

Name \_\_\_\_\_

Test 3

November 10, 2008

$$h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s} = 4.136 \times 10^{-15} \text{ eV} \cdot \text{s}$$

$$\hbar = 1.055 \times 10^{-34} \text{ J} \cdot \text{s} = 6.582 \times 10^{-16} \text{ eV} \cdot \text{s}$$

1D square well:

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

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

$$n = 1, 2, 3, \dots$$

Harmonic Osc.

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$n = 0, 1, 2, \dots$$

Reflection off a step:

$$R = \begin{cases} \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right)^2 & \text{if } E > V_0 \\ 1 & \text{if } E < V_0 \end{cases}$$

Barrier penetration:

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

**Part I: Multiple Choice [20 points]**

For each question, choose the best answer (2 points each)

- In three dimensions, under what condition would we conclude that a particle cannot be at the point  $\vec{r}$ ?
  - If the wave function  $\psi(\vec{r}) = 0$  there (only)**
  - If the wave function  $\psi(\vec{r})$  is negative (only)
  - If the wave function  $\psi(\vec{r})$  is pure imaginary (only)
  - A and B are both correct
  - A and C are both correct
- Which of the following is *not* possible for a single electron in hydrogen?
  - $l = 2$
  - $m = -1$
  - $m_s = 1/2$
  - $n = 0$**
  - All of these are possible
- The difference between a bound and an unbound state is
  - Bound states always go like  $1/x$  at infinity, unbound states do not
  - Bound states have less energy than the potential at infinity, unbound have more**
  - Bound states have complex wave functions, unbound states are real
  - Bound states have a wave function that vanishes outside of a region, unbound states do not
  - Bound states have positive energies, unbound states have negative energies
- The expectation value of the Hamiltonian,  $\langle H \rangle$ , would tell you the average result if you measured a particle's
  - Position
  - Momentum
  - Angular Momentum
  - Spin
  - Energy**

5. The spherical harmonics  $Y_{l,m}(\theta, \phi)$  would be useful in solving which of the following problems?
- The harmonic oscillator (only)
  - The 3D infinite square well (only)
  - Any spherically symmetric problem (only)**
  - Reflection off a barrier (only)
  - All of the above
6. Under what conditions do you get at least partial reflection off a step boundary?
- If the step  $V_0$  is greater than the incoming energy, but not if it is less
  - If the step  $V_0$  is any positive number, but not if it is negative
  - If the step  $V_0$  is any negative number, but not if it is positive
  - If the step  $V_0$  is positive or negative, but not if it is zero**
  - You always get some reflection, whether  $V_0$  is positive, negative, or zero
7. An electron in which subshell is most likely to be near the origin?
- 2p
  - 3s**
  - 3p
  - 4d
  - 4f
8. In addition to satisfying Schrödinger's equation in whatever regions we have, what other criterion or criteria is/are commonly required of the wave function?
- It must be normalizable (only)
  - It must be continuous (only)
  - The derivative must be continuous (only)
  - A and B are correct, but not C
  - A, B, and C are all correct**
9. Given above are the wave functions for the time-independent 1D square well. What do you need to do to get the time-dependent wave functions?
- Multiply them by  $e^{iE_n t/\hbar}$
  - Multiply them by  $e^{-iE_n t/\hbar}$**
  - Normalize them
  - Multiply them by the spherical harmonics  $Y_{l,m}(\theta, \phi)$
  - Multiply them by their complex conjugate
10. If you confine one particle in a very small region, but at zero temperature, which type of particle will result in the highest pressure in that region?
- The particle with the smallest mass**
  - The particle with the largest mass
  - The particle with the shortest wavelength
  - The particle with the lowest rest energy
  - Since it's at zero temperature, there will be zero pressure

**Part II: Short answer [20 points]**

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

- 11. I wish to have a particle penetrate a barrier using an energy  $E$  which is actually smaller than the height  $V_0$  of the barrier. If I want to increase the probability that it gets through, give at least three things I can adjust to make it easier. You can adjust any relevant parameters, including  $E$  and  $V_0$ , and any other property of the barrier or particle.**

The relevant formula is

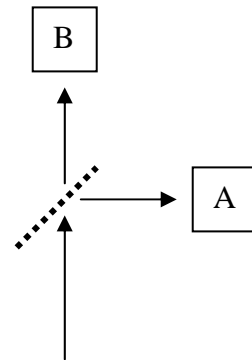
$$T \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) \exp\left(-2L\sqrt{2m(V_0 - E)}/\hbar\right)$$

the most important factors are the ones that go into the exponential. To make the probability increase, we want the argument of the exponential small. Since we can't adjust the constant  $\hbar$ , we can increase the probability by decreasing the thickness of the barrier  $L$ , decreasing  $V_0 - E$  by either increasing the energy or lowering the barrier, or by decreasing the mass of the particle.

- 12. Give a qualitative description explaining the difference between orbital angular momentum  $L$  and spin  $S$ .**

$L$  describes the angular momentum of one object around another, like the Earth around the Sun.  $S$  describes the intrinsic angular momentum, the angular momentum having to do with the particle itself rotating.

