Quantum Theory and Atomic Structure

Chapter 7

7.1 The Nature of Light

7.2 Atomic Spectra

7.3 The Wave-Particle Duality of Matter and Energy

7.4 The Quantum-Mechanical Model of the Atom

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The wavelength, \( \lambda \), is the crest-to-crest-distance in space. The frequency, \( \nu \), is the number of times per second that a crest passes a given point on the x-axis.

Electric field is perpendicular to an oscillating magnetic field & both are perpendicular direction to both direction of propagation.

---

In 1873, Maxwell found that light is an electromagnetic wave that travels at the speed of light, \( c \).

\[
\text{speed of light} = c = \lambda \cdot \nu = 3.00 \times 10^8 \text{ m/sec}
\]

The **wavelength**, \( \lambda \), is the crest-to-crest-distance in space.

The **frequency**, \( \nu \), is the number of times per second that a crest passes a given point on the x-axis.

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The **wavelength**, \( \lambda \), is the crest-to-crest-distance in space of the waveform taken at an instant in time.

The amplitude, \( A \), of the electric field is the maximum disturbance of the waveform.

The **frequency**, \( \nu \), is the number of times per second that a crest passes any given point on the x-axis (units of 1/sec called Hertz = Hz).

It is related to the period (sec) of the wave by \( f = 1/T \)

The frequency and wavelength of a wave are connected by the speed of light:

\[
c = \lambda \cdot \nu = 3.00 \times 10^8 \text{ m/s}
\]
The wavelength ($\lambda$) of electromagnetic radiation is expressed in many different units of length...know the conversions between them.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Symbol</th>
<th>Length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Angstrom</td>
<td>Å</td>
<td>$10^{-10}$</td>
</tr>
<tr>
<td>Nanometer</td>
<td>nm</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>Micrometer</td>
<td>µm</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Millimeter</td>
<td>mm</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Centimeter</td>
<td>cm</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>Meter</td>
<td>m</td>
<td>1</td>
</tr>
</tbody>
</table>

Electromagnetic radiation exists over a broad range of frequencies.

<table>
<thead>
<tr>
<th>$\lambda$ (nm)</th>
<th>0.10</th>
<th>10</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
<th>$10^6$</th>
<th>$10^7$</th>
<th>$10^8$</th>
<th>$10^9$</th>
<th>$10^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$ (Hz)</td>
<td>$10^{20}$</td>
<td>$10^{19}$</td>
<td>$10^{18}$</td>
<td>$10^{17}$</td>
<td>$10^{16}$</td>
<td>$10^{15}$</td>
<td>$10^{14}$</td>
<td>$10^{13}$</td>
<td>$10^{12}$</td>
<td>$10^{11}$</td>
</tr>
</tbody>
</table>

Gamma X-rays UV IR Microwave Radio Waves

Sample Problem 7.1 Interconverting Wavelength and Frequency

A dental hygienist uses x-rays ($\lambda = 1.00\,\text{Å}$) to take a series of dental radiographs while the patient listens to a radio station ($\lambda = 325\,\text{cm}$) and looks out the window at the blue sky ($\lambda = 473\,\text{nm}$). What is the frequency (in s$^{-1}$) of the electromagnetic radiation from each source? (Assume that the radiation travels at the speed of light, $3.00 \times 10^8\,\text{m/s}$.)

$$c = \lambda \nu$$

$$1.00\,\text{Å} \times \frac{10^{-10}\,\text{m}}{1\,\text{Å}} = 1.00 \times 10^{-10}\,\text{m}$$

$$\nu = \frac{3 \times 10^8\,\text{m/s}}{1.00 \times 10^{-10}\,\text{m}} = 3 \times 10^{18}\,\text{s}^{-1}$$

$$325\,\text{cm} \times \frac{10^{-2}\,\text{m}}{1\,\text{cm}} = 325 \times 10^{-2}\,\text{m}$$

$$\nu = \frac{3 \times 10^8\,\text{m/s}}{325 \times 10^{-2}\,\text{m}} = 9.23 \times 10^{17}\,\text{s}^{-1}$$

$$473\,\text{nm} \times \frac{10^{-9}\,\text{m}}{1\,\text{nm}} = 473 \times 10^{-9}\,\text{m}$$

$$\nu = \frac{3 \times 10^8\,\text{m/s}}{473 \times 10^{-9}\,\text{m}} = 6.34 \times 10^{14}\,\text{s}^{-1}$$

Experiments over 300 years show that electromagnetic radiation (light) exhibits both wave-like and particle-like properties.

