Assignment 8 – Solutions

Problems:
Chapter 12: 45, 52, 54, 56

Wave Mechanics and Particle in a Box

45. a. $\Delta p = m\Delta v = 9.11 \times 10^{-31}\text{ kg} \times 0.100\text{ m/s} = \dfrac{9.11 \times 10^{-32}\text{ kg m}}{\text{s}}$

$$\Delta p\Delta x \geq \frac{h}{4\pi},\ \Delta x = \frac{h}{4\pi\Delta p} = \frac{6.626 \times 10^{-34}\text{ J s}}{4 \times 3.142 \times (9.11 \times 10^{-32}\text{ kg m/s})} = 5.79 \times 10^{-4}\text{ m}$$

b. $\Delta x = \dfrac{h}{4\pi\Delta p} = \dfrac{6.626 \times 10^{-34}\text{ J s}}{4 \times 3.142 \times 0.145\text{ kg} \times 0.100\text{ m/s}} = 3.64 \times 10^{-33}\text{ m}$

c. The diameter of an H atom is roughly 1.0×10^{-8} cm. The uncertainty in position is much larger than the size of the atom.

d. The uncertainty is insignificant compared to the size of a baseball.

Orbitals and Quantum Numbers

52. Quantum numbers give the allowed solutions to Schrödinger equation. Each solution is an allowed energy level called a wave function or an orbital. Each wave function solution is described by three quantum numbers, n, ℓ, and m_ℓ. The physical significance of the quantum numbers are:

n: Gives the energy (it completely specifies the energy only for the H atom or ions with one electron) and the relative size of the orbitals.

ℓ: Gives the type (shape) of orbital.

m_ℓ: Gives information about the direction in which the orbital is pointing.

The specific rules for assigning values to the quantum numbers n, ℓ, and m_ℓ are covered in Section 12.9. In Section 12.10, the spin quantum number m_s is discussed. Since we cannot locate electrons, we cannot see if they are spinning. The spin is a convenient model. It refers to the ability of the two electrons that can occupy any specific orbital to produce two differently oriented magnetic moments.

54. b. For $\ell = 3$, m_ℓ can range from -3 to +3; thus +4 is not allowed.

c. n cannot equal zero.

d. ℓ cannot be a negative number.

The quantum numbers in part a are allowed.

56. 5p: three orbitals $3d_{z^2}$: one orbital 4d: five orbitals

$n = 5$: $\ell = 0$ (1 orbital), $\ell = 1$ (3 orbitals), $\ell = 2$ (5 orbitals), $\ell = 3$ (7 orbitals), $\ell = 4$ (9 orbitals); total for $n = 5$ is 25 orbitals.

$n = 4$: $\ell = 0$ (1), $\ell = 1$ (3), $\ell = 2$ (5), $\ell = 3$ (7); total for $n = 4$ is 16 orbitals.

Assignment 8 Additional Problems

A1. For a particle, the wavelength and speed are related by:

$$\lambda = \frac{h}{m\text{v}} \Longrightarrow \text{v} = \frac{h}{m\lambda}$$

The wavelength is equal to the circumference of the first Bohr orbit, which has a radius of a_0, hence $\lambda = 2\pi a_0$. Substituting:

$$\text{v} = \frac{h}{2\pi a_0 m} = \frac{6.626\times10^{-34}\ \text{J}\cdot\text{s}}{2\pi(0.529\times10^{-10}\ \text{m})(9.109\times10^{-31}\ \text{kg})} = 2.19\times10^{6}\ \text{m/s}$$

The kinetic energy is given by:

$$\text{KE} = \tfrac{1}{2}m\text{v}^2 = \tfrac{1}{2}(9.109\times10^{-31}\ \text{kg})(2.19\times10^{6}\ \text{m/s})^2 = 2.18\times10^{-18}\ \text{J}$$

A2. (a). The uncertainty principle states:

$$\Delta x\Delta p \geq \frac{h}{4\pi} \Longrightarrow \Delta x m\Delta v \geq \frac{h}{4\pi} \Longrightarrow \Delta\text{v} \geq \frac{h}{4\pi m\Delta x}$$

$$\Delta\text{v} \geq \frac{6.626\times10^{-34}\ \text{J}\cdot\text{s}}{4\pi(1.0\times10^{-9}\ \text{kg})(1.0\times10^{-6}\ \text{m})}$$

$$\geq 5.27\times10^{-20}\ \text{m/s}$$

Note that the mass should be in kg (1.0 μg = 1.0×10^{-6} g = 1.0×10^{-9} kg).

