Name ___________________

Test 3 Solutions
November 12, 2007

This test consists of three parts. Please note that in parts II and III, you can skip one question of those offered. Some possibly useful formulas can be found below.

$$h = 6.626\times10^{-34}\ \text{J}\cdot\text{s} = 4.136\times10^{-15}\ \text{eV}\cdot\text{s}$$
$$\hbar = 1.055\times10^{-34}\ \text{J}\cdot\text{s} = 6.582\times10^{-16}\ \text{eV}\cdot\text{s}$$

1D square well:
$$E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}$$
$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n x}{L}\right)$$
$$n = 1,2,3,\ldots$$

Harmonic Osc.
$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right)$$
$$n = 0,1,2,\ldots$$

Reflection off a step:
$$R = \begin{cases} \left(\dfrac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 & \text{if } E > V_0 \\ 1 & \text{if } E < V_0 \end{cases}$$

Barrier penetration:
$$T \approx 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)\exp\left(-2L\sqrt{2m\left(V_0-E\right)}\Big/\hbar\right)$$

Part I: Multiple Choice [20 points]
For each question, choose the best answer (2 points each)

1. Under what conditions can you solve Schrodinger's time independent equation, rather than his time dependent equation?
   A) When the potential *V* is spherically symmetric
   B) When the potential *V* is independent of time
   C) When the potential *V* is independent of space
   D) When you are working on problems in 1D, but not in 3D
   E) On Sundays and holidays

2. The formula for the wave functions of the 1D square well has a factor of $\sqrt{2/L}$ in it. What is the purpose of this factor?
   A) Schrodinger's equation will not be satisfied for any energy if this "normalization" factor isn't included
   B) Schrodinger's equation works, but gives the wrong energy if you leave out this factor
   C) This "normalization factor" assures that the probability that the particle is *somewhere* must be one.
   D) This factor is included to make sure the boundary conditions are satisfied
   E) This factor makes the computation of the derivatives easier; it isn't really necessary.

3. If I tell you I have a 7p electron, I am telling you the values of
   A) l and m B) l and m_s C) m and m_s D) m and n **E) n and l**

4. If an electron in a harmonic oscillator with angular frequency ω fell from level 3 to level 1, what would be the energy of the photon that came out?
   A) $\frac{1}{2}\hbar\omega$ **B)** $2\hbar\omega$ C) $\frac{3}{2}\hbar\omega$ D) $\frac{7}{2}\hbar\omega$ E) $5\hbar\omega$

5. Suppose at three points, the value of the wave function is $\psi(a) = A$, $\psi(b) = -A$, and $\psi(c) = iA$, where A is a real number and, of course, $i^2 = -1$. At which of these points is the particle most likely to be found?
   A) Point *a* is more likely than the other two
   B) Point *b* is more likely than the other two
   C) Point *c* is more likely than the other two
   D) Points *a* and *b* are equally likely, but point *c* is less likely
   E) All three points are equally likely

6. Which of the following expressions would be used to calculate the expectation value of the momentum *p*?
   A) $\langle p \rangle = \frac{\hbar}{i}\int \psi^* \frac{\partial \psi}{\partial x} dx$
   B) $\langle p \rangle = \frac{\hbar}{i}\int \psi \frac{\partial \psi}{\partial x} dx$
   C) $\langle p \rangle = \frac{\hbar}{i}\int \psi \frac{\partial \psi^*}{\partial x} dx$
   D) $\langle p \rangle = \frac{\hbar}{i}\int \frac{\partial}{\partial x}(\psi^* \psi) dx$
   E) $\langle p \rangle = \frac{\hbar}{i}\int \psi^* \psi \frac{\partial}{\partial x} dx$

7. To calculate the probability that a particle lies in a region $a < x < b$ in one dimension when we know the wave function ψ, we should
   A) Integrate $|\psi|^2$ from *a* to *b*
   B) Integrate ψ from *a* to *b*
   C) Integrate the derivative of ψ from *a* to *b*
   D) Take the difference of $|\psi|^2$ between *a* and *b*
   E) Take the difference of ψ between *a* and *b*

