongst you may worry that a function can increase monotonically but asymptote to a constant value instead of diverging as  $x \to \infty$ . This possibility, however, is ruled out by the fact that  $\partial \psi / \partial x$  is also increasing monotonically. Besides, we are about to argue that the  $\psi(x)$  we get cannot be normalized, and that would still be the case even if  $\psi(x)$  did approach some asymptotic value.

•  $\psi(x_0) > 0$  and  $\partial \psi / \partial x_{x=x_0} < 0$ . If we substitute V(x) with V(-x) in (13), following the same reasoning as in part (b) we obtain that  $\psi(-x)$  is a solution to Equation (13), that  $\psi(-x_0) > 0$  and that  $\partial \psi / \partial x_{x=-x_0} > 0$ . Thus, we fall in the first case again, and  $\psi \to \infty$  as  $x \to \infty$ .

For initial conditions where  $\psi(x_0) < 0$ , one can simply repeat the arguments above but with opposite signs. In every case the wavefunction diverges (*i.e.*  $\psi \to \pm \infty$ ) as  $x \to \infty$  of  $x \to -\infty$ . From this, we can say that a wavefunction with  $E < V_{min}$  cannot be normalized and thus is not a permissible wavefunction. Problem Set 4 8.04 Spring 2013 Solutions March 05, 2013

Problem 3. (20 points) Superposition in the Infinite Well

(**Background**) We wish to verify that an infinite potential well of width L has eigenfunctions given by

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x),\tag{15}$$

with energy  $E_n = \hbar^2 k_n^2/2m$ , where  $k_n = (n+1)\pi/L$ . We can do so by plugging the eigenfunctions into the energy eigenvalue equation:

$$\hat{E}\psi = E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$
(16)

where we have restricted ourselves to  $0 \le x \le L$ , so V(x) = 0. The left hand side is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\sqrt{\frac{2}{L}}\sin(k_n x)\right] = \frac{\hbar^2 k_n^2}{2m}\sqrt{\frac{2}{L}}\sin(k_n x) = E_n\phi_n,$$
 (17)

so our eigenfunctions are indeed solutions to the system. The fact that  $k_n = (n+1)\pi/L$  follows from the need to satisfy the boundary conditions  $\phi_n(0) = \phi_n(L) = 0$ .

(a) (2 points) Recall from our analysis of the Schrödinger equation that an energy eigenstate (a "stationary state") evolves in time in the following way:

$$\psi(x,t) = e^{-iEt/\hbar}\phi(x,0). \tag{18}$$

The wavefunction  $\psi_A$  is *not* an energy eigenstate. However, by the superposition principle we can find the time evolution of each of the three eigenstates that comprise  $\psi_A$ , and then add our results together to find  $\psi_A(x,t)$ . So if

$$\psi_A(x,0) = \sqrt{\frac{1}{6}}\phi_0(x) + \sqrt{\frac{1}{3}}\phi_1(x) + \sqrt{\frac{1}{2}}\phi_2(x), \tag{19}$$

then

$$\psi_A(x,t) = \sqrt{\frac{1}{6}} e^{-iE_0 t/\hbar} \phi_0(x) + \sqrt{\frac{1}{3}} e^{-iE_1 t/\hbar} \phi_1(x) + \sqrt{\frac{1}{2}} e^{-iE_2 t/\hbar} \phi_2(x), \qquad (20)$$

where  $E_0$ ,  $E_1$ , and  $E_2$  are given by the expression for  $E_n$  shown above.

