Solutions to Test 3
November 6, 2019

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

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

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

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

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

Part I: Multiple Choice [20 points]

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

1. Suppose a particle of energy E is impacting a step potential (infinite width) of height V_0. Under what circumstances will at least some of the incoming particles be reflected?
A) Only if $E > V_0$ B) Only if $E < V_0$ C) Only if $V_0 > 0$ **D) Only if** $V_0 \neq 0$ E) All V_0

2. For a particle with energy E in one dimension in a potential $V(x)$, under what conditions do we have a bound state?
A) $E < 0$ B) $E > 0$ **C)** $E < V(\pm\infty)$ D) $E > V(\pm\infty)$ E) $E + V(\pm\infty) < 0$

3. For an arbitrary operator $\mathcal{O}$, which expression should one use to find $\langle\mathcal{O}\rangle$?
A) $\int\psi^*\mathcal{O}\psi\,dx$ B) $\int\psi^*\psi\mathcal{O}\,dx$ C) $\int|\psi|^2\mathcal{O}\,dx$ D) $\int\psi\mathcal{O}\psi\,dx$ E) $\int\psi\mathcal{O}\psi^*\,dx$

4. If the ground state solution of the time-independent Schrödinger equation harmonic oscillator with angular frequency ω is $\psi_0(x)$, what would be the solution of the time-dependent Schrödinger equation for this wave function?
A) $\psi_0(x)e^{i\omega t}$ B) $\psi_0(x)e^{-i\omega t}$ C) $\psi_0(x)e^{i\omega t/2}$ **D)** $\psi_0(x)e^{-i\omega t/2}$ E) None of these

5. If a hydrogen atom has an electron with $n = 3$, what are all the values that l can take on?
A) $0,1,2,3$ **B)** $0,1,2$ C) $0,\pm1,\pm2,\pm3$ D) $0,\pm1,\pm2$ E) $\pm1,\pm2,\pm3$

6. If we put photons through one at a time through a mirror that reflects half of the probability, and then put up two detectors A and B to see which way that photon went, what would happen?
   A) You would get half a photon at A, and half a photon at B
   B) 50% of the time it would be at A, 50% at B, and never will it be neither or both
   C) 25% of the time there would be no photon, 50% at A or B, and 25% at both
   D) 50% of the time there will be a photon at both locations, and 50% at neither
   E) Always a full photon at both A and B, but each will have half the original energy

7. Given n, l, and m, which expression tells you the wave function for a state of hydrogen?
   A) $R_{n,l}(r)Y_{l,m}(\theta,\phi)$
   B) $R_{n,l}(r)Y_{n,m}(\theta,\phi)$
   C) $R_{l,m}(r)Y_{n,l}(\theta,\phi)$
   D) $R_{n,m}(r)Y_{l,m}(\theta,\phi)$
   E) $R_{l,n}(r)Y_{m,l}(\theta,\phi)$

8. When solving for the ground state of the harmonic oscillator, we initially had solutions that looked like $\exp\left(\pm m\omega x^2/2\hbar\right)$, but then we rejected $\exp\left(+m\omega x^2/2\hbar\right)$. Why?
   A) This would represent a particle coming in from $+\infty$, not what we want
   B) This did not satisfy Schrödinger's equation
   C) This wave function could not have the correct time dependence
   D) This wave function didn't satisfy the uncertainty relation
   E) This wave function cannot be normalized

9. In ordinary physics, to give initial conditions you would normally give $x\big|_{t=0}$ and $\left.\frac{dx}{dt}\right|_{t=0}$.
   What would initial conditions look like for a particle in quantum mechanics?
   A) Exactly the same thing
   B) $\Psi(x,t)\big|_{t=0}$ and $\left.\frac{\partial}{\partial t}\Psi(x,t)\right|_{t=0}$
   C) $\Psi(x,t)\big|_{t=0}$
   D) $\Psi(x,t)\big|_{t=0}$ and $x\big|_{t=0}$
   E) $\Psi(x,t)\big|_{t=0}$, $x\big|_{t=0}$ and $\left.\frac{dx}{dt}\right|_{t=0}$

10. If Ψ_1 and Ψ_2 are both solutions of Schrödinger's time-dependent equation, which of the following must also be a solution?
   A) $\Psi_1\Psi_2$ B) $\Psi_1\Psi_2^*$ C) $\Psi_1^*+\Psi_2^*$ D) Ψ_1/Ψ_2 **E)** $\Psi_1-i\Psi_2$

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. Explain qualitatively what the difference between spin and orbital angular momentum is. Also, for the electron, what is the value of S^2, the square of the spin?