8. What is the difference between a bound state and an unbound state?
   A) Bound states have $E > V(0)$, unbound states have $E < V(0)$
   B) Bound states have $E < V(0)$, unbound states have $E > V(0)$
   C) Bound states have $E > V(\pm\infty)$, unbound states have $E < V(\pm\infty)$
   D) Bound states have $E < V(\pm\infty)$, unbound states have $E > V(\pm\infty)$
   E) In quantum mechanics, because the position of a particle is uncertain, the distinction is meaningless

9. Why does the method of separation of variables work better for problems like the hydrogen atom when done in spherical coordinates (r,θ,ϕ) than it does when you work in Cartesian coordinate (x,y,z)?
   A) Because Schrodinger's equation treats the three directions (x,y,z) completely differently, while it treats (r,θ,ϕ) all the same
   B) Because the derivative terms are much simpler in spherical coordinates
   C) Because the energy term only gets simpler in spherical, not Cartesian coordinates
   D) Because the potential is a simple function of the spherical, but not the Cartesian coordinates
   E) Because Schrodinger's equation is naturally written in spherical coordinates

10. In class we divided up the hydrogen atom into a radial function $R(r)$ and an angular function $Y(\theta,\phi)$. Under what circumstances can we reuse these functions $Y(\theta,\phi)$ on another problem?
   A) They can be used on any problem in 3D, and they are always exactly the same
   B) They can be used on any problem in 3D, though their functional form will change
   C) They can be used on any spherically symmetric problem, and they are always exactly the same
   D) They can be used on any spherically symmetric problem, though their functional form will change
   E) They are worked out and can only be used for hydrogen-like atoms

Part II: Short answer [20 points]

Choose two of the following questions and give a short answer (1-3 sentences) (10 points each).

11. A particle with kinetic energy E is incident off of a barrier with height V_0. Under what conditions, if any, will the particle be (i) completely reflected, or (ii) completely transmitted. Consider the possibility that $V_0 < 0$, if necessary.

When the energy is less than the barrier, it was shown in class that you get total reflection (as can be seen from the formula). When the barrier is zero, you get total transmission. For all other values, including a negative barrier, you get partial reflection and partial transmission.

12. Suppose that, through an oversight, I gave you the formula for the wave functions for the infinite 1D square well, but I forgot to give you the energy formula E_n. How could you get the energy? Give any relevant formulas.

The wave functions should be solutions of Schrodinger's time independent equation, and therefore, we should have

$$E_n \psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

In fact, in this case the potential inside the well is just zero, so the second term can be dropped. Indeed, it is clear that when you take the derivative, you will get a factor of $\pi n/L$ each time, and the sin function will become first cos and then –sin, so we have $E_n = \pi^2 \hbar^2 n^2 / 2mL^2$, which agrees with the given formula.

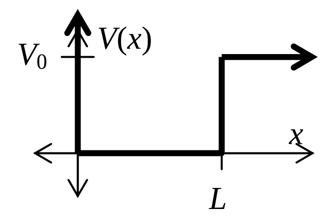
13. Explain, qualitatively, why it is possible in quantum physics for a particle with energy $E < V_0$ to penetrate to the other side of a barrier of height V_0 and arbitrary thickness L.

Classically, a particle cannot go into a region where the potential energy is greater than the total energy, but quantum mechanically, this just represents a place where there is a transition from an oscillating to an exponentially damped wave function. Hence the wave will grow ever smaller as it goes into the barrier, but if the barrier is finite in width, there will always be a small probability of leakage through the barrier.

Part III: Calculation: [60 points]

Choose three of the following four questions and perform the indicated calculations (20 points each).

14. We are attempting to find solutions of Schrodinger's Equation for the one-dimensional semi-infinite square well, with potential



$$V(x) = \begin{cases} \infty & \text{if } x < 0 \\ 0 & \text{if } 0 < x < L \\ V_0 & \text{if } x > L \end{cases}$$

and energy $0 < E < V_0$. This potential is sketched at right. So far, someone solving this has decided that the wave function must look like the following

$$\psi(x) = \begin{cases} 0 & \text{if } x < 0 \\ A\cos(kx) + B\sin(kx) & \text{if } 0 < x < L \\ Ce^{\alpha x} + De^{-\alpha x} & \text{if } x > L \end{cases}$$

(a) What constraint(s), if any, can be imposed on the coefficients *A–D* by considering the boundary conditions at $x = 0$?

The wave function must always be continuous at the boundaries, so since it vanishes for $x< 0$, it must vanish at $x = 0$. This can only happen if we choose sin(kx), not cos(kx), so we have $A = 0$.

