Phenomena: Different wavelengths of electromagnetic radiation were directed onto two different metal sample (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>K</th>
<th>Exp.</th>
<th>Wavelength of Light Directed at Sample</th>
<th>Intensity</th>
<th>Where Particles Ejected</th>
<th>Ejected Particle</th>
<th>Speed of Ejected Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.4×10^-7 m</td>
<td>Medium</td>
<td>Yes</td>
<td>e^-</td>
<td>4.9×10^4 m/s</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>3.3×10^-8 m</td>
<td>High</td>
<td>Yes</td>
<td>e^-</td>
<td>3.5×10^6 m/s</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.0 m</td>
<td>High</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3.3×10^-8 m</td>
<td>Low</td>
<td>Yes</td>
<td>e^-</td>
<td>3.5×10^6 m/s</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2.0 m</td>
<td>Medium</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>6.1×10^-12 m</td>
<td>High</td>
<td>Yes</td>
<td>e^-</td>
<td>2.7×10^8 m/s</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>5.5×10^4 m</td>
<td>High</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fe</th>
<th>Exp.</th>
<th>Wavelength of Light Directed at Sample</th>
<th>Where Particles Ejected</th>
<th>Ejected Particle</th>
<th>Speed of Ejected Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.4×10^-7 m</td>
<td>Medium</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>2</td>
<td>3.4×10^-11 m</td>
<td>High</td>
<td>Yes</td>
<td>e^-</td>
<td>1.1×10^8 m/s</td>
</tr>
<tr>
<td>3</td>
<td>3.9×10^3 m</td>
<td>Medium</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>4</td>
<td>2.4×10^-8 m</td>
<td>High</td>
<td>Yes</td>
<td>e^-</td>
<td>4.1×10^6 m/s</td>
</tr>
<tr>
<td>5</td>
<td>3.9×10^3 m</td>
<td>Low</td>
<td>No</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>6</td>
<td>2.6×10^-7 m</td>
<td>Low</td>
<td>Yes</td>
<td>e^-</td>
<td>1.1×10^5 m/s</td>
</tr>
<tr>
<td>7</td>
<td>3.4×10^-11 m</td>
<td>Low</td>
<td>Yes</td>
<td>e^-</td>
<td>1.1×10^8 m/s</td>
</tr>
</tbody>
</table>
Chapter 12: Quantum Mechanics and Atomic Theory

- Electromagnetic Radiation
- Quantum Theory
- Particle in a Box
- The Hydrogen Atom
- Quantum Numbers
- Orbitals
- Many-Electron Atoms
- Periodic Trends

**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: Consists of oscillating (time-varying) electric and magnetic fields that travel through space at $2.998 \times 10^8 \frac{m}{s}$ (c = speed of light) or just over 660 million mph.

Note: All forms of radiation transfer energy from one region of space into another.

Examples of Electromagnetic Radiation:
- Visible light
- Radio Waves
- X-Rays
Electromagnetic Radiation

- **Wavelength** ($\lambda$): Is the peak-to-peak distance.

  \[ \text{Note: Changing the wavelength changes the region of the spectrum (i.e. x-ray to visible).} \]

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

- **Frequency** ($\nu$): The number of cycles per second ($1 \text{ Hz} = 1 \frac{1}{s}$).
Chapter 12: Quantum Mechanics and Atomic Theory

Electromagnetic Radiation

Wavelength in meters

$10^{-12}$  $10^{-10}$  $10^{-8}$  $4 \times 10^{-7}$  $7 \times 10^{-7}$  $10^{-4}$  $10^{-2}$  $1$  $10^2$  $10^4$

Gamma rays  X rays  Ultraviolet  Infrared  Microwaves  Radio waves

Size of:

Atomic nuclei  Atoms  Molecules

Visibility

Paper clip  Human  Buildings

FM  Shortwave  AM

$4 \times 10^{-7}$  $5 \times 10^{-7}$  $6 \times 10^{-7}$  $7 \times 10^{-7}$
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.
**Black Body:** An object that absorbs and emits all frequencies of radiation without favor.

