Phenomena: Different wavelengths of electromagnetic radiation were directed onto two different metal samples (see picture). Scientists then recorded if any particles were ejected and if so what type of particles as well as the speed of the particle. What patterns do you see in the results that were collected?

<table>
<thead>
<tr>
<th>Exp.</th>
<th>Wavelength of Light</th>
<th>Intensity</th>
<th>Particles Ejected</th>
<th>Particle</th>
<th>Speed of Ejected Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$3 \times 10^{-7}$ m</td>
<td>Medium</td>
<td>Yes</td>
<td>e</td>
<td>$3 \times 10^{4}$ m/s</td>
</tr>
<tr>
<td>2</td>
<td>$3.3 \times 10^{-7}$ m</td>
<td>High</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>3</td>
<td>$2 \times 10^{-7}$ m</td>
<td>Low</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>4</td>
<td>$4 \times 10^{-7}$ m</td>
<td>Low</td>
<td>No</td>
<td>N/A</td>
<td>$2 \times 10^{7}$ m/s</td>
</tr>
</tbody>
</table>

**Big Idea:** The structure of atoms must be explained using quantum mechanics, a theory in which the properties of particles and waves merge together.

**Electromagnetic Radiation**

- **Wavelength ($\lambda$):** Is the peak-to-peak distance.
  
  *Note: Changing the wavelength changes the region of the spectrum (i.e. x-ray to visible).*

- **Amplitude:** Determines brightness of the radiation.

- **Frequency ($\nu$):** The number of cycles per second ($1 \text{ Hz} = 1 \text{ s}^{-1}$).

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**Examples of Electromagnetic Radiation:**

- Visible light
- Radio waves
- X-rays

**Quantum Theory**

- If white light is passed through a prism, a continuous spectrum of light is found. However, when the light emitted by excited hydrogen atoms is passed through a prism the radiation is found to consist of a number of components or spectra lines.
Quantum Theory

- **Black Body**: An object that absorbs and emits all frequencies of radiation without favor.

  **Heated Black Bodies**

  \[ T \lambda_{\text{max}} = 2.9 K \mathrm{mm} \quad I_{\text{tot}} = 5.67 \times 10^{-8} \frac{W}{\mathrm{m}^2 \cdot \lambda^4} \]

  *Note: \( \lambda_{\text{max}} \) is the most prevalent wavelength, not the longest wavelength.*

Quantum Theory

- **Max Planck**: Proposed that the exchange of energy between matter and radiation occurs in quanta, or packets of energy. His central idea was that a charged particle oscillating at a frequency \( \nu \), can exchange energy with its surroundings by generating or absorbing electromagnetic radiation only in discrete packets of energy.

  - **Quanta**: Packet of energy (implies minimum energy that can be emitted).
  - Charged particles oscillating at a frequency \( \nu \), can only exchange energy with their surroundings in discrete packets of energy.

Quantum Theory

- **Photoelectric Effect**: Ejection of electrons from a metal when its surface is exposed to ultra violet radiation.

  - **Findings of the Photoelectric Effect**
    1. No electrons are ejected unless the radiation has a frequency above a certain threshold value characteristic of the metal.
    2. Electrons are ejected immediately, however low the intensity of the radiation.
    3. The kinetic energy of the ejected electrons increases linearly with the frequency of the incident radiation.

  - **Albert Einstein**
    - Proposed that electromagnetic radiation consists of massless "particles" (photons)
    - Photons are packets of energy
    - Energy of a single photon = \( h \cdot \nu \)

  - **Work Function (\( \Phi \))**: The minimum amount of energy required to remove an electron from the surface of a metal.
    - If \( E_{\text{photo}} < \Phi \), no electron ejected
    - If \( E_{\text{photo}} > \Phi \), electron will be ejected

  *Note: This relationship is not intensity dependent.*
Chapter 12: Quantum Mechanics and Atomic Theory

Quantum Theory

With what speed will the fastest electrons be emitted from a surface whose threshold wavelength is 600 nm, when the surface is illuminated with light of wavelength $4.0 \times 10^{-7}$ m?

H atoms only emit/absorb certain frequencies. What is causing these properties?

- Electrons can only exist with certain energies.
- The spectral lines are transitions from one allowed energy level to another.

Finding energy levels of H atom

- $\Delta E = E_{\text{final}}(\nu) - E_{\text{initial}}(\nu) = h \nu$ (found experimentally)
- $\nu_{\text{final}} = \frac{3.29 \times 10^{15} \nu}{(2 - \frac{1}{n^2})}$

Energy level of H atom

- $E = -2.178 \times 10^{-19} \left( \frac{1}{n^2} \right)$ for n=1, 2, 3, ...