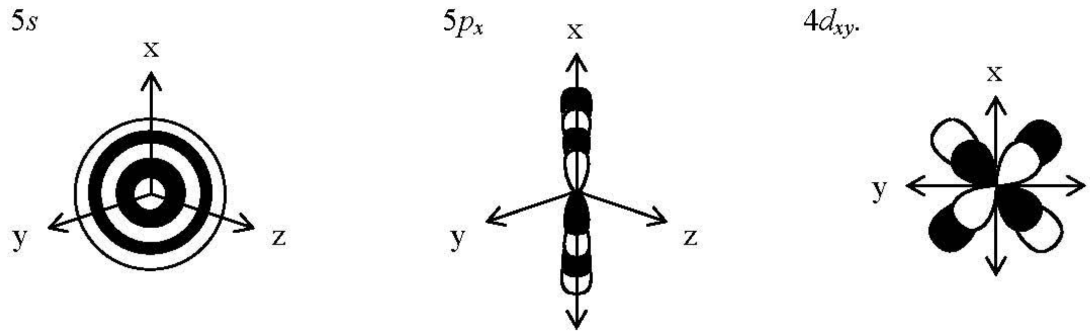
(b). Using Δx = 0.10 nm = 1.0×10^{-10} m:

$$\Delta\text{v} \geq \frac{6.626\times10^{-34}\ \text{J}\cdot\text{s}}{4\pi(1.0\times10^{-9}\ \text{kg})(1.0\times10^{-10}\ \text{m})}$$

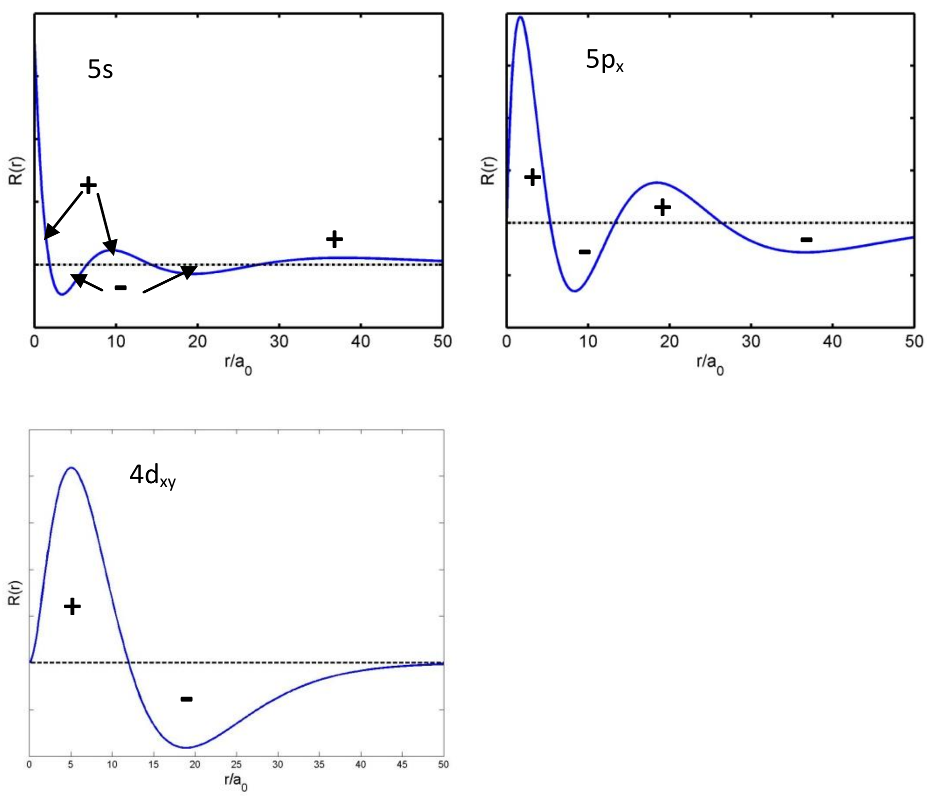
$$\geq 5.27\times10^{-16}\ \text{m/s}$$

This is a very small number, which implies that even a speck of dust weighing 1.0 μg is large enough to be governed by classical mechanics rather than quantum mechanics.

A3. The wave function has a positive value in the unshaded regions and a negative value in the shaded regions. A nodal plane is present at each changeover point.



A4. The graphs below show the radial part of each wavefunction. Keep in mind that these graphs show ONLY the radial nodes (since any angular nodes go through the origin).



