Name ___________________

Solutions to Test 3
November 7, 2018

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.

$$h = 6.626\times10^{-34}\ \text{J}\cdot\text{s} = 4.136\times10^{-15}\ \text{eV}\cdot\text{s}$$
$$\hbar = 1.055\times10^{-34}\ \text{J}\cdot\text{s} = 6.582\times10^{-16}\ \text{eV}\cdot\text{s}$$
$$1\ \text{eV} = 1.602\times10^{-19}\ \text{J}$$

Barrier penetration:
$$T \approx 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\alpha L}$$
$$\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

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

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

Euler's formula
$$e^{ix} = \cos x + i\sin x$$

Spherical Coords.
$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$
$$0 \le r < \infty$$
$$0 \le \theta \le \pi$$
$$0 \le \phi < 2\pi$$

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

1. If the total angular momentum squared has a value of $L^2 = 20\hbar^2$, what is l?
   A) 4 B) 5 C) 20 D) 380 E) 420

2. An electron with $n = 4$, $l = 2$, and $m = 1$ would be described as what type of electron?
   A) 4p B) 2p C) 2f D) 4f **E) 4d**

3. Which of the following tells you the probability density of finding a particle at the point $\vec{r}$ at time t in three dimensions?
   A) $\psi(\vec{r})$ B) $\psi^*(\vec{r})$ C) $[\psi(\vec{r})]^2$ D) $|\psi(\vec{r})|$ **E)** $|\psi(\vec{r})|^2$

4. If an electron in an atom has $l = 2$, what is a complete list of the values that m can take on?
   A) ±2 **B)** $\pm2, \pm1, 0$ C) $0, 1, 2$ D) $\pm2, \pm\frac{3}{2}, \pm1, \pm\frac{1}{2}, 0$ E) None of these

5. Which of the following corresponds to the momentum operator p_{op} in quantum mechanics in one dimension?
   A) $\frac{\hbar}{i}\frac{\partial}{\partial x}$ B) $-\frac{\hbar}{i}\frac{\partial}{\partial x}$ C) x D) $\hbar x$ E) none of these

6. How come we don't solve Schrödinger's equation for hydrogen by factoring the wave function into functions of *x*, *y*, and *z*: $\Psi(\vec{r}) = X(x)Y(y)Z(z)$?
   A) Because the derivative terms end up mixing these factors together into an intractable mess
   B) Because there are three Schrödinger's equations in 3D, and this can't solve all three at once
   C) Because it should be a *sum* of functions in 3D, not a product
   D) Because the potential for hydrogen can't be naturally written in Cartesian coordinates, and this factorization doesn't help
   E) It can be written this way; that's exactly how we solved it

7. To find the average energy you would expect if you measured a particle, you should calculate the expectation value of the
   A) Position B) Momentum C) Momentum squared **D) Hamiltonian** E) None of these

8. Suppose $\Psi_1(\vec{r},t)$ and $\Psi_2(\vec{r},t)$ are both solutions of Schrödinger's time-dependent equation. Which of the following is guaranteed to also be a solution?
   A) $\Psi_1^*(\vec{r},t) + \Psi_2^*(\vec{r},t)$
   B) $\Psi_1(\vec{r},t) \cdot \Psi_2(\vec{r},t)$
   C) $\Psi_1(\vec{r},t) / \Psi_2(\vec{r},t)$
   D) $\Psi_1(\vec{r},t) - \Psi_2(\vec{r},t)$
   E) None of these

9. For the harmonic oscillator with potential $V(x) = \frac{1}{2} m\omega^2 x^2$, why are there only bound states, no unbound states?
   A) Because the force never vanishes, the particle must always be bound
   B) Because e^{ikx} is not a solution to Schrödinger's equation, there can't be unbound states
   C) Because the potential at infinity is infinity, the energy can't exceed the potential there
   D) Because all solutions have positive energy, there can't be unbound states
   E) They both exist, we just only found the unbound states

10. When you try to penetrate a finite-thickness barrier of size *L*, and your energy *E* is smaller than the height of the barrier, how does the barrier thickness affect the probablity of getting through?
   A) The probability grows exponentially as the thickness increases
   B) The probability shrinks exponentially as the thickness increases
   C) The probability is inversely proportional to the thickness
   D) The probability is inversely proportional to the thickness squared
   E) The probability is always zero in this case

Part II: Short answer [20 points]

Choose two of the following three questions and give a short answer (2-4 sentences) (10 points each).

