Name ___________________

Solutions to Test 3
November 9, 2009

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

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

1. In a scanning tunneling microscope, current flows even though the tip of the microscope is above the surface you are scanning because
   A) Electrons can cross a barrier by quantum mechanical tunneling, even if they apparently have insufficient energy to make it across
   B) Since no one is observing the individual electrons, they are not required to conserve energy
   C) Because the tip is held steady (small uncertainty in momentum), its position is uncertain, and therefore it must occasionally dip down and touch the surface
   D) Photons dislodge electrons from the surface (the photoelectric effect), which are then absorbed by the tip of the microscope
   E) Quantum mechanically, electrons have an uncertainty in their energy, so some of them accidentally have enough energy to leap across the barrier

2. If $\Psi(\vec{r},t)$ is a solution of Schrödinger's equation, so also will be
   A) $\Psi^*(\vec{r},t)$ B) $\left|\Psi(\vec{r},t)\right|^2$ **C)** $c\Psi(\vec{r},t)$ D) $\Psi^2(\vec{r},t)$ E) None of the preceding

3. A muon is an elementary particle much like an electron, but about 200 times heavier. Suppose we confine a muon to a small space of size L in one dimension. If it has the minimum possible energy, how would its energy be compared to an electron confined in the same space?
   A) It would be 40,000 times smaller
   B) It would be 200 times smaller
   C) It would be the same
   D) It would be 200 times bigger
   E) It would be 40,000 times bigger

4. How does Schrödinger's equation in 3D differ from Schrödinger's equation in 1D?
   A) There are three wave functions instead of just one (only)
   B) The wave function is a function of all three variables, x, y, and z (only)
   C) The term $\partial^2/\partial x^2$ has to be replaced with $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ (only)
   D) Both B and C are correct
   E) A, B, and C are all correct

5. The expectation value of some operator like the position $\langle x \rangle$ tells you
   A) The average value you would get if you repeated the experiment many times
   B) The value you will get if you measure the position
   C) The most likely position x where you would find the particle
   D) The uncertainty, or spread in the position of the particle
   E) The actual position of the particle, though measuring it disturbs it and it may no longer be there.

6. Suppose you place two electrons in an atom. What restrictions are there on how the four quantum numbers n, l, m and m_s for the two electrons are related to each other?
   A) They can't have the same value of n
   B) They can't have the same value of l
   C) They can't have the same value of m
   D) They can't have the same value of m_s
   E) Though they can match on one or more of the quantum numbers, they can't match on all four

7. Which condition on the energy E tells you you are dealing with a bound state?
   A) $E > 0$ B) $E < 0$ C) $E < V(0)$ D) $E > V(\pm\infty)$ **E)** $E < V(\pm\infty)$

8. If you take the expectation value of the Hamiltonian, you will find the average value of the
   A) Momentum
   B) Position
   C) Total energy
   D) Potential energy
   E) Kinetic energy

9. According to the standard Copenhagen interpretation of quantum mechanics, when a single photon hits a half-silvered mirror, what happens to its wave function? Assume no measurement has yet occurred.
   A) Half the time it is reflected, half the time it is transmitted, and you can't predict which.
   B) It will be either reflected or transmitted, depending on the *phase* of the photon when it hits the mirror.
   C) It will either go through or not, depending on the exact *position* where it hits the mirror
   D) It gets split in half, with half the wave function going each way, at least until a measurement occurs
   E) It alternates, one photon going one way, the next going the other, so it is predictable but different for each successive photon

10. If we list the electrons in an atom with two or more electrons, we always start with $1s^2$. Why is it that the 1s electrons are the first ones that are filled?
   A) These states have electrons with angular momentum $\hbar$, which by Bohr's hypothesis will be the first electron states
   B) These states have the lowest energy
   C) These states are closest to the outside, so the most accessible as the electron enters the atom
   D) These two states are far apart from each other, and the electrons like to avoid each other
   E) They are following God's commands in Gen. 1:32, "And God said, go thou forth together, and fill the innermost shell of the atom. And God saw that it was good. And the evening and the morning were the eighth day."

Part II: Short answer [20 points]

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

11. The wave function must satisfy Schrödinger's equation. What other conditions must it satisfy?

The wave function must be continuous everywhere, it must have a continuous derivative everywhere (except possibly when the potential is infinite), and it must be normalized, so that the integral of the square of its magnitude must be one. This last condition can sometimes be relaxed for unbound states, but certainly it must always not diverge as you go to plus or minus infinitey.

12. What is it about the hydrogen atom that makes it sensible to factor the wave function into radial and angular components, $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$? Why didn't we do this, for example, for a particle in a 3D box?

It makes sense to do this for hydrogen because the potential is spherically symmetric, the same in all dimensions. A 3D box, in contrast, is *not* spherically symmetric, and is best solved in Cartesian coordinates.