Since the potential is infinite at this point, there is no constraint on the derivative of the wave function

(b) What constraint(s), if any, can be imposed on the coefficients *A–D* by considering the behavior of the wave function at $x \rightarrow \infty$?

The wave function must be normalizable, and this is impossible if the function blows up to infinity. Therefore, the C term is unacceptable, and we have $C = 0$.

(c) What constraint(s), if any, can be imposed on the coefficients *A–D* by considering the boundary conditions at $x = L$?

The potential is finite, and hence the wave function must both be continuous and have a continuous derivative at $x = L$. Taking advantage of the fact that $A = C = 0$, this simplifies to

$$\psi(L) = B\sin(kL) = De^{-\alpha L} \quad \text{and} \quad \psi'(L) = Bk\cos(kL) = -\alpha De^{-\alpha L}$$

These equation can be combined to show that $\tan(kL)/k = 1/\alpha$, but this was not asked for.

15. At t = 0, a particle has a wave function $\Psi(x)$ with the following expectation values:

$$\langle x\rangle = -\tfrac{3}{2}a \qquad \langle x^2\rangle = 3a^2 \qquad \langle x^3\rangle = -5a^3 \qquad \langle x^4\rangle = 10a^4$$

$$\langle p\rangle = \frac{\hbar}{a}\ , \qquad \langle p^2\rangle = \frac{3\hbar^2}{2a^2}\ , \qquad \langle p^3\rangle = \frac{2\hbar^3}{a^3}\ , \qquad \langle p^4\rangle = \frac{3\hbar^4}{a^4}\ ,$$

where a is a constant with units of length.

(a) What is the uncertainty in position Δx? What is the uncertainty in momentum Δp?

The uncertainty in position is given by

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = 3a^2 - \left(\tfrac{3}{2}a\right)^2 = \tfrac{3}{4}a^2\,, \qquad \text{so} \qquad \Delta x = \tfrac{\sqrt{3}}{2}a$$

Similarly

$$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2 = \frac{3\hbar^2}{2a^2} - \left(\frac{\hbar}{a}\right)^2 = \frac{\hbar^2}{2a^2}\,, \qquad \text{so} \qquad \Delta p = \frac{\hbar}{a\sqrt{2}}$$

(b) Check that the uncertainty relationship is satisfied.

$$(\Delta x)(\Delta p) = \frac{a\sqrt{3}}{2}\frac{\hbar}{a\sqrt{2}} = \tfrac{1}{2}\sqrt{\tfrac{3}{2}}\hbar \geq \tfrac{1}{2}\hbar$$

Yes, this certainly is true.

(c) If the particle has mass m and is in a potential $V(x) = Ax^3 + Bx^4$, what would be the average value of the energy E if you measured it?

The average value of the energy is the expectation value of the Hamiltonian. The Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + Ax^3 + Bx^4$$

The average energy, therefore, is

$$\bar{E} = \langle H\rangle = \frac{\langle p^2\rangle}{2m} + A\langle x^3\rangle + B\langle x^4\rangle = \frac{3\hbar^2}{4ma^2} - 5Aa^3 + 10Ba^4$$

16. A doubly ionized Lithium atom (Li^{+2}, Z = 3 with one electron) is found to be in a bound state with energy E = -3.40 eV.

(a) What is the principal quantum number n for this electron?

The energy of a hydrogen-like atom is given by

$$E_n = -\frac{(13.6\text{ eV})Z^2}{n^2}$$

We therefore have

$$(13.6\text{ eV})Z^2 = (3.40\text{ eV})n^2$$

or, rearranging a little, we have

$$n^2 = 4.00Z^2 = 4.00 \cdot 9 = 36.0$$

So n = 6.

(b) What are the possible quantum numbers for l, m, and m_s for this electron? Just give me the range for each one.

The quantum number l runs from 0 to n – 1, so in this case, our choices are l = 0, 1, 2, 3, 4, 5. The quantum number m runs from – l to l, so depending on the value of l, this could be anywhere from -5 to +5, or explicitly, l = -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5. As always, the quantum number m_s = +½ or – ½ .

(c) What possible values could occur if you measured L^2, L_Z, S^2, and S_Z for this electron?