11. Suppose you have found a solution $\psi(x)$ to Schrödinger's time-independent equation. Unfortunately, it turns out that the function is not normalized probably. What should you do? You will need to include one or more formulas in your answer.

Fortunately, any multiple of $\psi(x)$ will also satisfy Schrödinger's time-independent equation, so we simply try to multiply by an appropriate constant to make it normalized. Assume that $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = A$, then we can define $\hat{\psi}(x) = \psi(x)/\sqrt{A}$, then $\hat{\psi}(x)$ will satisfy Schrödinger's equation and will have $\int_{-\infty}^{\infty} |\hat{\psi}(x)|^2 \, dx = 1$.

12. When solving Schrödinger's equation, it is often necessary to solve it in different regions, and then piece the potential together at the boundaries. What are appropriate boundary conditions if (i) you have solutions on both sides of the boundary, or (ii) the potential is infinite on one side of the boundary.

Generally, the solutions to Schrödinger's equation, must be continuous, have a first derivative, and that derivative must be continuous. Hence we demand that the function and its derivative match on the two sides of the boundary. If the potential is infinite on one side of the boundary, the wave function must vanish there, and demanding that the wave function be continues then implies that it must vanish as you approach the other side of the boundary.

13. According to our computations for hydrogen, the 3p, 3d, and 4s energies are related by $E_{3p} = E_{3d} < E_{4s}$. Explain qualitatively why this doesn't work for more complicated atoms, and give the correct general heirarchy for these levels, according to our more sophisticated model.

The hydrogen-like model ignores interactions between electrons. The most important effect is that the innermost (1s) electrons are so close to the nucleus that effectively they almost completely screen the nucleus, effectively reducing its charge, and hence the outer electrons don't have as negative an energy as one would expect. However, for electrons with small values of the total angular quantum number *l* (such as the 4s, and to a lesser extent, the 3p), the electron does penetrate a little into the innermost part of the atom, allowing the electron to experience the full attractiveness of the nucleus and lowering the energy. So the 4s energy is lowered, below the 3d, and the 3p is lowered compared to 3d as well, so the final heirarchy is $E_{3p} < E_{4s} < E_{3d}$.

Part III: Calculation: [60 points] Choose three of the following four questions and perform the indicated calculations (20 points each).

14. An atom contains a single electron in the state n = 6, but the nuclear charge is unknown. The amount of energy required to extract the electron from the atom is measured to be $E = 3.40\text{ eV}$

(a) What is the value of the nuclear charge Z?

We use the formula for the energy of a hyarogen-like atom, $E = -(13.6\text{ eV})Z^2/n^2$. If it takes 3.40 eV to get the electron to be freed, the initial energy must be $E = -3.40\text{ eV}$. We therefore have

$$-3.40\text{ eV} = -\frac{(13.6\text{ eV})Z^2}{n^2} = -\frac{(13.6\text{ eV})Z^2}{6^2},$$

$$Z^2 = \frac{(3.40\text{ eV})6^2}{13.6\text{ eV}} = 9.00,$$

$$Z = 3.$$

The answer has to be an integer, so we have Z = 3.

(b) If the atom were to emit one photon, starting in this state, what would be the smallest energy E that that emitted photon could have, and what would be the final value of n?