13. Classically, if an object is approaching a barrier of finite height and finite width, it is guaranteed to be reflected if the object has insufficient energy to make it over the barrier. Explain what, if anything, is different in quantum mechanics. Explain how come we don't normally notice this effect in everyday life.

In quantum mechanics, the wave function does not vanish when it reaches the barrier, but instead starts to decrease rapidly. If the barrier is finite in width, it is possible for the wave function to reemerge, albeit with a much diminished amplitude, on the other side of the wave, leading to a probability of penetration roughly given by the formula at the beginning of the exam,

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

However, in everyday practical situations, the exponential factor makes this almost indistinguishable from zero, so we don't notice.

Part III: Calculation: [60 points]

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

14. A group of 9000 electrons of energy $E = 25\text{ eV}$ are fired at a step barrier of unknown height V_0. It is discovered that 5000 of them make it through.

(a) [4] What is the reflection probability *R*?

It is obvious that $\frac{5}{9}$ of them are transmitted, and therefore $\frac{4}{9}$ of them are reflected. The reflection probability is then $R = \frac{4}{9}$.

(b) [16] What is the barrier height V_0? You should get two answers.

To solve this problem, we use the formula

$$R = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2 = \frac{4}{9}$$

since the other formula ($R = 1$) clearly doesn't apply. Take the square root of both sides, remembering that every number has two square roots, so we have

$$\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} = \pm \frac{2}{3}$$

We now split this into two problems, which we attempt to solve in parallel. We cross multiply to give

$$3\left(\sqrt{E} - \sqrt{E - V_0}\right) = 2\left(\sqrt{E} + \sqrt{E - V_0}\right) \quad \text{or} \quad 3\left(\sqrt{E} - \sqrt{E - V_0}\right) = -2\left(\sqrt{E} + \sqrt{E - V_0}\right),$$
$$3\sqrt{E} - 3\sqrt{E - V_0} = 2\sqrt{E} + 2\sqrt{E - V_0} \quad \text{or} \quad 3\sqrt{E} - 3\sqrt{E - V_0} = -2\sqrt{E} - 2\sqrt{E - V_0},$$
$$\sqrt{E} = 5\sqrt{E - V_0} \quad \text{or} \quad 5\sqrt{E} = \sqrt{E - V_0}.$$

We now square this and simplify, solving for V_0.

$$E = 25\left(E - V_0\right) \quad \text{or} \quad 25E = E - V_0,$$
$$25V_0 = 24E \quad \text{or} \quad 24E = -V_0,$$
$$V_0 = \tfrac{24}{25}E \quad \text{or} \quad V_0 = -24E,$$
$$V_0 = +24\text{ eV} \quad \text{or} \quad V_0 = -600\text{ eV}.$$

These are our two solutions, as advertised.

15. The harmonic oscillator has potential $V(x) = \frac{1}{2} m\omega^2 x^2$ and ground state wave function

$$\psi(x) = N \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

where *N* is a constant

(a) [15] Show explicitly that this satisfies Schrödinger's time-independent equation for the appropriate energy.

We simply substitute this into Schrödinger's time independent equation.

$$\begin{aligned}
E\psi(x) &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) \\
&= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} N \exp\left(-\frac{m\omega x^2}{2\hbar}\right) + \frac{1}{2} m\omega^2 x^2 N \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \\
&= -\frac{\hbar^2 N}{2m}\frac{d}{dx}\left[-\frac{m\omega}{\hbar} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)\right] + \frac{1}{2} m\omega^2 x^2 N \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \\
&= -\frac{\hbar^2 N}{2m}\left[-\frac{m\omega}{\hbar}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) + \left(\frac{m\omega}{\hbar}\right)^2 x^2 \exp\left(-\frac{m\omega x^2}{2\hbar}\right)\right] \\
&\quad + \frac{1}{2} m\omega^2 x^2 N \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \\
&= N \exp\left(-\frac{m\omega x^2}{2\hbar}\right)\left[\frac{\hbar\omega}{2} - \frac{m\omega^2}{2} x^2 + \frac{1}{2} m\omega^2 x^2\right] \\
&= \tfrac{1}{2}\hbar\omega\psi(x).
\end{aligned}$$

The energy, therefore, is $E = \frac{1}{2}\hbar\omega$, as it should be for the ground state of the Harmonic oscillator.

(b) [5] Using this solution of the time-*independent* equation, find a solution to the time-*dependent* Schrödinger equation.

