Physics 390: Homework set #3 Solutions

Reading: Tipler & Llewellyn, Chapter 6

Questions:

1. If the ground-state energy of an electron in a box were of the same magnitude as hydrogen in the ground state, how would the width of the box compare to the Bohr radius?

Solution: For a particle in a box, the ground state energy is

$$E = \frac{\hbar^2 \pi^2}{2mL^2} \Longrightarrow L = \frac{\hbar \pi}{\sqrt{2mE}} = \frac{\hbar c \pi}{\sqrt{2mc^2 E}}$$

Taking the electron mass for m and E=13.6 eV, we have

$$L = \frac{\pi (197 \text{ eV} \cdot \text{nm})}{\sqrt{2(511 \times 10^3 \text{ eV})(13.6 \text{ eV})}}$$

= 0.17 nm.

This is pretty close (within about a factor of 3) of the Bohr radius, $a_0 = 0.0529$ nm. Note, the Bohr radius is smaller than the length scale that emerges from this particle in a box calculation. This says that the Coulomb potential binds the electron more tightly than the crude approximation of a particle in a box would suggest.

2. (a) In the systems we have considered, do any two energy eigenfunctions that are proportional to each other have the same energy eigenvalues? (b) Can you find two wave functions that are not proportional to each other, yet still have the same energy eigenvalues? What distinguishes the functions?

Solution:

(a) Any two eigenfunctions that are proportional to each other have the same eigenvalue. Let ψ be a solution to the Schrödinger equation with energy E, so that $\hat{H}\psi = E\psi$. Now let $\phi = C\psi$ be a function that's proportional to ψ . We have

$$\ddot{H}\phi = \ddot{H}(C\psi) = C\ddot{H}\psi = CE\psi = E(C\psi) = E\phi.$$

(b) Yes, we have encountered an example: The free-particle wave functions $\psi_1 = Ae^{i(kx-\omega t)}$ and $\psi_2 = Ae^{-i(kx+\omega t)}$. These both describe a particle with energy $E = \hbar^2 k^2/2m$, but they are not proportional. The first describes a particle moving to the right, while the second describes a particle moving to the left.

When we study two- or three-dimensional particles in a box wavefunctions, or the hydrogen atom, we'll see additional examples:

- The two-dimensional particle in a box wavefunctions, $\psi_{nm} = (2/L) \sin(n\pi x/L) \sin(m\pi y/L)$. Both ψ_{nm} and ψ_{mn} have the same energy, $E_{nm} = E_{mn} = \frac{\hbar^2 \pi^2}{2mL^2} (n^2 + m^2)$. For $n \neq m$, the functions are not proportional; they correspond to different numbers of standing waves in the x and y directions.
- Up to small corrections, the H-atom energy depends only on the principal quantum number n, but for a given n there can be different wavefunctions that correspond to different values of the angular momentum and/or its projection onto the z-axis.

3. Does Equation 6-27 imply that we know the momentum of the particle exactly? If so, what does that imply about our knowledge of its position? How can you reconcile this with our knowledge that the particle must be in the well?

Solution: Equation 6-27 gives the relationship between energy and momentum for the particle in a box: $k^2 = (p/\hbar)^2 = 2mE/\hbar^2$. So what happens if the particle is in an energy eigenstate, i.e. a state with definite energy $E_n = p_n^2/2m = n^2\hbar^2\pi^2/2mL^2$? This does not mean that the particle has a definite momentum. Rather, the particle has a definite momentum squared. The momentum itself is uncertain because it can have either sign—the particle could be moving to the left or to the right with equal probability. This is why we found $\langle p \rangle = 0$ when we computed it in class. We saw then that the uncertainty relations are indeed satisfied for the particle in a box.

Formally, the momentum is not well-defined because the energy eigenstates, $\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$, are not eigenstates of momentum. That is, when we act on ψ_n with the momentum operator $-i\hbar \frac{\partial}{\partial x}$, we do not get back a multiple of ψ_n .

4. In this problem you will verify the Heisenberg uncertainty relations for the ground state of the quantum harmonic oscillator, for which (Equation 6-58)

$$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar}.$$

(a) Show that the normalization condition $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ requires $A_0 = (m\omega/\hbar\pi)^{1/4}$. Solution: We need

$$1 = \int_{-\infty}^{\infty} \psi_0^* \psi_0 \, dx = A_0^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} \, dx.$$

Let $u = \sqrt{m\omega/\hbar} x$. Then

$$1 = A_0^2 \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} e^{-u^2} du = A_0^2 \sqrt{\frac{\hbar}{m\omega}} \cdot \sqrt{\pi} \Longrightarrow A_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}.$$

In the last step I used the result of Appendix B in the text to do the gaussian integral.