**Heated Black Bodies**

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

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

Theory

- Scientists used classical physics arguments to derive an expression for the energy density (Rayleigh Jens Law).

\[
\text{Energy Density } \propto \frac{T}{\lambda^4}
\]

The Problem With Explaining Black Body Radiation Using Classical Mechanics

- Classical mechanics put no limits on minimum wavelength therefore at very small \( \lambda \), \( E \) would be a huge value even for low temperatures.
Quantum Theory

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

- **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 = $h \cdot \nu$
Quantum Theory

- **Photoelectric Effect**
  - Electromagnetic radiation consists of streams of photons traveling with frequency, $\nu$, and energy $h \cdot \nu$.
  - Photons collide with metal.
  - If the photons have enough energy, electrons will be removed from the metal.

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

**Note:** This relationship is not intensity dependent.
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 $4.0 \times 10^{-7} \text{ m}$?
Quantum Theory

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.
Quantum Theory

- **Finding energy levels of H atom**
  - \( \Delta E = E_{upper(2)} - E_{lower(1)} = h\nu_{emitted} \)
  - \( \nu_{emitted} = 3.29 \times 10^{15} \text{Hz} \left( \frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \) (Found experimentally)

**Note:** In this equation \( n_2 \) is always the large number which corresponds to the higher energy level.

- \(-h(3.29 \times 10^{15} \text{Hz}) \left( \frac{1}{n_2^2} - \frac{1}{n_1^2} \right) = -(6.626 \times 10^{-34} \text{J} \cdot \text{s})(3.29 \times 10^{15} \text{Hz}) \left( \frac{1}{n_2^2} - \frac{1}{n_1^2} \right)\)

**Note:** The negative sign appeared because a negative sign was taken out of parenthesis.

- \(-2.178 \times 10^{-18} J \left( \frac{1}{n_2^2} - \frac{1}{n_1^2} \right) = E_{upper(2)} - E_{lower(1)}\)

- **Energy level of H atom**
  - \( E = -2.178 \times 10^{-18} J \left( \frac{1}{n^2} \right) \quad n=1, 2, 3, \ldots \)

- **Energy level of other 1e⁻ systems**
  - \( E = -2.178 \times 10^{-18} J \left( \frac{Z^2}{n^2} \right) \quad n=1, 2, 3, \ldots \)
**Quantum Theory**

**Student Question**

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

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

a) $-1.664 \times 10^{24}$ m
b) $-5.399 \times 10^{-8}$ m
c) $1.621 \times 10^{-7}$ m
d) $4.864 \times 10^{-7}$ 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.
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.
Quantum Theory

Student Question

What is the wavelength of an electron traveling at \( \frac{1}{1000} \) the speed of light?

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

a) \( 2.42 \times 10^{-9} \text{ m} \)

b) \( 2.42 \times 10^{-12} \text{ m} \)

c) \( 4.12 \times 10^{11} \text{ m} \)

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.
Quantum Theory

- **Wavefunction ($\psi$):** A solution of the Schrödinger equation; the probability amplitude.  
  
  **Note:** This gives you a representation of the particle’s trajectory.

- **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.  
  
  **Examples:**  
  $\psi = \sin(x)$  
  
  **Note:** This value must be between 0 and 1.
Particle in a Box

Particle in a 1-D Box

- **Boundary Conditions**
  - $x = 0 \psi = 0$
  - $x = L \psi = 0$

- **What is the wavefunction?**
  - $\sin(x) (\sin(0) = 0 \text{ and } \sin(\pi) = 0)$
  - $\psi(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$

**Note:** $n$ is a quantum number. Quantum numbers are integers or $1/2$ integers that label a wavefunction.

**Note:** The term $\left(\frac{2}{L}\right)^{1/2}$ is there for normalization in order to get $\psi^2 = 1$.  

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Chapter 12: Quantum Mechanics and Atomic Theory

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Page 22
Particle in a Box

What are the allowed energy levels?