Energy level of other 1e- systems

- $E = -2.178 \times 10^{-19} \left( \frac{1}{n^2} \right)$ for n=1, 2, 3, ...

Student Question

What is the wavelength of the radiation emitted by an Li$^+$ atom when an electron transitions between $n=4$ to the $n=2$ levels?

Helpful Hint: $c = 2.998 \times 10^8 \text{m/s}$

a) -1.664 x 10^24 m
b) -5.399 x 10^-8 m
c) 1.621 x 10^-7 m
d) 4.864 x 10^-7 m
e) None of the Above

Quantum Theory

Constructive Interference: When the peaks of waves coincide, the amplitude of the resulting wave is increased.

Destructive Interference: When the peak of one wave coincides with the trough of another wave, the resulting wave is decreased.


d) When light passes through a pair of closely spaced slits, circular waves are generated at each slit. These waves interfere with each other.

\where they interfere constructively, a bright line is seen on the screen behind the slits; where the interference is destructive, the screen is dark.
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Student Question

What is the wavelength of an electron traveling at the speed of light?

Helpful information: \( m_e = 9.109 \times 10^{-31} \text{ kg} \) and \( h = 6.626 \times 10^{-34} \text{ J s} \)

a) 2.42\times10^{-9} \text{ m}

b) 2.42\times10^{-12} \text{ m}

c) 4.12\times10^{11} \text{ m}

d) None of the Above

Quantum Theory

Particles have wave-like properties, therefore, classical mechanics are incorrect.

Classical Mechanics:
- Particles have a defined trajectory.
- Location and linear momentum can be specified at every moment.

Quantum Mechanics:
- Particles behave like waves.
- Cannot specify the precise location of a particle.

Note: For the hydrogen atom, the duality means that we are not going to be able to know the speed of an electron orbiting the nucleus in a definite trajectory.

Wavefunction (\( \Psi \)): A solution of the Schrödinger equation; the probability amplitude.

Examples:
\( \Psi = \sin(x) \)

Probability Density (\( |\Psi|^2 \)): A function that, when multiplied by volume of the region, gives the probability that the particle will be found in that region of space.

Note: This must be between 0 and 1.

Plug 2\text{nd} derivative back into wavefunction

\[ \frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} \sin \left( \frac{m}{L}x \right) = E \left( \frac{m}{L} \right)^2 \sin \left( \frac{m}{L}x \right) \]

Cancel out

\[ \frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} = E \left( \frac{m}{L} \right)^2 \]

Simplify

\[ \hbar = \frac{\sqrt{2mE}}{L} \]

\[ E = \frac{\hbar^2}{2m} \left( \frac{m}{L} \right)^2 \]

Note: The term \( \left( \frac{m}{L} \right)^2 \) is there for normalization in order to get \( \Psi^2 = 1 \).
Atomic Orbitals: A region of space in which there is a high probability of finding an electron in an atom.

The wavefunction of an electron is given in spherical polar coordinates:

- \( r \) = distance from the center of the atom
- \( \theta \) = the angle from the positive z-axis, which can be thought of as playing the role of the geographical "latitude"
- \( \phi \) = the angle about the z-axis, the geographical longitude

Note: The wavefunctions of electrons are the atomic orbitals.

Wavefunction of an electron in a 1-electron atom:

\[
\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)
\]

- \( R(r) \) = Radial Wavefunction
- \( Y(\theta, \phi) \) = Angular Wavefunction

Scientists have solved for the energy of the H-atom:

- \( E \) = Energy of electron in hydrogen atom
- \( n \) = principle quantum number can be 1, 2, 3, ...
- \( h \) = Planck’s constant \( 6.62608 \times 10^{-34} \text{J} \cdot \text{s} \)

Pictured: The permitted energy levels of a hydrogen atom. The levels are labeled with the quantum number \( n \) which ranges from \( n = 1 \) (ground state) to \( n = \infty \).

Quantum Numbers

- **Principle Quantum Number** \( n \)
  - Related To: Size and Energy
  - Allowed Values: 1, 2, 3, ..., \( \infty \) (shells)

Example:

\( 3p \) \( n = 3 \)
### Angular Momentum Quantum Number ($\ell$)

- **Related To:** Shape
- **Allowed Values:** $0, 1, 2, \ldots, n - 1$ (subshells)

<table>
<thead>
<tr>
<th>Value of $\ell$</th>
<th>Orbital Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$s$</td>
</tr>
<tr>
<td>1</td>
<td>$p$</td>
</tr>
<tr>
<td>2</td>
<td>$d$</td>
</tr>
<tr>
<td>3</td>
<td>$f$</td>
</tr>
</tbody>
</table>

What are the possible $\ell$ values given the following $n$ values?