(b) (4 points) First we rewrite  $E_1$  and  $E_2$  in terms of  $E_0$ :

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{(n+1)^2 \pi^2 \hbar^2}{2mL^2} \quad \Rightarrow \quad E_1 = 4E_0, \ E_2 = 9E_0.$$
(21)

With this our previous answer becomes

$$\psi_A(x,t) = \sqrt{\frac{1}{6}} e^{-iE_0 t/\hbar} \phi_0(x) + \sqrt{\frac{1}{3}} e^{-i4E_0 t/\hbar} \phi_1(x) + \sqrt{\frac{1}{2}} e^{-i9E_0 t/\hbar} \phi_2(x).$$
(22)

We now compute  $\langle \hat{E} \rangle$  using two methods (both of which, naturally, give the same result). For the first method, recall that if a properly normalized wavefunction is decomposed into a sum of energy eigenstates

$$\psi = \sum_{n} c_n \phi_n, \tag{23}$$

then the probability of measuring energy  $E_n$  is given by  $|c_n|^2$ , *i.e.* the norm-squared of the coefficient in front of the corresponding eigenfunction. For example, in our case the probabilities of measuring  $E_0$ ,  $E_1$ , and  $E_2$  are

$$\mathbb{P}(E_0) = |c_0|^2 = \left(\sqrt{\frac{1}{6}}e^{-iE_0t/\hbar}\right)^* \left(\sqrt{\frac{1}{6}}e^{-iE_0t/\hbar}\right) = \frac{1}{6}e^{+iE_0t/\hbar}e^{-iE_0t/\hbar} = \frac{1}{6}$$
(24a)

$$\mathbb{P}(E_1) = |c_1|^2 = \left(\sqrt{\frac{1}{3}}e^{-i4E_0t/\hbar}\right)^* \left(\sqrt{\frac{1}{3}}e^{-i4E_0t/\hbar}\right) = \frac{1}{3}e^{+i4E_0t/\hbar}e^{-i4E_0t/\hbar} = \frac{1}{3}$$
(24b)

$$\mathbb{P}(E_2) = |c_2|^2 = \left(\sqrt{\frac{1}{2}}e^{-i9E_0t/\hbar}\right)^* \left(\sqrt{\frac{1}{2}}e^{-i9E_0t/\hbar}\right) = \frac{1}{2}e^{+i9E_0t/\hbar}e^{-i9E_0t/\hbar} = \frac{1}{2} \quad (24c)$$

Notice that the probabilities add up to 1, as they should since  $\phi_0$ ,  $\phi_1$ , and  $\phi_2$  are the only eigenstates that comprise  $\psi_A$ . The expectation value  $\langle \hat{E} \rangle$  is simply the weighted average of the measured energy:

$$\langle \hat{E} \rangle = \sum_{n} E_{n} \mathbb{P}(E_{n}) = \frac{1}{6} E_{0} + \frac{1}{3} E_{1} + \frac{1}{2} E_{2} = \frac{1}{6} E_{0} + \frac{4}{3} E_{0} + \frac{9}{2} E_{0} = 6E_{0}.$$
 (25)

The second method is more complicated, but it is instructive to see that it works. We start with the definition of  $\langle \hat{E} \rangle$ :

$$\langle \hat{E} \rangle \equiv \int_{-\infty}^{\infty} \psi_A^* \hat{E} \psi_A dx.$$
 (26)

Now, because we've written  $\psi_A$  in terms of a superposition of eigenstates of  $\hat{E}$ , the quantity  $\hat{E}\psi_A$  is simple:

$$\hat{E}\psi_A = \hat{E}\left(\sqrt{\frac{1}{6}}e^{-iE_0t/\hbar}\phi_0(x) + \sqrt{\frac{1}{3}}e^{-i4E_0t/\hbar}\phi_1(x) + \sqrt{\frac{1}{2}}e^{-i9E_0t/\hbar}\phi_2(x)\right)$$
(27a)

$$= \left(\sqrt{\frac{1}{6}}e^{-iE_0t/\hbar}\hat{E}\phi_0(x) + \sqrt{\frac{1}{3}}e^{-i4E_0t/\hbar}\hat{E}\phi_1(x) + \sqrt{\frac{1}{2}}e^{-i9E_0t/\hbar}\hat{E}\phi_2(x)\right) \quad (27b)$$

$$= \left(\sqrt{\frac{1}{6}}e^{-iE_0t/\hbar}E_0\phi_0(x) + \sqrt{\frac{1}{3}}e^{-i4E_0t/\hbar}E_1\phi_1(x) + \sqrt{\frac{1}{2}}e^{-i9E_0t/\hbar}E_2\phi_2(x)\right) (27c)$$