- 13. A single photon is sent into a half-silvered mirror, and then sent towards two detectors, which we will assume have 100% detection efficiency. What is the probability, for a single photon, that each of the detectors see it? What is the probability that they both see it? What is the probability that neither sees it?**

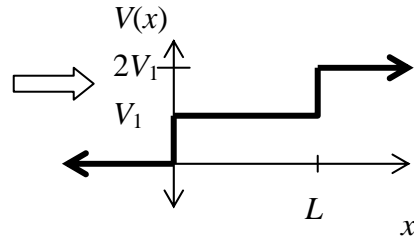


According to quantum mechanics, the particle either goes one way or the other, never both, so there is a 50% probability it goes into A and not B, 50% probability that it goes into B but not A, and a 0% probability that it goes into neither or goes into both.

**Part III: Calculation: [60 points]**

**14. At right is the “double step barrier,” defined by**

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_1 & \text{if } 0 < x < L \\ 2V_1 & \text{if } x > L \end{cases}$$



**A particle of energy  $E = \frac{3}{2}V_1$  is incident from the left on this barrier.**

**(a) Show that the equations**

$$\psi = Ae^{-\alpha x} \quad \text{and} \quad \psi = Be^{\alpha x}$$

**where  $\alpha$  is a real constant will work in one of the two regions  $0 < x < L$  or  $L < x$ , and determine an equation for  $\alpha$ .**

It is easy to see that each time you take a derivative, you get a factor of  $\pm\alpha$ , so if you do it twice, we have  $d^2\psi/dx^2 = \alpha^2\psi$ . Plugging this into Schrödinger's time-independent equation, we have

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

$$\hbar^2 \alpha^2 / 2m = V(x) - E = V(x) - \frac{3}{2}V_1$$

Obviously, the left side is positive, so we must make sure  $V(x) > \frac{3}{2}V_1$ , which only works for  $x > L$ , where we find

$$\hbar^2 \alpha^2 = 2m(2V_1 - \frac{3}{2}V_1) = mV_1$$

$$\alpha = \sqrt{mV_1}/\hbar.$$

**(b) Show that the equations**

$$\psi = Ce^{ikx} \quad \text{and} \quad \psi = De^{-ikx}$$

**where  $k$  is a real constant will work in the other of the two regions  $0 < x < L$  or  $L < x$ , and determine an equation for  $k$ .**

Taking two derivatives we find for each of these wave functions  $d^2\psi/dx^2 = -k^2\psi$ . We know this time we need  $0 < x < L$ , where  $V(x) = V_1$ , so

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

$$\hbar^2 k^2 / 2m = E - V(x) = \frac{3}{2}V_1 - V_1 = \frac{1}{2}V_1$$

$$k = \sqrt{mV_1}/\hbar$$

(c) Although they work in Schrödinger's equation, one of the four constants  $A$ ,  $B$ ,  $C$ , and  $D$  is not "physically meaningful", and would be set to zero in solving this problem. Which one, and why?

The  $A$  term represents a wave that blows up at positive infinity, and would create a wave function that can't be normalized. Hence this term is not physically relevant, and we set  $A = 0$ .

**15. A proton with mass  $m = 1.672 \times 10^{-27}$  kg is trapped within a one-dimensional infinite square well of size  $L = 1.00 \times 10^{-11}$  m. It is initially in the  $n = 1$  state.**

**(a) What is the energy of the initial state, in eV (1 eV =  $1.602 \times 10^{-19}$  J)?**

We simply use the formula for the energy, namely

$$E_1 = \frac{\pi^2 \hbar^2 1^2}{2mL^2} = \frac{\pi^2 (1.055 \times 10^{-34} \text{ J}\cdot\text{s})^2}{2(1.672 \times 10^{-27} \text{ kg})(1.00 \times 10^{-11} \text{ m})^2} = \frac{3.285 \times 10^{-19} \text{ J}}{1.602 \times 10^{-19} \text{ J/eV}} = 2.051 \text{ eV}$$

**(b) The proton suddenly makes a transition to the  $n = 3$  state. To do so, will it absorb or emit a photon of light? What is the energy of that photon?**

The new energy is just

$$E_3 = \frac{\pi^2 \hbar^2 3^2}{2mL^2} = 9E_1$$

Since this is an increase of energy, the photon must be absorbed. The energy of the photon is the difference in energy, or

$$\Delta E = E_3 - E_1 = 8(2.051 \text{ eV}) = 16.40 \text{ eV}$$

**(c) A photon of the same energy causes a transition of *another* proton, this one in a harmonic oscillator. It has the exact right energy to shift from the  $n = 2$  state to the  $n = 4$  state. What is the angular frequency  $\omega$  for this harmonic oscillator?**

The harmonic oscillator has energy  $E_n = \hbar\omega(n + \frac{1}{2})$ . The difference in energy between level 4 and level 2 is then

$$\Delta E = E_4 - E_2 = \hbar\omega(4 + \frac{1}{2}) - \hbar\omega(2 + \frac{1}{2}) = 2\hbar\omega$$