1. $n = 1$
2. $n = 2$
3. $n = 3$

What type of orbital is associated with the following quantum numbers?

1. $n = 1$ and $\ell = 0$
2. $n = 2$ and $\ell = 1$
3. $n = 3$ and $\ell = 0$

### Magnetic Quantum Number ($m_\ell$)

- **Related To:** Orientation in space (specifies exactly which orbital [e.g., $p_z$])
- **Allowed Values:** $\ell, \ell - 1, \ldots, 0, \ldots, -\ell$ (orbitals)

What are the possible values of $m_\ell$ given the following $n$ and $\ell$ values?

1. $n = 1$ and $\ell = 0$
2. $n = 2$ and $\ell = 1$
3. $n = 2$ and $\ell = 0$

### Electron Spin Quantum Number ($m_s$)

- **Related To:** Spin of the electron
- **Allowed Values:** $+\frac{1}{2}$ (spin up $\uparrow$) or $-\frac{1}{2}$ (spin down $\downarrow$)
Chapter 12: Quantum Mechanics and Atomic Theory

Orbitals

What does an s-orbital \((l = 0)\) look like?
- \(n = 1\) and \(l = 0\)
- \(R(r) = \frac{2e^{-r/a_0}}{a_0^{3/2}}\) (radial wavefunction)
- \(Y(\theta, \phi) = \frac{1}{2\pi}e^{i\nu}Y_{\ell}^m(\theta, \phi)\) (angular wavefunction)
- \(\psi(r, \theta, \phi) = \frac{2}{a_0^{3/2}}\frac{1}{2\pi}e^{i\nu}Y_{\ell}^m(\theta, \phi)\)
- \(\psi^2(r, \theta, \phi) = \frac{1}{a_0^{3/2}}e^{-2r/a_0}\)

The three s-orbitals \((l = 0)\) of lowest energy
- The simplest way of drawing an atomic orbital is as a boundary surface, a surface within which there is a high probability (typically 90%) of finding the electron. The darker the shaded region within the boundary surfaces, the larger the probability of the electron being found there.

Many-Electron Atoms

The electrons in many-electron atoms occupy orbitals like those of hydrogen but the energy of the orbitals differ.
- Differences between the many-electron orbital energies and hydrogen atom orbital energies:
  - The nucleus of the many-electron orbitals have more positive charge attracting the electrons, thus lowering the energy.
  - The electrons repel each other raising the energy.

The number of electrons in an atom affects the properties of the atom.

Potential Energy for He atom (2 p and 2 e)

\[
V = \frac{2}{4\pi \epsilon_0} \frac{2}{4\pi \epsilon_0} + \frac{e^2}{4\pi \epsilon_0 r_1 r_2}
\]

- \(r_1\) = distance between electron 1 and the nucleus
- \(r_2\) = distance between electron 2 and the nucleus
- \(r_{12}\) = distance between the two electrons

Note: If with 1 electron has no electron-electron repulsion and the electron will have the same energy if is the 2s or 2p orbital (all orbitals within one shell degenerate).
Many-Electron Atoms

Why do the energies change?

- **Shielding:** The repulsion experienced by an electron in an atom that arises from the other electrons present and opposes the attraction exerted by the nucleus.

- **Effective Nuclear Charge \((Z_{\text{eff}})\):** The net nuclear charge after taking into account the shielding caused by other electrons in the atom.

**Note:** s electrons can penetrate through the nucleus while p and d electrons cannot.

Order of Orbital Filling

- 1s
- 2s 2p
- 3s 3p 3d
- 4s 4p 4d 4f
- 5s 5p 5d 5f
- 6s 6p 6d 6f
- 7s 7p 7d 7f

**Electron Configuration:** A list of an atom’s occupied orbitals with the number of electrons that each contains.

- In the ground state, the electrons occupy atomic orbitals in such a way that the total energy of the atom is a minimum.
- We might expect that atoms would have all their electrons in the 1s orbital, however this is only true for H and He.

**Pauli Exclusion Principle:** No more than two electrons may occupy any given orbital. When two electrons occupy one orbital, the spins must be paired.

**Electronic Configurations:**

- **He**
  - Step 1:
  - Step 2:
  - Step 3:

- **Be**
  - Step 1:
  - Step 2:
  - Step 3:

**Writing Electron Configurations**

- **Step 1:** Determine the number of electrons the atom has.
- **Step 2:** Fill atomic orbitals starting with lowest energy orbitals first and proceeding to higher energy orbitals.
- **Step 3:** Determine how electrons fill the orbitals.