In the first equality, we used the fact that  $\hat{E}$  contains only spatial derivatives, so it passes right through the  $e^{-iEt/\hbar}$  factors. In the second equality, we used the fact that the  $\phi(x)$ 's are energy eigenstates, so  $\hat{E}\phi_n(x) = E_n\phi_n(x)$ . We now need to multiply by  $\psi_A^*$  and integrate with respect to x. Since the only x dependence remaining in our expression comes from the eigenfunctions  $\phi_n(x)$ , all our terms are of the form  $\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx$ . What's more, most of these terms are zero, because<sup>5</sup> our eigenfunctions are orthonormal, in the sense that

$$\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = \frac{2}{L} \int_{-L}^{L} \sin(k_m x)\sin(k_n x)dx = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n. \end{cases}$$
(28)

With this, our expression reduces to

$$\langle \hat{E} \rangle = \frac{1}{6} E_0 \int_{-\infty}^{\infty} \phi_0^* \phi_0 dx + \frac{1}{3} E_1 \int_{-\infty}^{\infty} \phi_1^* \phi_1 dx + \frac{1}{2} E_2 \int_{-\infty}^{\infty} \phi_2^* \phi_2 dx \qquad (29a)$$

$$= \frac{1}{6}E_0 + \frac{1}{3}E_1 + \frac{1}{2}E_2 = 6E_0,$$
(29b)

just like we had before. Note that since our calculation was performed using the full time-dependent wavefunction  $\psi_A(x,t)$ , we see that  $\langle \hat{E} \rangle$  does *not* change with time.

- (c) (2 points) The probability of measuring an energy equal to  $\langle \hat{E} \rangle$  is zero. The postulates of quantum mechanics tell us that we can only measure energies corresponding to the energy eigenstates that make up  $\psi_A$ . This is true at t = 0 as well as at  $t = t_1$ , because the eigenstates that are superimposed to form  $\psi_A$  simply time-evolve independently as stationary states.
- (d) (2 points) As alluded to in part (b), only  $E_0$ ,  $E_1 = 4E_0$ , and  $E_2 = 9E_0$  are values that can be measured. The probabilities are given in Equations 24a to 24c, and do not change with time (which can be seen from the fact that the time dependence cancels out of the calculations leading up to the probabilities).
- (e) (2 points) After measuring the energy of the particle to be  $E_2$  at  $t = t_1$ , the wavefunction collapses to the corresponding eigenfunction  $\phi_2$ . Thus, at times  $t > t_1$ , we have

$$\psi_A(x,t) = e^{-iE_2 t/\hbar} \phi_2(x).$$
(30)

Since the system is now in an energy eigenstate, any future measurement is *certain* to yield energy  $E_2$ . Formally,

$$\mathbb{P}(E_2) = |c_2|^2 = e^{+iE_2t/\hbar} e^{-iE_2t/\hbar} = 1.$$
(31)

(f) (4 points) If  $\psi_B$  is to yield the same set of measured energies with the same probabilities as  $\psi_A$ , the complex coefficients in front of each eigenfunction must have the same

<sup>&</sup>lt;sup>5</sup>This can be proved by direct integration, either by using trigonometric identities or by expressing the sines in complex exponentials.