Get the allowed energy levels from Schrödinger’s equation

\[-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\]

Note: \( V(x) = 0 \) for the particle in a box

\[-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} = E\psi\]

Take 1\textsuperscript{st} derivative of \( \sin\left(\frac{n\pi x}{L}\right)\)

\[\frac{d}{dx}\left(\frac{d}{dx}\sin\left(\frac{n\pi x}{L}\right)\right) = \frac{d}{dx} \frac{n\pi}{L} \cos\left(\frac{n\pi x}{L}\right)\]

Take 2\textsuperscript{nd} derivative of \( \sin\left(\frac{n\pi x}{L}\right)\)

\[\frac{d}{dx} \frac{n\pi}{L} \cos\left(\frac{n\pi x}{L}\right) = -\left(\frac{2\pi}{L}\right)^2 \sin\left(\frac{n\pi x}{L}\right)\]
Plug 2nd derivative back into wavefunction

\[ \frac{\hbar^2}{2m} \left( \frac{2}{L} \right)^{1/2} \left( \frac{n\pi}{L} \right)^2 \sin \left( \frac{n\pi x}{L} \right) = E \left( \frac{2}{L} \right)^{1/2} \sin \left( \frac{n\pi x}{L} \right) \]

Cancel out

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

Simplify

\[ \hbar = \frac{h}{2\pi} \]

\[ E = \frac{\hbar^2}{2^2\pi^2 n^2 \pi^2} \frac{n^2 \pi^2}{2mL^2} = \frac{\hbar^2 n^2}{8mL^2} \]
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”
- \( \varphi \) = 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
General wavefunction expression for a hydrogen atom:
\[ \psi_{n\ell m}(r, \theta, \varphi) = \sqrt{\frac{(2\pi)^3}{n\lambda_0}} \frac{(n-\ell-1)!}{2n(n+\ell)!} e^{-\rho/2} \rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho) \cdot Y_{\ell m}(\theta, \varphi) \]

### Table 1.2 Hydrogen Wavefunctions (Atomic Orbitals), \( \psi = RY \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( l )</th>
<th>( R_{n\ell}(r) )</th>
<th>( l )</th>
<th>( m )</th>
<th>( Y_{\ell m}(\theta, \phi) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>( 2 \left( \frac{Z}{\lambda_0} \right)^{3/2} e^{-Zr/\lambda_0} )</td>
<td>0</td>
<td>0</td>
<td>( \left( \frac{1}{4\pi} \right)^{1/2} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{2\sqrt{2}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( 2 - \frac{Zr}{\lambda_0} \right) e^{-Zr/2\lambda_0} )</td>
<td>1</td>
<td>( x )</td>
<td>( \left( \frac{3}{4\pi} \right)^{1/2} \sin \theta \cos \phi )</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>( \frac{1}{2\sqrt{6}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( 2 - \frac{Zr}{\lambda_0} \right) e^{-Zr/2\lambda_0} )</td>
<td>( y )</td>
<td>( z )</td>
<td>( \frac{3}{4\pi} )</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>( \frac{1}{9\sqrt{3}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( 3 - \frac{Zr}{\lambda_0} + \frac{2Zr^2}{9\lambda_0^2} \right) e^{-Zr/3\lambda_0} )</td>
<td>( z )</td>
<td>( 0 )</td>
<td>( \frac{3}{4\pi} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{2\sqrt{6}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( 2 - \frac{Zr}{\lambda_0} \right) e^{-Zr/3\lambda_0} )</td>
<td>( xy )</td>
<td>( +2 )</td>
<td>( \frac{15}{16\pi} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{81\sqrt{30}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( \frac{Zr}{\lambda_0} \right)^{2} e^{-Zr/3\lambda_0} )</td>
<td>( yz )</td>
<td>( -1 )</td>
<td>( \frac{15}{16\pi} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{81\sqrt{30}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( \frac{Zr}{\lambda_0} \right)^{2} e^{-Zr/3\lambda_0} )</td>
<td>( zx )</td>
<td>( +1 )</td>
<td>( \frac{15}{16\pi} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{81\sqrt{30}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( \frac{Zr}{\lambda_0} \right)^{2} e^{-Zr/3\lambda_0} )</td>
<td>( x^2 - y^2 )</td>
<td>( -2 )</td>
<td>( \frac{15}{16\pi} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( \frac{1}{81\sqrt{30}} \left( \frac{Z}{\lambda_0} \right)^{3/2} \left( \frac{Zr}{\lambda_0} \right)^{2} e^{-Zr/3\lambda_0} )</td>
<td>( z^2 )</td>
<td>( 0 )</td>
<td>( \frac{5}{16\pi} )</td>
</tr>
</tbody>
</table>