Assignment 8 Challenge Problem

1. Why JJ did NOT observe diffraction.

   a. What are the (i) velocity and (ii) wavelength of the electrons in the beam?

$$E_{\text{kinetic}} = \frac{1}{2} m_e v^2$$

$$v = \sqrt{\frac{2E_{\text{kinetic}}}{m_e}} = \sqrt{\frac{2(1.2 \times 10^{-17}\ \text{J})}{(9.109 \times 10^{-31}\ \text{kg})}} = 5.13 \times 10^6\ \text{m/s}$$

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{J s}}{(9.109 \times 10^{-31}\ \text{kg})(5.13 \times 10^6\ \text{m/s})} = 1.42 \times 10^{-10}\ \text{m} = 0.142\ \text{nm}$$

b. The light beam should go directly through the slit without showing any signs of diffraction and hit the screen with a bright spot directly in front of the slit. In order for diffraction to be observed, the slit width must be approximately equal to (within about a factor of 1000) the wavelength of the electrons.

c. The wavelength calculated in (a) is 1.42×10^{-10} m, so therefore the slit width has to be approximately 1.42×10^{-10} m in order for diffraction to be observed. In fact, a slit smaller than about 1×10^{-7} m is required.

d. JJ did not observe diffraction because any slit the electrons passed through in his experiment was too wide. The electrons would not have been diffracted, but passed straight through as though they were simply particles.

2. Why George DID observe diffraction.

a. When waves pass through a narrow slit, they diffract, that is, they spread out in all directions on the other side of the slit, rather than traveling in straight lines as particles would. When the waves emanating from the two slits overlap, they exhibit another fundamental property of waves: interference. When two waves overlap in phase, they add together, or create constructive interference, which is observed as a bright spot. When two waves overlap out of phase, they cancel each other out, resulting in destructive interference, or a dark spot. In the two slit experiment, constructive interference is observed at any point on the screen where the difference in the path lengths from the two slits to that point is equal to an integral multiple of the wavelength of the light (or electrons). At these points, the waves will be in phase, and constructive interference (a bright spot) will be observed. One such bright spot always lies directly between the two slits, where the path lengths are equal. The locations of the other bright spots depend on the wavelength of light (electrons).

b. Using the wavelength for the electron calculated in 1a, calculate d, the distance between the "two slits".

$$n\lambda = d \sin\theta$$

$$d = \frac{n\lambda}{\sin\theta} = \frac{1.42 \times 10^{-10}\ \text{m}}{\sin(41.2^\circ)} = 2.16 \times 10^{-10}\ \text{m}$$

c. The distance, d, corresponds to the distance between Ni nuclei. Note that the nuclei are very small and the size of the Ni atoms (and therefore the distance between them in the crystal) is determined by the orbitals that are populated with electrons, but because the electrons themselves are extremely small, the majority of the atoms are empty space. Therefore, for the most part, the beam of electrons can pass through the crystal without hitting the nuclei (remember Rutherford's gold foil experiment – most of the particles went straight through.) The nuclei arranged in a regular pattern in the crystal form the 'slits' that the electrons pass through. The value in 2b is physically reasonable because it is the same size as we would expect for the diameter of a Ni atom: ~200 pm or 2×10^{-10} m (see Chapter 12 for atomic radii). The answer is also consistent with part 1 because it is approximately equal to the wavelength calculated for the electrons (1.42×10^{-10} m), therefore we expect to observe diffraction.

3. What would Heisenberg say about this?

a. If the uncertainty in the velocity of an electron from 1a is 2.69×10^{5} m/s, what is the uncertainty in its position?

$$\Delta p \times \Delta x \geq \frac{h}{4\pi} \quad \text{or} \quad m\Delta v \times \Delta x \geq \frac{h}{4\pi}$$

$$\Delta x \geq \frac{h}{4\pi m \Delta v}$$

$$\Delta x \geq \frac{6.626\times10^{-34}\ \text{J s}}{4\pi(9.109\times10^{-31}\ \text{kg})(2.69\times10^{5}\ \text{m/s})}$$

$$\geq 2.15\times10^{-10}\ \text{m}$$

b. No. The uncertainty in the electron's position is about the same size as the distance between nuclei. Therefore, it is not possible to determine exactly which pair of Ni nuclei an electron passes between.

c. If a single electron were fired at the Ni crystal, it would not pass straight through the crystal. Instead, it would be detected at a single, random point on the screen. The electron is detected at a random position because when it passes through the crystal it is diffracted due to its wave-like properties. It then appears at a single point because when hitting the screen the electron displays particle-like properties. If we were to do this experiment many times with many individual electrons, we would see that the electrons would cluster at positions that correspond to the intensity maxima in the diffraction pattern. This means that the diffraction pattern generated by a continuous wave with the wavelength of the electrons can be interpreted as a probability distribution; there is a greater probability that an electron will hit the screen at a point corresponding to a maximum (bright spot) in the diffraction pattern and a lower probability that it will hit at a point corresponding to a minimum (dark spot) in the pattern.