norm-squared  $(|c_n|^2)$ , because those determine the probabilities. The coefficients must therefore differ by at most a phase factor of the form  $e^{i\theta}$ . One example would be

$$\psi_B(x,0) = \sqrt{\frac{1}{6}}\phi_0(x) + \sqrt{\frac{1}{3}}\phi_1(x) - \sqrt{\frac{1}{2}}\phi_2(x), \qquad (32)$$

where the only difference between this and  $\psi_A$  is a minus sign (*i.e.* phase factor  $e^{i\pi}$ ) in the last coefficient. One can check that this is in fact orthogonal to  $\psi_A$  by computing the "dot product" between the two wavefunctions:

$$\int_{-\infty}^{\infty} \psi_A^*(x,0)\psi_B(x,0)dx = \int_{-\infty}^{\infty} \psi_A^*(x,0)\left(\sqrt{\frac{1}{6}}\phi_0(x) + \sqrt{\frac{1}{3}}\phi_1(x) - \sqrt{\frac{1}{2}}\phi_2(x)\right)dx$$
(33a)

$$= \int_{-\infty}^{\infty} \left( \sqrt{\frac{1}{6}} \phi_0^*(x) + \sqrt{\frac{1}{3}} \phi_1^*(x) + \sqrt{\frac{1}{2}} \phi_2^*(x) \right) \left( \sqrt{\frac{1}{6}} \phi_0(x) + \sqrt{\frac{1}{3}} \phi_1(x) - \sqrt{\frac{1}{2}} \phi_2(x) \right) dx \quad (33b)$$

$$= \frac{1}{6} \int_{-\infty}^{\infty} \phi_0^* \phi_0 dx + \frac{1}{3} \int_{-\infty}^{\infty} \phi_1^* \phi_1 dx - \frac{1}{2} \int_{-\infty}^{\infty} \phi_2^* \phi_2 dx = \frac{1}{6} + \frac{1}{3} - \frac{1}{2} = 0,$$
(33c)

where we have once again used the orthonormality of  $\phi_n$ 's to simplify our algebra. Since the "dot product" is zero<sup>6</sup>, the wavefunctions must be linearly independent.

(g) (4 points) One possible solution would be

$$\psi_C(x,0) = \sqrt{\frac{3}{8}}\phi_0 + \sqrt{\frac{5}{8}}\phi_2.$$
(34)

Following the usual prescription for finding the probabilities for measuring the different possible energies, we have

$$\mathbb{P}(E_0) = |c_0|^2 = \frac{3}{8}$$
(35a)

$$\mathbb{P}(E_2) = |c_2|^2 = \frac{5}{8}.$$
 (35b)

Since the individual eigenfunctions  $\phi_n$  are orthogonal to each other,  $\psi_B$  must be linearly independent of  $\psi_A$  since it does not contain  $\phi_2$ . The quantity  $\langle \hat{E} \rangle$  is exactly what we want it to be:

$$\langle \hat{E} \rangle = \frac{3}{8} E_0 + \frac{5}{8} E_2 = 6E_0.$$
 (36)

Another example (among the infinite number of possibilities!) would be

$$\psi_D(x,0) = a\left(\sqrt{\frac{1}{6}}\phi_0(x) - \sqrt{\frac{1}{3}}\phi_1(x)\right) + b\phi_3,\tag{37}$$

<sup>6</sup>Note that while this is a *sufficient* condition, it is not *necessary*.

which is orthogonal to  $\psi_A$  by construction (try it!). We can find a and b by insisting that our wavefunction be properly normalized and that  $\langle \hat{E} \rangle$  comes out to our desired value. Using similar techniques as before, we have

$$1 = \int_{-\infty}^{\infty} \psi_D^* \psi_D dx = \frac{a^2}{6} \int_{-\infty}^{\infty} \phi_0^* \phi_0 dx + \frac{a^2}{3} \int_{-\infty}^{\infty} \phi_1^* \phi_1 dx + b \int_{-\infty}^{\infty} \phi_3^* \phi_3 dx = \frac{a^2}{2} + b^2 \quad (38)$$

and

$$6E_0 = \langle \hat{E} \rangle = E_0 \mathbb{P}(E_0) + E_1 \mathbb{P}(E_1) + E_3 \mathbb{P}(E_3) = E_0 \left(\frac{3}{2}a^2 + 16b^2\right).$$
(39)