Note: In each case, \( \lambda_0 = 4\pi\varepsilon_0^2m_e^2 \), or close to 52.9 pm; for hydrogen itself, \( Z = 1 \).

*In all cases except \( m_l = 0 \), the orbitals are sums and differences of orbitals with specific values of \( m_l \).*
The Hydrogen Atom

Schrödinger Equation for the H-atom

\[-\frac{\hbar^2}{2\mu r^2} \frac{1}{\sin \theta} \left[ \sin \theta \frac{d}{dr} \left( r^2 \frac{d\psi}{dr} \right) + \frac{d}{d\theta} \left( \sin \theta \frac{d\psi}{d\theta} \right) + \frac{1}{\sin \theta} \frac{d^2\psi}{d\phi^2} \right] + V(r)\psi = E\psi\]

- \( V(r) = \frac{(-e)(+e)}{4\pi \varepsilon_o r} = \frac{-e^2}{4\pi \varepsilon_o r} \)
- \( V(r) = \) Columbic potential energy between the proton and electron
- \( \mu = \) Reduced mass (proton and electron)

Scientists have solved for the energy of the H-atom

\[ E = \frac{-\hbar R}{n^2} = -2.178 \times 10^{-18} \frac{1}{n^2}, \quad R = \frac{m_e e^4}{8\hbar^3 \varepsilon_o^2} = 3.290 \times 10^{15} \text{Hz} \]

- \( n = \) principle quantum number can be 1, 2, 3, ...
- \( h = \) planks constant \( 6.62608 \times 10^{-34} \text{J} \cdot \text{s} \)
The Hydrogen Atom

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 $n = \infty$. 

[Diagram of energy levels with labels $0$, $-\frac{1}{9} \hbar R$, $-\frac{1}{4} \hbar R$, $-\hbar R$, $n = \infty$, $n = 3$, $n = 2$, $n = 1$, Balmer series, Lyman series]
**Principle Quantum Number** \( (n) \)

- Related To: Size and Energy
- Allowed Values: 1, 2, 3, ... (shells)

**Note:** The larger the \( n \), the larger the size, the larger the orbital, and the larger the energy.

**Note:** When identifying the orbital, the \( n \) value comes in front of the orbital type.

**Example:**

\[ 3p \quad n = 3 \]
Angular Momentum Quantum Number \((l)\)
- Related To: Shape
- Allowed Values: 0, 1, 2, ..., \(n - 1\) (subshells)

What are the possible \(l\) 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 \(l = 0\)
2) \(n = 2\) and \(l = 1\)
3) \(n = 3\) and \(l = 0\)
Quantum Numbers

**Magnetic Quantum Number** \((m_l)\)

- **Related To:** Orientation in space (specifies exactly which orbital [ex: \(p_x\)])
- **Allowed Values:** \(l, l - 1, \ldots, 0, \ldots, -l\) (orbitals)