In general, the solution of the time-dependent Schrödinger equation are

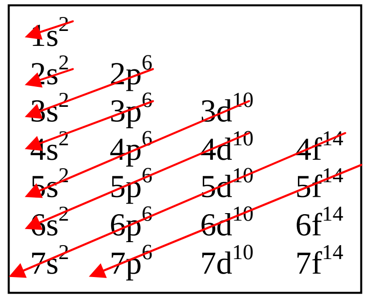
$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

In this case, the energy is $E = \frac{1}{2}\hbar\omega$, which simplifies slightly the phase factor at the end, and we have

$$\Psi(x,t) = \psi(x) e^{-i\omega t/2} = N \exp\left(-\frac{m\omega x^2}{2\hbar}\right) e^{-i\omega t/2}.$$

16. A certain electron is in a d-subshell in its atom.

(a) [5] Assuming the atom is in its ground state, what is the *minimum* value of *Z* such that the atom would have a d electron at all? Assume our rules for filling up quantum states is correct (and show your work).



The electrons are supposed to fill in the atom in the order

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6\ \ldots$$

It follows that to have any d electrons, you need to have more than 20 electrons, which means you need at least *Z* =21, corresponding to Sc, or scandium.

(b) [7] What do we know about the value of *n*, *l*, *m*, and m_s for this electron? For each of these, you can give either the value or a list of possible values (the list might be infinite). Note that this part of the problem is uncoupled from part (a), this need not be the lowest energy d electron.

A d electron has $l = 2$, by definition. Since *n* must be greater than *l*, *n* must be an integer 3 or greater. Since this part of the problem doesn't say we have scandium, there's no guarantee that $n = 3$.

The value of *m* is restricted to lie between $-l$ and l, and therefore can only take on the values -2, -1, 0, +1, or +2.

The value of m_s is always restricted to take on the value $m_s = \pm\frac{1}{2}$.

(c) [8] If you measured the total orbital angular momentum L^2, the orbital angular momentum around the *z*-axis L_z, the total spin squared S^2, and the spin around the *z*-axis S_z, what possible values might you get? In each case, your answer might be a definite value or a list of possible values.

We have $L^2 = (l^2 + l)\hbar^2 = (2^2 + 2)\hbar^2 = 6\hbar^2$. There is no ambiguity here.

We also have $L_z = m\hbar$, so the possible outcomes are $L_z \in \{-2\hbar, -\hbar, 0, \hbar, 2\hbar\}$.

For S_z, we have $S_z = m_s\hbar$, the possible outcomes will be $S_z \in \{-\frac{1}{2}\hbar, \frac{1}{2}\hbar\}$.

For S^2, we have $S^2 = (s^2 + s)\hbar^2$, but all electrons have $s = \frac{1}{2}$, so $S^2 = \frac{3}{4}\hbar^2$

17. A particle in one dimension has wave function

$$\psi(x) = \begin{cases} \sqrt{\dfrac{15}{16a^5}}\left(a^2 - x^2\right) & \text{for } -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

where *a* is a constant with units of length. This wave function is already properly normalized, and has $\langle x \rangle = 0$ and $\langle x^2 \rangle = \frac{1}{7}a^2$.

(a) [10] What is the expectation value of the momentum $\langle p \rangle$ and momentum squared $\langle p^2 \rangle$?

The wave function is real, and hence by our general rules, it must have $\langle p \rangle = 0$. To find $\langle p^2 \rangle$, we sandwich the operator between the complex conjugate of the wave function and the wave function, which gives us

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, p_{op}^2 \psi(x)\, dx = \int_{-a}^{a} \sqrt{\frac{15}{16a^5}}\left(a^2 - x^2\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \sqrt{\frac{15}{16a^5}}\left(a^2 - x^2\right) dx$$

$$= -\frac{15\hbar^2}{16a^5}\int_{-a}^{a}\left(a^2 - x^2\right)\frac{d^2}{dx^2}\left(a^2 - x^2\right)dx = -\frac{15\hbar^2}{16a^5}\int_{-a}^{a}\left(a^2 - x^2\right)(-2)\,dx$$

$$= \frac{15\hbar^2}{8a^5}\left(a^2 x - \tfrac{1}{3}x^3\right)\Big|_{x=-a}^{a} = \frac{15\hbar^2}{8a^5}\left[\left(a^3 - \tfrac{1}{3}a^3\right) - \left(-a^3 + \tfrac{1}{3}a^3\right)\right] = \frac{15\hbar^2}{8a^5}\frac{4a^3}{3} = \frac{5\hbar^2}{2a^2}.$$

That was a bit hairy, but the rest is easy!

(b) [6] What are the uncertainties Δx and Δp in the position and momentum?

To find the uncertainties, we simply use

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{a^2}{7}} = \frac{a}{\sqrt{7}},$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{5\hbar^2}{2a^2}} = \frac{\hbar}{a}\sqrt{\frac{5}{2}}.$$

(c) [4] Does this wave satisfy the Heisenberg uncertainty relation?

We simply look at the product

$$\Delta x \Delta p = \frac{\hbar}{a}\frac{a}{\sqrt{7}}\sqrt{\frac{5}{2}} = \hbar\sqrt{\tfrac{5}{14}} = 0.5976\hbar$$

According to the uncertainty principle, this must exceed $\frac{1}{2}\hbar$, and indeed it does.