These two equations can be solved simultaneously, giving  $a = \sqrt{20/13}$  and  $b = \sqrt{3/13}$  and

$$\psi_D(x,0) = \sqrt{\frac{10}{39}}\phi_0(x) - \sqrt{\frac{20}{39}}\phi_1(x) + \sqrt{\frac{3}{13}}\phi_3.$$
(40)

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Problem 4. (25 points) "Sloshing" Superposition State in the Infinite Potential Well

(a) (3 points) Without loss of generality we can set the potential well width to unity L = 1 and we also can define a dimensionless time  $\tau = \omega_0 t$  ( $\omega_1 = 2\omega_0$ ). Then our wavefunction becomes:

$$\psi(x,\tau) = \sin(\pi x) e^{-i\tau} + \sin(2\pi x) e^{-i2\tau}.$$
(41)

Below there is a plot of the associated probability density  $|\psi(x,\tau)|^2$  with the dimensionless time  $\tau$  running from 0 to  $3\pi$ . We observe that after a period  $T = 2\pi$  the probability density pattern starts to repeat itself.



(b) (4 points) Our wavefunction is

$$\psi(x,t) = \sqrt{\frac{1}{L}} \sin \frac{\pi}{L} x \quad e^{-i\omega_0 t} + \sqrt{\frac{1}{L}} \sin\left(\frac{2\pi}{L} x\right) e^{-i\omega_1 t}.$$
(42)

To check that it is properly normalized, we compute  $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx$ . First,

$$|\psi(x,t)|^2 = \frac{1}{L} \left[ \sin\left(\frac{\pi}{L}x\right) e^{-i\omega_0 t} + \sin\left(\frac{2\pi}{L}x\right) e^{-i\omega_1 t} \right]^* \left[ \sin\left(\frac{\pi}{L}x\right) e^{-i\omega_0 t} + \sin\left(\frac{2\pi}{L}x\right) e^{-i\omega_1 t} \right]$$
(43a)

$$= \frac{1}{L} \left[ \sin^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} + \left[ e^{i(\omega_0 - \omega_1)t} + e^{-i(\omega_0 - \omega_1)t} \right] \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \right]$$
(43b)

$$= \frac{1}{L} \left[ \sin^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} + 2\cos[(\omega_0 - \omega_1)t] \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \right].$$
(43c)

Integrating this gives

$$\sum_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \frac{1}{L} \left[ \underbrace{\int_0^L \sin^2 \frac{\pi x}{L} dx}_{=L/2} + \underbrace{\int_0^L \sin^2 \frac{2\pi x}{L} dx}_{=L/2} + 2\cos[(\omega_0 - \omega_1)t] \underbrace{\int_0^L \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} dx}_{=0} \right] = 1$$
(44)

so the wavefunction is properly normalized, and will remain so for all time because all time dependence disappeared in our final result. Note that we really could've said right from the beginning that the  $\sin(\pi x/L) \sin(2\pi x/L)$  cross-term integrates to zero, because the two pieces of  $\psi(x, t)$  are different energy eigenstates of the system that are orthogonal to each other.

(c) (3 points) The probability distribution  $\mathbb{P}(x,t)$  is given by Equation 43c above, so

$$\mathbb{P}(x,t) = |\psi(x,t)|^2 = \frac{1}{L} \left[ \sin^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} + 2\cos[(\omega_0 - \omega_1)t] \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \right].$$
(45)

The system will return to its original configuration after

$$T = \frac{2\pi}{\omega_0 - \omega_1}.\tag{46}$$

(d) (3 points) Since  $\omega_n = E_n \hbar$ , our time of interest is

$$t_* = \pi \hbar / [2(E_1 - E_0)] = \pi / [2(\omega_1 - \omega_0)], \tag{47}$$

which is a quarter (1/4) of the period T. Shown below is a plot of the probability distribution at that time. The x-axis is in units of L while the y-axis is in units of 1/L.