What are the possible values of \(m_l\) given the following \(n\) and \(l\) values:

1) \(n = 1\) and \(l = 0\)
2) \(n = 2\) and \(l = 1\)
3) \(n = 2\) and \(l = 0\)
Quantum Numbers

Chapter 12: Quantum Mechanics and Atomic Theory

Note: The quantum number $m_l$ is an alternative label for the individual orbitals: in chemistry, it is more common to use x, y, and z instead.
Quantum Numbers

### TABLE 1.3 Quantum Numbers for Electrons in Atoms

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Values</th>
<th>Specifies</th>
<th>Indicates</th>
</tr>
</thead>
<tbody>
<tr>
<td>principal</td>
<td>$n$</td>
<td>1, 2, \ldots</td>
<td>shell</td>
<td>size</td>
</tr>
<tr>
<td>orbital angular momentum*</td>
<td>$l$</td>
<td>0, 1, \ldots, $n - 1$</td>
<td>subshell: $l = 0, 1, 2, 3, 4, \ldots$</td>
<td>shape</td>
</tr>
<tr>
<td>magnetic</td>
<td>$m_l$</td>
<td>$l, l - 1, \ldots, -l$</td>
<td>orbitals of subshell</td>
<td>orientation</td>
</tr>
<tr>
<td>spin magnetic</td>
<td>$m_s$</td>
<td>$+\frac{1}{2}, -\frac{1}{2}$</td>
<td>spin state</td>
<td>spin direction</td>
</tr>
</tbody>
</table>

*Also called the *azimuthal quantum number.*

- A summary of the arrangements of shells, subshells, and orbitals in an atom and the corresponding quantum numbers.
The following set of quantum numbers is not allowed: \( n = 3, l = 0, m_l = -2 \). Assuming that the \( n \) and \( m_l \) values are correct, change the \( l \) value to an allowable combination.

a) \( l = 1 \)
b) \( l = 2 \)
c) \( l = 3 \)
d) \( l = 4 \)
e) None of the Above
Quantum Numbers

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

- Related To: Spin of the electron
- Allowed Values: $\pm \frac{1}{2}$ (spin up $\uparrow$) or $-\frac{1}{2}$ (spin down $\downarrow$)
What does an s-orbital ($l = 0$) look like?

- $n = 1$ and $l = 0$

- $R(r) = \frac{2e^{-r/a_o}}{a_o^{3/2}}$ (radial wavefunction)

- $Y(\theta, \phi) = \frac{1}{2\pi^{1/2}}$ (angular wavefunction)

- $\psi(r, \theta, \phi) = \frac{2e^{-r/a_o}}{a_o^{3/2}} \cdot \frac{1}{2\pi^{1/2}} = \frac{e^{-r/a_o}}{(\pi a_o^3)^{1/2}}$

- $\psi^2(r, \theta, \phi) = \frac{e^{-2r/a_o}}{\pi a_o^3}$
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.
What do p-orbitals \((l = 1)\) look like?
What do d-orbitals \((l = 2)\) look like?
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.
Many-Electron Atoms

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

<table>
<thead>
<tr>
<th>Potential Energy for He atom (2 p and 2 e⁻)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Attraction of electron 1 to the nucleus</td>
</tr>
<tr>
<td>Attraction of electron 2 to the nucleus</td>
</tr>
<tr>
<td>Repulsion between the two electrons</td>
</tr>
</tbody>
</table>

\[ V = -\frac{2e^2}{4\pi\varepsilon_0 r_1} - \frac{2e^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0 r_{12}} \]

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

Note: H 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).
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_{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.

Amount of Shielding

<table>
<thead>
<tr>
<th>S</th>
<th>P</th>
<th>D</th>
<th>F</th>
</tr>
</thead>
</table>

Distance from nucleus

Chapter 12: Quantum Mechanics and Atomic Theory
Many-Electron Atoms

Order of Orbital Filling

1s  2s  2p  3s  3p  4s  3d  4p  5s  4d  5p
Many-Electron Atoms

- **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.