**Note:** Electrons that are farther apart repel each other less.

**Note:** Electrons with parallel spins tend to avoid each other more.
**Periodic Trends**

**Effective Nuclear Charge** \( (Z_{\text{eff}}) \) The net nuclear charge after taking into account the shielding caused by other electrons in the atom.

*Why*: Going across the periodic table, the number of core electrons stays the same but the number of protons increases. The core electrons are responsible for most of the shielding, therefore the \( Z_{\text{eff}} \) gets larger as you go across a period. Although going down a group adds more core electrons it also adds more protons therefore \( Z_{\text{eff}} \) is pretty much constant going down a group.

**Atomic Radii**: Half the distance between the centers of neighboring atoms in a solid of a homonuclear molecule.

*Why*: Going across a period the \( Z_{\text{eff}} \) increases, therefore the pull on the electrons increases and the atomic radii decrease. Going down a group, more atomic shells are added and the radii increase.

**First Ionization Energy**: The minimum energy required to remove the first electron from the ground state of a gaseous atom, molecule, or ion.

\[ X(g) \rightarrow X^+(g) + e^- \]

*Why*: Going across a period the \( Z_{\text{eff}} \) increases therefore it is harder to remove an electron and the first ionization energy increases. However, going down a group the electrons are located farther from the nucleus and they can be removed easier.

**Electron Affinity**: \( (E_{\text{ea}}) \) The energy released when an electron is added to a gas-phase atom.

\[ X(g) + e^- \rightarrow X^-(g) \]

*Why*: Going across a period the \( Z_{\text{eff}} \) increases therefore the atom has a larger positive charge and releases more energy when an electron is added to the atom. Going down a group the electron is added farther from the nucleus and the electron affinity decreases. This trend does not hold true for the noble gases.

Note: This trend has the most atoms that do not obey it.
Take Away From Chapter 12

- **Big Idea:** The structure of atoms must be explained using quantum mechanics, a theory in which the properties of particles and waves merge together.

- **Electromagnetic Radiation** (27)
  - Be able to change between frequency and wavelength
    \[ c = \lambda \nu \]
  - Be able to assign what area of the electromagnetic spectrum radiation comes from.

- **Quantum Theory**
  - Know that electromagnetic radiation has both wave and matter properties. (32)
  - Photoelectric effect (particle property) \([9,30,31]\)
  - Know what the wave function of a material is.
  - Diffraction (wave property)
  - Be able to calculate the energy carried in an electromagnetic wave (21)
  - \[ E = h \nu \]
  - Know that matter has both wave and matter properties.
  - Be able to calculate the wavelength of matter. \([34,36,37]\)
  - \[ \lambda = \frac{h}{p} \]
  - Know that the Heisenberg uncertainty principle determines the accuracy in which we can measure momentum and position. \([53]\)
  - \[ \Delta p \Delta x \geq \frac{\hbar}{2} \]

- **Orbitals**
  - Know that when atomic orbitals are drawn they represent the area in which e- have a 90% chance of being in. \([71]\)
  - Know the what s, p, and d orbitals look like.

- **Quantum Numbers** (62, 66, 68, 69, 78, 79)
  - Know that the quantum number \(n\) gives the size and energy
  - Allowed values of \(n = 1, 2, \ldots\)
  - Know that the quantum number \(l\) gives the orbital type (shape)
  - Allowed values of \(l = 0, 1, 2, \ldots, n - 1\)
  - Know that the quantum number \(m_l\) gives the orbital orientation (ex: p, )
  - Allowed values of \(m_l = -l, \ldots, 0, \ldots, l\)
  - Know that a fourth quantum number was needed to have theory match experiment, \(m_s\)
  - Allowed values of \(m_s = \pm \frac{1}{2}\) and \(\pm \frac{3}{2}\)

- **Particle in a Box**
  - Know that the wavefunction of different systems can be found using boundary conditions.
  - Particle in a box wavefunction \[ \psi = (\frac{\pi}{L})^{1/2} \sin \left( \frac{n \pi x}{L} \right) \]
  - Know that the square of the wavefunction tells us the probability of the particle being in a certain location. \([70]\)
  - Know that the Schrödinger equation allows us to match wavefunctions with allowed energy values.
  - Particle in a box \[ E = \frac{n^2 \pi^2}{L^2} \]

- **The Hydrogen Atom**
  - Know that when quantum mechanics is applied to 1 electron systems the observed energy and the theoretical energies match. \([44, 45, 46, 48, 50, 51, 147]\)
  - \[ E = -2.178 \times 10^{-18} (n^2) \]