(e) (3 points) To get the probability of finding the particle in the left half of the well, we integrate the probability distribution over the left half only:

$$\int_{0}^{\frac{L}{2}} |\psi(x,t)|^{2} dx = \frac{1}{L} \int_{0}^{\frac{L}{2}} \left[ \sin^{2} \frac{\pi x}{L} + \sin^{2} \frac{2\pi x}{L} + 2\cos[(\omega_{0} - \omega_{1})t] \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \right] dx \quad (48a)$$

$$= \frac{1}{2} + \frac{4}{3\pi} \cos[(\omega_{0} - \omega_{1})t]. \quad (48b)$$

(f) (3 points) The expectation value  $\langle \hat{x} \rangle$  is once again determined by integration:

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$
(49a)

$$= \frac{1}{L} \int_0^L \left[ x \sin^2 \frac{\pi x}{L} + x \sin^2 \frac{2\pi x}{L} + 2x \cos[(\omega_0 - \omega_1)t] \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \right] dx \quad (49b)$$

$$= L\left(\frac{1}{2} - \frac{16}{9\pi^2}\cos[(\omega_0 - \omega_1)t]\right).$$
(49c)

From the form of  $\langle \hat{x} \rangle$ , we see that the average value of x moves symmetrically and periodically about the middle of the well *i.e.* it "sloshes".

(g) (2 points) Plugging x = L/2 into our probability distribution (Equation 43c) gives

$$\mathbb{P}(L/2,t) = \frac{1}{L} \left[ \sin^2 \frac{\pi}{2} + \sin^2 \pi + 2\cos[(\omega_0 - \omega_1)t] \sin \frac{\pi}{2} \sin \pi \right] = \frac{1}{L}, \quad (50)$$

which is independent of time.

(h) (4 points) Let's take a look at our wavefunction at x = L/2:

=

$$\psi\left(x=\frac{L}{2},t\right) = \sqrt{\frac{1}{L}}\sin\left(\frac{\pi}{L}\frac{L}{2}\right)e^{-i\omega_0 t} + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi}{L}\frac{L}{2}\right)e^{-i\omega_1 t}$$
(51)

$$= \sqrt{\frac{1}{L}} \sin\left(\frac{\pi}{2}\right) e^{-i\omega_0 t} + \sqrt{\frac{1}{L}} \sin(\pi) e^{-i\omega_1 t}$$
(52)

$$= \sqrt{\frac{1}{L}}e^{-i\omega_0 t} + 0. \tag{53}$$

We see that at x = L/2 and regardless of time the second eigenfunction is always zero (it has a node). So for x = L/2 our wavefunction is composed only from the first eigenfunction, which being a stationary state always gives a constant probability distribution. While we would normally find  $|\psi(x,t)|^2$  first and then plug in x = L/2, here we perform the substitution first for computational convenience. Note that this would *not* be legitimate if we were interested in working out expectation values, for then we would have to perform an integral, and it makes a difference whether we plug in a specific value for x first and then integrate or we integrate first and then evaluate.

We can modify things so that the probability density at x = L/2 becomes timedependent by adding a third eigenstate which has a value different from zero at x = L/2. In this way the first eigenstate can interfere with the one we added, resulting in a time-dependent probability density at x = L/2. That is, we can say

$$\psi(x,t) = \sqrt{\frac{2}{3L}} \sin\left(\frac{\pi}{L}x\right) e^{-i\omega_0 t} + \sqrt{\frac{2}{3L}} \sin\left(\frac{2\pi}{L}x\right) e^{-i\omega_1 t} + \sqrt{\frac{2}{3L}} \sin\left(\frac{3\pi}{L}x\right) e^{-i\omega_2 t},\tag{54}$$

where the coefficients in front of each eigenstate have been modified so that the wavefunction is normalized. Let us now check whether the probability density for this wavefunction is constant at x = L/2. So:

$$\psi(L/2,t) = \sqrt{\frac{2}{3L}}e^{-i\omega_0 t} - \sqrt{\frac{2}{3L}}e^{-i\omega_2 t}$$
 (55a)

$$\Rightarrow \mathbb{P}(L/2,t) = |\psi(L/2,t)|^2 = \frac{2}{3L} \left[ 2 - \left( e^{i(\omega_0 - \omega_2)t} + e^{-i(\omega_0 - \omega_2)t} \right) \right]$$
(55b)

$$= \frac{4}{3L} \left( 1 + \cos[(\omega_0 - \omega_2)t]) \right),$$
 (55c)

which is time-dependent, since  $\omega_0 \neq \omega_2$ .