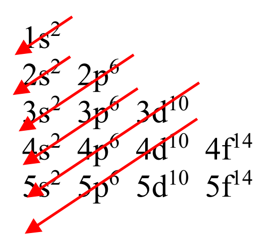
Orbital angular momentum is the angular momentum of a particle going around another, such as the electron orbiting the nucleus in hydrogen. Spin is the internal angular momentum, representing the angular momentum of the object spinning around itself. For an electron, we have $s = \frac{1}{2}$, so that we then have

$$S^2 = \left(s^2 + s\right)\hbar^2 = \left(\tfrac{1}{4} + \tfrac{1}{2}\right)\hbar^2 = \tfrac{3}{4}\hbar^2 \ .$$

12. When we were solving Schrödinger's equation for the step potential with a particle impacting from the left, we had solutions $Ae^{ikx} + Be^{-ikx}$ for $x < 0$, and $Ce^{ik'x} + De^{-ik'x}$ for $x > 0$. Explain what each of these terms would represent, and why we set one of them to zero. No equations are necessary.

The A term represents the incoming wave on the left, and the B term is the reflected wave, also on the left. On the right side, C represents a wave moving to the right, and therefore is the transmitted wave. But D would represent an incoming wave coming from the right, which makes no sense for this problem, so we set $D = 0$.

13. Give the electronic configuration ($1s^2$ …) for Mn (Z=25). Assume the standard rules apply.



We fill up the quantum state according to the standard rules, as sketched at right. The electron configuration is:

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^5$$

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

14. A beam of 148,000 electrons ($m = 5.11\times10^5\ \text{eV}/c^2 = 9.11\times10^{-31}\ \text{kg}$ **) with energy** $E = 1.45\ \text{eV}$ **is attempting to penetrate a barrier of height 5.80 eV. It is found that only 135 of them make it through.**

(a) What is the probability *P* of the particles making it through?

The probability is the fraction that make it through, which is just

$$T = \frac{135}{148,000} = 9.12\times10^{-4}\ .$$

(b) What is the damping coefficient α **?**

The damping coefficient is given by

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{\sqrt{2\left(5.11\times10^5\ \text{eV}/c^2\right)\left(5.80\ \text{eV} - 1.45\ \text{eV}\right)}}{\hbar}$$

$$= \frac{2108\ \text{eV}}{\left(6.582\times10^{-16}\ \text{eV}\cdot\text{s}\right)\left(2.998\times10^8\ \text{m/s}\right)} = 1.069\times10^{10}\ \text{m}^{-1} = 10.69\ \text{nm}^{-1}\ .$$

(c) What is the thickness of the barrier in nm?

We equate the probability found in part (a) to the formula for the penetration probability, so we have

$$T = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\alpha L} = 16\frac{1.45\ \text{eV}}{5.80\ \text{eV}}\left(1 - \frac{1.45\ \text{eV}}{5.80\ \text{eV}}\right)e^{-2\alpha L} = 16(0.250)(0.750)e^{-2\alpha L} = 3.000e^{-2\alpha L}\ ,$$

$$e^{2\alpha L} = \frac{3.000}{T} = \frac{3.00}{9.12\times10^{-4}} = 3289\ ,$$

$$2\alpha L = \ln(3289) = 8.098\ ,$$

$$L = \frac{8.098}{2\alpha} = \frac{8.098}{2\left(10.69\ \text{nm}^{-1}\right)} = 0.379\ \text{nm}.$$

15. A particle is trapped in the *n* = 3 wave function of the infinite square well with allowed region $0 < x < L$. Some possibly helpful integrals are given below.

(a) What is the energy of this particle?

We simply substitute *n* = 3 in the formula to find

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

(b) What is the probability density that the particle is at the point *x*? Demonstrate that the wave function is properly normalized.

The probability density is the square of the magnitude of the wave function, and is therefore given by

$$\left|\psi_3\left(x\right)\right|^2 = \frac{2}{L}\sin^2\left(\frac{3\pi x}{L}\right)$$

We then integrate this probability density over the whole of the allowed region to obtain

$$\int \left|\psi_3\left(x\right)\right|^2 dx = \frac{2}{L}\int_0^L \sin^2\left(\frac{3\pi x}{L}\right)dx = \frac{2}{L}\left[\frac{x}{2} - \frac{1}{4\left(3\pi/L\right)}\sin\left(\frac{6\pi x}{L}\right)\right]_0^L$$

$$= \frac{2}{L}\left[\frac{L}{2} - \frac{L}{4\pi}\sin\left(6\pi\right) - \frac{0}{2} + \sin\left(0\right)\right] = \frac{2}{L}\cdot\frac{L}{2} = 1.$$

Obviously this worked out.

(c) What is the probability that the particle is in the region $x < \frac{1}{4}L$?

To find this probability, we integrate the probability density over the region indicated, which will give

$$P\left(x < \tfrac{1}{4}L\right) = \int_{-\infty}^{\frac{1}{4}L} \left|\psi_1\left(x\right)\right|^2 = \frac{2}{L}\int_0^{\frac{1}{4}L} \sin^2\left(\frac{3\pi x}{L}\right)dx = \frac{2}{L}\left[\frac{x}{2} - \frac{1}{4\left(3\pi/L\right)}\sin\left(\frac{6\pi x}{L}\right)\right]_0^{L/4}$$

$$= \frac{2}{L}\left[\frac{L}{2\cdot 4} - \frac{L}{12\pi}\sin\left(\frac{6\pi}{4}\right) - \frac{0}{2} + \frac{L}{12\pi}\sin\left(0\right)\right] = \frac{1}{4} - \frac{1}{6\pi}\cdot\left(-1\right) = \frac{1}{4} + \frac{1}{6\pi}$$

$$\approx 0.303 = 30.3\%.$$

Possibly useful integrals: $\int \sin\left(\alpha x\right)dx = -\frac{1}{\alpha}\cos\left(\alpha x\right)$, $\int \sin^2\left(\alpha x\right)dx = \frac{x}{2} - \frac{1}{4\alpha}\sin\left(2\alpha x\right)$.