- (b) What value do you expect for $\langle x \rangle$? Use a symmetry argument rather than a calculation. **Solution:** The potential $V(x) = \frac{1}{2}m\omega^2 x^2$ is symmetric about x = 0. So we expect the particle to spend equal amounts of time on the left and on the right. Thus we expect $\langle x \rangle = 0$.
- (c) Compute $\langle x^2 \rangle$. Then compute $\Delta x \equiv \sqrt{\langle x^2 \rangle \langle x \rangle^2}$. Solution:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi_0^* x^2 \psi_0 \, dx = A_0^2 \int_{-\infty}^{\infty} x^2 e^{-m\omega x^2/\hbar} \, dx = A_0^2 \left(\frac{\hbar}{m\omega}\right)^{3/2} \int_{-\infty}^{\infty} u^2 e^{-u^2} \, du = A_0^2 \left(\frac{\hbar}{m\omega}\right)^{3/2} \frac{\sqrt{\pi}}{2} dx$$

where I again used the technique of Appendix B to evaluate the integral. Using the result of part (a) for A_0 , we have

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \Longrightarrow \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{\hbar}{2m\omega}}.$$

- (d) What value do you expect for $\langle p \rangle$? Use a symmetry argument rather than a calculation. Solution: Again by the symmetry of the potential, we expect the particle to be moving to the left as often as to the right. So $\langle p \rangle = 0$, as can be easily verified by a direct calculation.
- (e) Conservation of energy for the harmonic oscillator can be used to relate p^2 to x^2 . Use this relation, along with the value of $\langle x^2 \rangle$ from part (c), to find $\langle p^2 \rangle$.

Solution: We know that $E = E_k + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. For the ground state, $E = \frac{1}{2}\hbar\omega$. So taking the expectation value of both sides,

$$\langle E \rangle = \frac{1}{2}\hbar\omega = \frac{1}{2m}\langle p^2 \rangle + \frac{1}{2}m\omega^2 \langle x^2 \rangle = \frac{1}{2m}\langle p^2 \rangle + \frac{1}{2}m\omega^2 \cdot \frac{\hbar}{2m\omega} = \frac{1}{2m}\langle p^2 \rangle + \frac{1}{4}\hbar\omega.$$

Solving for $\langle p^2 \rangle$, we have

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

(f) Using the results of parts (d) and (e), evaluate Δp .

Solution: $\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{m\omega\hbar}{2}}.$

(g) Finally, using the results of parts (c) and (e), evaluate $\Delta x \Delta p$ for the harmonic oscillator. Is the result consistent with the uncertainty relationship?

Solution:

$$\Delta x \Delta p = \left(\sqrt{\frac{\hbar}{2m\omega}}\right) \left(\sqrt{\frac{m\omega\hbar}{2}}\right) = \frac{\hbar}{2}$$

This is consistent with the Heisenberg uncertainty relation $\Delta x \Delta p \ge \hbar/2$. The value obtained here is the minimum possible value of $\Delta x \Delta p$ allowed by the uncertainty principle. In this sense, the wave function of the ground state of the harmonic oscillator, which is known as a Gaussian wave packet, is the most "compact" wave packet that can be constructed.

Problems: 3, 6, 25, 42, 43, 50

Problem 6-3: The wave function $\psi(x) = Ae^{-x^2/2L^2}$ is a solution to the Schrödinger equation with energy $E = \hbar^2/2mL^2$.

(a) To find the potential, we use the fact that $\psi(x)$ is a solution to the Schrödinger equation, which we can write as

$$V(x)\psi = E\psi + \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}.$$
(1)

So compute the second derivative of ψ :

$$\begin{aligned} \frac{d\psi}{dx} &= -\frac{x}{L^2} \cdot A e^{-x^2/2L^2} \\ &= -\frac{x}{L^2} \psi. \\ \frac{d^2\psi}{dx^2} &= -\frac{1}{L^2} \psi - \frac{x}{L^2} \frac{d\psi}{dx} \\ &= -\frac{1}{L^2} \psi + \frac{x}{L^2} \frac{x}{L^2} \psi \\ &= \frac{1}{L^2} \left(\frac{x^2}{L^2} - 1\right) \psi. \end{aligned}$$

We can now write down the left-hand side of Equation (1):

$$E\psi + \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \frac{\hbar^2}{2mL^2}\psi + \frac{\hbar^2}{2mL^2}\left(\frac{x^2}{L^2} - 1\right)\psi$$
$$= \frac{\hbar^2}{2mL^4}x^2\psi$$
$$= V(x)\psi,$$

where in the last step I used the Schrödinger equation, Equation (1). So

$$V(x) = \frac{1}{2} \left(\frac{\hbar^2}{mL^4}\right) x^2.$$

This is the equation of a parabola centered at x = 0.