## Problem Set 4 8.04 Spring 2013

Problem 5. (35 points) Qualitative Properties of Energy Eigenstates

Let's first summarize the main ingredients to plot an energy eigenstate:<sup>7</sup>

- The wavefunction for the *n*th energy level has n-1 nodes,
- inside the well,<sup>8</sup> where the potential is shallower, the wavelength of the oscillation is longer and the amplitude is greater than where the potential is deeper,<sup>9</sup>
- outside the well,<sup>10</sup> the exponential decay is greater where the potential is higher,
- if the potential is symmetric with respect to a given point, eigenstates are alternatively even and odd, the ground state being even.

<sup>&</sup>lt;sup>7</sup>Mostly taken from A. P. French and E. F. Taylor, "Qualitative plots of bound state wave functions," Am. J. Phys. 39, 961-962 (1971).

<sup>&</sup>lt;sup>8</sup>By which we mean regions where the potential V is less than the total energy E.

<sup>&</sup>lt;sup>9</sup>These two features are due to the fact that in shallower regions the speed of the particle is lower, and therefore the wavelength is longer, and the probability density to find the particle there is higher.

<sup>&</sup>lt;sup>10</sup>Meaning, where V > E.

(a) **(7 points)** 



(b) (7 points)



Notice that the first excited level has a nonvanishing slope at its node. This is a general feature of eigenstates. To see why, consider the eigenstate equation

$$-\frac{\hbar^2}{2m}\psi'' + (V(x) - E)\psi = 0, \qquad (56)$$

and assume that  $\psi$  has a node at x = 0, i.e.  $\psi(0) = 0$ . Let's also assume that  $\psi(x)$ 

and V(x) can be expanded as a Taylor series about x = 0:

$$\psi(x) = ax + bx^2 + cx^3 + \cdots, \qquad \frac{2m}{\hbar^2}(E - V(x)) = A + Bx + \cdots.$$

Substituting the above expansions in (56) we get

$$2b + 6cx + A(ax + bx^{2}) + Bx(ax) + \dots = 0,$$

and thus

$$b = 0, \qquad 6c + aA = 0,$$

which means

$$\psi(x) = a\left(x - \frac{A}{6}x^3 + \cdots\right).$$

In particular, it is easy to see that all the coefficients of the Taylor expansion of  $\psi(x)$  are proportional to a. Therefore, if a = 0, the whole Taylor expansion of  $\psi$  is zero, and thus  $\psi(x) = 0$  everywhere. We conclude that the slope of  $\psi(x)$  at x = 0 cannot vanish, at least as far as it can be expanded as a Taylor series.

(c) (i) **(6 points)** 



(ii) (6 points)



## (iii) (6 points)



(3 points) The ground state of the double-well system is symmetric. One way to see this is to start with the  $V_0 = 0$  case, and to imagine slowly dialing up the value of  $V_0$ . Initially we just have a single infinite potential well, and for this we know from our explicit eigenfunction solutions that the ground state is symmetric and the first excited state is anti-symmetric. As  $V_0$  is slowly increased, we expect the wavefunctions to evolve continuously to the states for the double well system, which means the ground state and the first excited state should remain symmetric and anti-symmetric respectively. Note that this all hinges on the fact that even as we increase  $V_0$ , the potential remains symmetric, so our eigenfunctions can be taken to be either symmetric or antisymmetric (see previous problem). Thus, for a general potential which is not symmetric we do not expect the ground state to necessarily be symmetric.

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