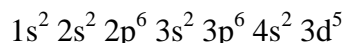
Solving for  $\omega$ , we have

$$\omega = \frac{\Delta E}{2\hbar} = \frac{16.40 \text{ eV}}{2(6.582 \times 10^{-16} \text{ eV}\cdot\text{s})} = 1.246 \times 10^{16} \text{ s}^{-1}$$

16. The element manganese has  $Z = 25$  electrons. It follows our rules for electron configuration exactly.

(a) Give the electron configuration for manganese, starting “ $1s^2 \dots$ ”

We use our little chart, sketched at right, and keep counting until we get to 25 electrons:



<del><math>1s^2</math></del>				
<del><math>2s^2</math></del>	<del><math>2p^6</math></del>			
<del><math>3s^2</math></del>	<del><math>3p^6</math></del>	<del><math>3d^{10}</math></del>		
<del><math>4s^2</math></del>	<del><math>4p^6</math></del>	<del><math>4d^{10}</math></del>	<del><math>4f^{14}</math></del>	
<del><math>5s^2</math></del>	<del><math>5p^6</math></del>	<del><math>5d^{10}</math></del>	<del><math>5f^{14}</math></del>	
<del><math>6s^2</math></del>	<del><math>6p^6</math></del>	<del><math>6d^{10}</math></del>	<del><math>6f^{14}</math></del>	
<del><math>7s^2</math></del>	<del><math>7p^6</math></del>	<del><math>7d^{10}</math></del>	<del><math>7f^{14}</math></del>	

(b) If you measured the orbital angular momentum squared,  $L^2$  of each of the electrons, what values would you get, and how many of each value would you get? You may give your answer in a table ( $L^2$ , number of electrons) if you wish.

$L^2$	#
0	8
$2\hbar^2$	12
$6\hbar^2$	5

The orbital angular momentum  $L^2$  is given by  $L^2 = \hbar^2(l^2 + l)$ , where  $l = 0$  for an s-electron,  $l = 1$  for a p-electron, and  $l = 2$  for a d-electron.

(c) If you measured the orbital angular momentum  $L_z$  of one of the electrons, what is the largest (most positive) possible value you could get? What is the smallest (most negative) possible value you could get? I am only looking for one number for each of these questions, not a list of all the electrons.

The  $L_z$  values are given by  $m\hbar$ , where  $m$  runs from  $-l$  to  $l$ . The largest value of  $l$  we have is  $l = 2$ , so we could find an electron with  $m$  as low as  $-2$  or as high as  $+2$ . So the lowest/highest values are  $\pm 2\hbar$ .

(d) If you measured the internal angular momentum (spin) squared,  $S^2$  of each of the electrons, what values would you get, and how many of each value would you get?

All electrons are spin  $\frac{1}{2}$ , so  $S^2 = \hbar^2(s^2 + s) = \frac{3}{4}\hbar^2$ . If you want it as a table, the table appears at right, but that's a bit silly.

$S^2$	#
$\frac{3}{4}\hbar^2$	25

**17. A particle in one dimension has wave function**

$$\psi(x) = \frac{a\sqrt{2a/\pi}}{a^2 + x^2}$$

where  $a$  is a constant with units of length. Several possibly useful integrals are given below. This wave function has already been properly normalized.

(a) What is the expectation value of the position and position squared,  $\langle x \rangle$  and  $\langle x^2 \rangle$ ?

To calculate these quantities, we simply sandwich  $x$  or  $x^2$  between the wave function and its complex conjugate and integrate

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi dx = \frac{2a^3}{\pi} \int_{-\infty}^{\infty} \frac{x dx}{(x^2 + a^2)^2} = 0,$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi dx = \frac{2a^3}{\pi} \int_{-\infty}^{\infty} \frac{x^2 dx}{(x^2 + a^2)^2} = \frac{2a^3}{\pi} \frac{\pi}{2a} = a^2.$$

(b) What is the uncertainty  $\Delta x$  in the position?

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{a^2 - 0} = a$$

(c) What is the expectation value of the momentum  $\langle p \rangle$ ?

$$\langle p \rangle = \frac{\hbar}{i} \int_{-\infty}^{\infty} \psi^* \frac{d}{dx} \psi dx = \frac{\hbar}{i} \frac{2a^3}{\pi} \int_{-\infty}^{\infty} \frac{1}{(a^2 + x^2)} \frac{-2x}{(a^2 + x^2)^2} dx = 0$$

Then again, we could simply have remembered that when the wave function is real, we always get  $\langle p \rangle = 0$ .

(d) The momentum squared has expectation value  $\langle p^2 \rangle = \hbar^2/2a^2$ . What is the uncertainty  $\Delta p$  in the position? Check that the Heisenberg uncertainty principle is satisfied.

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\hbar^2/2a^2 - 0} = \frac{\hbar}{a\sqrt{2}},$$

$$\Delta x \Delta p = a \cdot \frac{\hbar}{a\sqrt{2}} = \frac{1}{\sqrt{2}} \hbar > \frac{1}{2} \hbar$$

Yes, it worked.