(b) The classical system with this type of potential is the simple harmonic oscillator: $V = \frac{1}{2}kx^2$. So the "spring constant" of this quantum system is $k = \hbar^2/mL^4$.

Problem 6-6:

(a) For a free electron, the potential V(x) = 0, so the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi.$$

Substituting the second derivative of $\psi(x) = A \sin(2.5 \times 10^{10} \ x)$

$$\frac{d^2\psi}{dx^2} = -(2.5 \times 10^{10})^2\psi$$

into the Schrödinger equation gives

$$(2.5 \times 10^{10})^2 \left(\frac{\hbar^2}{2m}\right) \psi = E\psi,$$

and, since $E = E_k = p^2/2m$ for a free particle,

$$p^2 = 2m \left[(2.5 \times 10^{10})^2 \left(\frac{\hbar^2}{2m} \right) \right]$$
 and $p = (2.5 \times 10^{10})\hbar = \underline{2.64 \times 10^{-24} \text{ kg} \cdot \text{m/s}}.$

(b) The total energy E is then

$$E = p^2/2m = \left(2.64 \times 10^{-24} \text{ kg} \cdot \text{m/s}\right)^2/(2) \left(9.11 \times 10^{-31} \text{ kg}\right) = 3.82 \times 10^{-18} \text{ J} = \underline{23.9 \text{ eV}}.$$

(c) The Compton wavelength is given by

$$\lambda = h/p = 6.63 \times 10^{-34} \text{ J} \cdot \text{s}/2.64 \times 10^{-24} \text{ kg} \cdot \text{m/s} = 2.5 \times 10^{-10} \text{ m} = 0.251 \text{ nm}.$$

Problem 6-25: Let's assume that $V_1 < E < V_2$, and let's define 4 regions to consider here:

Region I $(V = V_2)$: $-\infty < x < 0$ Region II (V = 0): $0 \le x < x_1$ Region III $(V = V_1)$: $x_1 \le x < x_2$ Region IV $(V = V_2)$: $x_2 \le x < \infty$

For regions I and IV, ψ is exponentially falling, curvature is positive.

For region II: ψ is oscillatory; E_k is relatively large, so p is relatively large and therefore λ is relatively small. The amplitude is relatively small because the kinetic energy E_k , and hence the velocity of the particle is relatively large.

For region III: ψ is oscillatory; E_k is relatively small, so p is relatively small and therefore λ is relatively large. The amplitude is relatively large because the kinetic energy E_k , and hence the velocity of the particle is relatively small.

These findings are summarized in this graph:



Problem 6-42: The situation is as shown here:

(

(a) For
$$x > 0$$
,
 $E = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 k_2^2}{2m} - V_0 = 2V_0 \implies \frac{\hbar^2 k_2^2}{2m} = 3V_0.$
So $k_2 = \sqrt{6mV_0}/\hbar$. Since $k_1 = \sqrt{4mV_0}/\hbar$, then $\underline{k_2 = \sqrt{3/2k_1}}$.
(b)

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(1 - \sqrt{3/2})^2}{(1 + \sqrt{3/2})^2} = 0.0102$$

So 1.02% of the incident particles are reflected at the boundary.



- (c) T = 1 R = 0.99.
- (d) Approximately 99% of the particles, or 990,000, would continue on. Classically, 100% of the particles would continue on.

Problem 6-43: From Eqns. 6-68 and 6-69

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \qquad T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

we get

$$T + R = \frac{4k_1k_2}{(k_1 + k_2)^2} + \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(4k_1 + k_1^2 - 2k_1k_2 + k_2^2)}{(k_1 + k_2)^2}$$
$$= \frac{(k_1^2 + 2k_1k_2 + k_2^2)}{(k_1 + k_2)^2}$$
$$= \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2} = 1.$$

Problem 6-50:

(a) For particles in an infinite square well the energy levels are given by

$$E_n = \frac{n^2 h^2}{8ml^2}$$
 and $E_{n+1} = \frac{(n+1)^2 h^2}{8ml^2}$.
 $E_{n+1} - E_n$ $n^2 + 2n + 1 - n^2$ $2n + 1$ $2 + 1/2$

 So

$$\frac{E_{n+1} - E_n}{E_n} = \frac{n^2 + 2n + 1 - n^2}{n^2} = \frac{2n+1}{n^2} = \frac{2+1/n}{n}.$$

For large n, $1/n \ll 2$, and

$$\frac{E_{n+1} - E_n}{E_n} \approx \frac{2}{n}.$$

(b) For n = 1000, the fractional energy difference is

$$\frac{2}{1000} = 0.002 = \underline{0.2\%}.$$

(c) It means that the energy difference between adjacent levels per unit energy for large n is getting smaller, as the corresponding principle requires.