When the atom emits a photon, it falls to a lower level, so the final n must be less than 6. The smallest amount it could fall would be to n = 5, so this must be the final state. The energy emitted is the initial energy divided by the final energy, so

$$\Delta E = E_6 - E_5 = -\frac{(13.6\text{ eV})3^2}{6^2} + \frac{(13.6\text{ eV})3^2}{5^2} = (-3.40\text{ eV}) + (4.90\text{ eV}) = 1.496\text{ eV}.$$

(c) If the atom were to absorb one photon, starting in this state, what would be the smallest energy E that that absorbed photon could have, and what would be the final value of n?

In this case, the energy must be increasing, so n must be larger than 6. The smalles amount of energy that can be absorbed is when n increases as little as possible, to n = 7, and the energy absorbed in this case must be the final energy minus the initial energy, so

$$\Delta E = E_7 - E_6 = -\frac{(13.6\text{ eV})3^2}{7^2} + \frac{(13.6\text{ eV})3^2}{6^2} = (-2.50\text{ eV}) + (3.40\text{ eV}) = 0.902\text{ eV}.$$

15. A group of electrons with kinetic energy $E = 8.00\text{ eV}$ impacts a sudden step potential of unknown height V_0. It is found that of 9.00×10^6 electrons, 8.00×10^6 of them successfully penetrate the barrier.

(a) What is the reflection probability *R*?

Since $\frac{8}{9}$ of the electrons are transmitted, it is clear that $\frac{1}{9}$ of them are reflected, so $R = \frac{1}{9} = 11.1\%$.

(b) What is the value (or possible values) of the potential height V_0?

We now simply equate the reflection probability to our formula, which is

$$\left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = R = \frac{1}{9},$$

$$\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}} = \pm\frac{1}{3},$$

$$3\sqrt{E}-3\sqrt{E-V_0} = \pm\sqrt{E}\pm\sqrt{E-V_0},$$

$$(3\mp1)\sqrt{E} = (3\pm1)\sqrt{E-V_0},$$

$$(3\mp1)^2 E = (3\pm1)^2 (E-V_0).$$

At this point it is probably good to break it into two cases and do them separately

$$4E = 16(E-V_0) \quad\text{or}\quad 16E = 4(E-V_0),$$

$$16V_0 = 12E \quad\text{or}\quad 12E = -4V_0,$$

$$V_0 = \tfrac{3}{4}E \quad\text{or}\quad V_0 = -3E,$$

$$V_0 = \tfrac{3}{4}(8.00\text{ eV}) \quad\text{or}\quad V_0 = -3(8.00\text{ eV}),$$

$$V_0 = 6.00\text{ eV} \quad\text{or}\quad V_0 = -24.00\text{ eV}.$$

16. A particle has wave function $\psi(x) = \begin{cases} 2\lambda^{3/2} x e^{-\lambda x} & \text{for } x > 0, \\ 0 & \text{for } x < 0. \end{cases}$

This wave function is properly normalized and has $\langle p^2 \rangle = \hbar^2 \lambda^2$**. A possibly useful integral is below.**

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

Real wave functions always have $\langle p \rangle = 0$, so there is nothing to calculate. For $\langle x \rangle$ and $\langle x^2 \rangle$, we compute

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x)\, dx = 4\lambda^3 \int_0^{\infty} x e^{-\lambda x} x x e^{-\lambda x} dx = 4\lambda^3 \int_0^{\infty} x^3 e^{-2\lambda x} dx = \frac{4\lambda^3 3!}{(2\lambda)^4} = \frac{4 \cdot 6\lambda^3}{16\lambda^4} = \frac{3}{2\lambda},$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x)\, dx = 4\lambda^3 \int_0^{\infty} x e^{-\lambda x} x^2 x e^{-\lambda x} dx = 4\lambda^3 \int_0^{\infty} x^4 e^{-2\lambda x} dx = \frac{4\lambda^3 4!}{(2\lambda)^5} = \frac{4 \cdot 24\lambda^3}{32\lambda^4} = \frac{3}{\lambda^2}.$$

(b) Find the uncertainties Δx **and** Δp**, and check that it satisfies the uncertainty principle.**

We calculate the uncertainties using the formulas

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

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{3}{\lambda^2} - \left(\frac{3}{2\lambda}\right)^2} = \frac{1}{\lambda}\sqrt{3 - \frac{9}{4}} = \frac{1}{\lambda}\sqrt{\frac{3}{4}} = \frac{\sqrt{3}}{2\lambda}.$$

The uncertainty relation then just says

$$(\Delta x)(\Delta p) = \lambda \hbar \frac{\sqrt{3}}{2\lambda} = \frac{\sqrt{3}}{2}\hbar > \frac{1}{2}\hbar.$$

So it is satisfied, as it must me.