**Note:** Paired spins means $\uparrow$ and $\downarrow$ electron ($\uparrow\downarrow$)
Many-Electron Atoms

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.

<table>
<thead>
<tr>
<th>Subshell</th>
<th>l</th>
<th>Smallest n</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>p</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>d</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>f</td>
<td>3</td>
<td>4</td>
</tr>
</tbody>
</table>
Many-Electron Atoms

- **Electron Configurations:**
  - **He**
    - Step 1:
    - Step 2:
    - Step 3:
  - **Be**
    - Step 1:
    - Step 2:
    - Step 3:
Many-Electron Atoms

**Electron Configurations:**

- **C**
  - Step 1:
  - Step 2:
  - Step 3: __ __ __ 2p __ __ __ 2p __ __ __ 2p
    \[
    \uparrow \downarrow 2s \quad \uparrow \downarrow 2s \quad \uparrow \downarrow 2s \\
    \uparrow \downarrow 1s \quad \uparrow \downarrow 1s \quad \uparrow \downarrow 1s
    \]

**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.
Periodic Trends

- **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.
Periodic Trends

- **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.
1\textsuperscript{st} Ionization Energy Data

Why don’t B and Al fit the 1\textsuperscript{st} ionization energy trend?
Periodic Trends

- **Electron Affinity**: \( (E_{ea}) \)
  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 \( Z_{eff} \) 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.
Periodic Trends

Electron Affinity of the First 20 Elements

EA (kJ/mole)

Atomic Number

H, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ar

Chapter 12: Quantum Mechanics and Atomic Theory
**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.

Numbers correspond to end of chapter questions.
Take Away From Chapter 12

- **Quantum Theory**
  - Know that electromagnetic radiation has both wave and matter properties. (32)
    - Photo electric effect (particle property) (29,30,31)
    - Know what the work 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)
    - \( \lambda = \frac{h}{mv} \)
  - Know that the Heisenberg uncertainty principle determines the accuracy in which we can measure momentum and position. (53)
    - \( \Delta p \Delta x \geq \frac{1}{2} \hbar \)

Numbers correspond to end of chapter questions.
Chapter 12: Quantum Mechanics and Atomic Theory

Take Away From Chapter 12

- **Particle in a Box**
  - Know that the wavefunction of different systems can be found using boundary conditions.
  - Particle in a box wavefunction $\psi = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$
  - Know that the square of the wavefunction tells us the probability of the particle being in a certain location. (70)
  - Know the most likely location of a particle in a box (ex: $n = 1$ particle most likely in center of box, $n = 2$ particle most likely on sides of box)
  - Know that the Schrödinger equation allows us to match wavefunctions with allowed energy values.
  - Particle in a box $E = \frac{n^2\hbar^2}{8mL}$ (57,58,59,61)

- **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)
  - $E = -2.178 \times 10^{-18} \left(\frac{Z^2}{n^2}\right)$

Numbers correspond to end of chapter questions.
Take Away From Chapter 12

- **Quantum Numbers** \((62, 66, 68, 69, 78, 79)\)
  - Know that the quantum number \(n\) gives the size and energy
    - Allowed values of \(n = 1, 2, ...\)
  - 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: \(p_x\))
    - 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 \(m_s = +\frac{1}{2} and -\frac{1}{2}\)

Numbers correspond to end of chapter questions.
Take Away From Chapter 12

- **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.

- **Many-Electron Atoms**
  - Be able to write both the full and shorthand electron configurations of atoms. (80, 81, 84, 88, 96, 98)
  - Be able to predict the number of unpaired electrons in a system. (97)

- **Periodic Trends**
  - Know the trends of effective nuclear charge, atomic radii, ionization energy, and electron affinity. (13, 14, 103, 104, 106, 112, 114, 119, 120, 139)

Numbers correspond to end of chapter questions.