$L^2 = \hbar^2(l^2+l)$, so plugging in our values for l, the possible values are 0, $2\hbar^2$, $6\hbar^2$, $12\hbar^2$, $20\hbar^2$, and $30\hbar^2$. The values for L_z are $m\hbar$, which works out to $-5\hbar$, $-4\hbar$, $-3\hbar$, $-2\hbar$, $-\hbar$, 0, $\hbar$, $2\hbar$, $3\hbar$, $4\hbar$, and $5\hbar$. The value for S^2 is always $\frac{3}{4}\hbar^2$, no matter what, and the values for S_z are $\pm\frac{1}{2}\hbar$.

(d) L_Z is actually measured, and found to have a value of $L_Z = -3\hbar$. How, if at all, would your answers change for part (c) (other than, obviously, your answer for L_Z).

L_Z is $m\hbar$, so we must have m = -3. Since m runs from $-l$ to l, we must therefore have l at least as big as 3, which narrows it down to l = 3, 4, or 5, and therefore L^2 will be one of $12\hbar^2$, $20\hbar^2$, and $30\hbar^2$. S^2 and S_Z remain the same, and of course L_Z is $-3\hbar$.

17. A particle in one dimension has wave function given by

$$\psi(x) = \begin{cases} Ne^{-\alpha x} & \text{if } x > 0 \\ Ne^{\beta x} & \text{if } x < 0 \end{cases}$$

where α and β are positive real constants. Some useful integrals can be found below.

(a) What is the normalization constant *N*? Assume *N* is positive.

For all parts of this problem, we will have to break the integral up into the two regions. For example, for the normalization, we have

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = N^2 \int_{-\infty}^{0} e^{2\beta x} dx + N^2 \int_{0}^{\infty} e^{-2\alpha x} dx = N^2 \left(\frac{1}{2\beta} + \frac{1}{2\alpha} \right) = N^2 \frac{\alpha+\beta}{2\alpha\beta}$$

This equation is satisfied if

$$N = \sqrt{\frac{2\alpha\beta}{\alpha+\beta}}$$

(b) Find the expectation values $\langle x \rangle$, $\langle x^2 \rangle$, and $\langle p \rangle$.

We perform the same computation as before, but we stick an extra x or x^2 into the integral.

$$\langle x \rangle = N^2 \left(\int_{-\infty}^{0} x e^{2\beta x} dx + \int_{0}^{\infty} x e^{-2\alpha x} dx \right) = N^2 \left(-\frac{1}{(2\beta)^2} + \frac{1}{(2\alpha)^2} \right) = \frac{2\alpha\beta}{\alpha+\beta} \cdot \frac{\beta^2 - \alpha^2}{4\alpha^2\beta^2} = \frac{\beta - \alpha}{2\alpha\beta},$$

$$\langle x^2 \rangle = N^2 \left(\int_{-\infty}^{0} x^2 e^{2\beta x} dx + \int_{0}^{\infty} x^2 e^{-2\alpha x} dx \right) = N^2 \left(\frac{2}{(2\beta)^3} + \frac{2}{(2\alpha)^3} \right) = \frac{2\alpha\beta}{\alpha+\beta} \cdot \frac{\alpha^3 + \beta^3}{4\alpha^3\beta^3}$$

$$= \frac{\alpha^2 - \alpha\beta + \beta^2}{2\alpha^2\beta^2}.$$

Because the wave function is real, we automatically have $\langle p \rangle = 0$, or explicitly,

$$\langle p \rangle = \frac{\hbar}{i} \int_{-\infty}^{\infty} \psi(x) \frac{d\psi(x)}{dx} dx = \frac{\hbar N^2}{i} \left(\int_{-\infty}^{0} e^{\beta x} \beta e^{\beta x} dx - \int_{0}^{\infty} e^{-\alpha x} \alpha e^{-\alpha x} dx \right) = \frac{\hbar N^2}{i} \left(\frac{\beta}{2\beta} - \frac{\alpha}{2\alpha} \right) = 0$$

(c) What is the probability that the particle lies in the region *x*> 0?

To calculate this, we redo the original integral but restrict it to the relevant region.

$$P(x > 0) = N^2 \int_{0}^{\infty} e^{-2\alpha x} dx = \frac{N^2}{2\alpha} = \frac{2\alpha\beta}{2\alpha(\alpha+\beta)} = \frac{\beta}{\alpha+\beta}.$$