Possibly useful integral: $\int_0^{\infty} x^n e^{-Ax} dx = n!/A^{n+1}$.

Wave functions for next problem:

$$R_{2,1} = \frac{r}{2\sqrt{6a^5}} e^{-r/2a}, \quad Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}, \quad Y_{2,\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\phi}.$$

17. Chemists prefer using real wave functions for atoms. For example, one of the states they use is $\psi = \frac{1}{\sqrt{2}}\left(\psi_{2,1,-1} - \psi_{2,1,+1}\right)$. Some hydrogen wave functions are written below.

(a) Write explicitly this wave function ψ as a function of (r,θ,ϕ), and show that it is real.

We start with $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$, so we have

$$\psi(r,\theta,\phi) = \frac{1}{\sqrt{2}}\left(\psi_{2,1,-1} - \psi_{2,1,+1}\right) = \frac{1}{\sqrt{2}}R_{21}(r)\left[Y_{1,-1}(\theta,\phi) - Y_{1,1}(\theta,\phi)\right]$$
$$= \frac{1}{\sqrt{2}}\frac{r}{2\sqrt{6a^5}}e^{-r/2a}\left[\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} + \sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}\right] = \frac{1}{\sqrt{2}}\frac{re^{-r/2a}}{2\sqrt{16\pi a^5}}\sin\theta\left(e^{-i\phi} + e^{i\phi}\right)$$
$$= \frac{re^{-r/2a}}{8\sqrt{2\pi a^5}}\sin\theta\left(\cos\phi - i\sin\phi + \cos\phi + i\sin\phi\right) = \frac{re^{-r/2a}}{4\sqrt{2\pi a^5}}\sin\theta\cos\phi.$$

The final expression is manifestly real.

(b) Find the value(s) of (r,θ,ϕ) where the particle is most likely to be.

This will occur any place where the function is at a maximum positive value or maximum negative value. To find the location, we just focus on the three factors and insist that their derivatives relative to the corresponding variables vanishes. The numerical factors are irrelevant. We therefore have

$$0 = \frac{d}{dr}\left(re^{-r/2a}\right) = e^{-r/2a} - \frac{r}{2a}e^{-r/2a} = \left(1 - \frac{r}{2a}\right)e^{-r/2a},$$
$$0 = \frac{d}{d\theta}\sin\theta = \cos\theta,$$
$$0 = \frac{d}{d\phi}\cos\phi = -\sin\phi.$$

The first equation has a root at $r = 2a$. The only place cosine vanishes between 0 and π is $\frac{1}{2}\pi$. For the final equation, sine vanishes at both 0 and π. Thus the two points where the wave function is maximum are $(r,\theta,\phi) = \left(2a,\frac{1}{2}\pi,0\right)$ and $\left(2a,\frac{1}{2}\pi,\pi\right)$.

(c) Find the corresponding cartesian coordinates (x,y,z).

We first note that for both points, $z = r\cos\theta = 0$ and $y = r\sin\theta\sin\phi = 0$. For x we have

$$x = r\sin\theta\cos\phi = 2a\sin\left(\tfrac{1}{2}\pi\right)\cos(0) = 2a \quad \text{or} \quad x = r\sin\theta\cos\phi = 2a\sin\left(\tfrac{1}{2}\pi\right)\cos(\pi) = -2a.$$

Hence the points are $(x,y,z) = (\pm 2a,0,0)$.