16. A particle has the normalized wave function $\psi(x) = \begin{cases} \sqrt{\dfrac{8}{3a}} \sin^2\left(\dfrac{\pi x}{a}\right) & 0 < x < a\,, \\ 0 & \text{otherwise.} \end{cases}$

This wave function has $\langle p^2 \rangle = 4\pi^2\hbar^2 / (3a^2)$**. Some possibly useful integrals are below.**

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

Because the wave function is real, we automatically have $\langle p \rangle = 0$. For the other expressions, we simply do all the integrals.

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \frac{8}{3a} \int_0^a \sin^2\left(\frac{\pi x}{a}\right) x \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{8}{3a} \cdot \frac{a^2}{4} = \frac{a}{2},$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi \, dx = \frac{8}{3a} \int_0^a \sin^2\left(\frac{\pi x}{a}\right) x^2 \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{8}{3a} \cdot a^3 \left(\frac{1}{8} - \frac{15}{64\pi^2}\right) = a^2 \left(\frac{1}{3} - \frac{5}{8\pi^2}\right).$$

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

We calculate these as usual:

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2 \left(\frac{1}{3} - \frac{5}{8\pi^2}\right) - \frac{a^2}{4} = a^2 \left(\frac{1}{12} - \frac{5}{8\pi^2}\right),$$

$$\Delta x = a\sqrt{\frac{1}{12} - \frac{5}{8\pi^2}} \approx 0.141a,$$

$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{4\pi^2\hbar^2}{3a^2} - 0^2 = \frac{4\pi^2\hbar^2}{3a^2},$$

$$\Delta p = \frac{2\pi\hbar}{a\sqrt{3}} \approx \frac{3.63\hbar}{a}.$$

We then check the product of these two expressions, which is

$$(\Delta x)(\Delta p) = a\sqrt{\frac{1}{12} - \frac{5}{8\pi^2}} \cdot \frac{2\pi\hbar}{a\sqrt{3}} = \hbar\sqrt{\frac{\pi^2}{9} - \frac{5}{6}} \approx 0.513\hbar.$$

The uncertainty principle states that this must exceed $0.5\hbar$, which it does.

Possibly useful integrals:

$$\int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{1}{2}a, \quad \int_0^a x \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{1}{4}a^2, \quad \int_0^a x^2 \sin^2\left(\frac{\pi x}{a}\right) dx = \left(\frac{1}{6} - \frac{1}{4\pi^2}\right) a^3,$$

$$\int_0^a \sin^4\left(\frac{\pi x}{a}\right) dx = \frac{3}{8}a, \quad \int_0^a x \sin^4\left(\frac{\pi x}{a}\right) dx = \frac{3}{16}a^2, \quad \int_0^a x^2 \sin^4\left(\frac{\pi x}{a}\right) dx = \left(\frac{1}{8} - \frac{15}{64\pi^2}\right) a^3.$$

17. An electron in a hydrogen atom has its total angular momentum measured, and it is found to have a value of $L^2 = 12\hbar^2$.

(a) Based on this, deduce the value of one of the variables (n, l, m, m_s) describing the various states of the electron.

The total angular momentum is described by the variable *l*, and takes the values $L^2 = (l^2 + l)\hbar^2$, where *l* is a non-negative integer. Equating $12\hbar^2 = (l^2 + l)\hbar^2$, and solving for *l*, we conclude that $l = 3$.

(b) If the angular momentum around the *z*-axis L_z were measured, what would be the possible values?

The quantity L_z is given by $L_z = m\hbar$, where *m* takes on the values $-l, -l+1, \ldots, l$. For $l = 3$, we conclude that

$$L_z \in \{-3\hbar, -2\hbar, -\hbar, 0, \hbar, 2\hbar, 3\hbar\}$$

(c) If the spin around the *z*-axis S_z were measured, what would be the possible values?

The spin takes on the values $S_z = m_s\hbar$, where $m_s = \pm\frac{1}{2}$, so $S_z = \pm\frac{1}{2}\hbar$.

(d) If the energy of this state were measured, what would be the <u>minimum</u> (most negative *E*) that could be measured?

In general, we always have $l = 0, 1, \ldots, n-1$, so we have $n > l$. With $l = 3$, we must have $n > 3$. The smallest value will be $n = 4$, and this will be the lowest (most negative energy). Substituting into the energy equation, we have

$$E = -\frac{13.6 \text{ eV}}{n^2} = -\frac{13.6 \text{ eV}}{16} = -0.850 \text{ eV}.$$