- **WAVE**
  - Waves “bend”
  - Beam of waves
  - Crests of waves

- **PARTICLE**
  - Trajectory of a pebble
  - Particles “fly straight”

Light can interact “constructively and destructively” interfere forming light and dark regions (fringes) on a wall.

**SINGLE SLIT**: When light is passed through a tiny single slit one bright line appears. No interference of light waves (particle like)!

**DOUBLE SLIT**: two slits spaced closely together a pattern of bright and dark appears showing that light is an wave that interferes.
It has been known since the 1600's that light acts like a wave; it can be diffracted by passing light through small slits producing an interference pattern.

In the early 1900's there were mysteries involving light and matter that the physicists could not explain including:

I. **Black-body Radiation Problem** - the frequencies and intensities of light emitted by heated solids at a given temperature.

II. The **Photo-Electric Effect** - the ejection of electrons from certain metals upon exposure of light depended on the frequency of light, not its intensity (how bright).

III. **Line Emission and Absorption Spectra** - compounds, gases emitted only emitted or absorb very specific frequencies (colors) of light.

**MYSTERY #2:** When a photoelectric tube is bombarded with electromagnetic radiation (light), only specific frequencies eject electrons from the surface of the light sensitive plate to generate current.

**Detailed Explanation of the Photoelectric Effect.**

- Light acts like a particle and are "quantized energy packets" called photons.
- 1 photon has energy \( E = h \nu \).
- Photon has to have a certain minimum energy to eject an electron from the metal.
- \( E = h \nu = KE + \text{Binding Energy} \)
- If a photon does not have enough energy no electrons are ejected no matter how intense the light is (the number of photons per unit time)
- Greater intensity of the wrong frequency (more photons) does not overcome the electron binding energy. It is the energy (frequency) and not the intensity that is key.

**Planck postulated that energy and matter exist in fixed quantities or “quanta” of energy and not continuous energy states.**

\[ E = n \ h \nu \]

\( n = \) whole number

\( h = \) Planck’s constant = \( 6.63 \times 10^{-34} \text{ J s} \)

Energy (joules)

Matter exists in quantized states as opposed to continuous set of energy states.

Light can be absorbed from \( n = 1 \) to any other higher \( n \). Light can be emitted if electron falls from one level to another.

It can also be emitted from one \( n \) to another.
Learning Check: Photon-Energy and Photo Electric Effect Work-Function Calculations

1. Calculate the energy, in joules per photon, of radiation that has a frequency of $4.77 \times 10^{14}$ s$^{-1}$.

$$E = h\nu = 6.63 \times 10^{-34} \text{ J s} \times 4.77 \times 10^{14} \text{ s}^{-1} = 3.16 \times 10^{-19} \text{ J}$$

2. If the energy of an infrared krypton laser is $2.484 \times 10^{-19}$ joules per photon, determine the wavelength of the radiation.

$$E = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J s})(3.00 \times 10^{8} \text{ m/s})}{2.484 \times 10^{-19} \text{ J}} = 8.01 \times 10^{-7} \text{ m}$$

3. Calculate the maximum kinetic energy of an electron ejected by the photon in part (b) from a metal with a binding energy of 3.7 eV.

$$KE = E - Binding \text{ Energy} = 8.01 \times 10^{-7} \text{ J} - 5.19 \times 10^{-19} \text{ J} = 8.01 \times 10^{-7} \text{ J}$$

MYSTERY #3: Narrow bands of colors of light are emitted when gases are excited by high voltage in a tube. The colors are characteristic and reproducible for different elements.

Classical physics predicts a "continuous spectrum" (top). We observe discrete wavelengths, however, which correspond to discrete energy levels. These levels are "quantized".

All elements display a characteristic emission spectra that we can use to fingerprint all elements.

<table>
<thead>
<tr>
<th>Element</th>
<th>Spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>alkali metals</td>
</tr>
<tr>
<td>Na</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td></td>
</tr>
<tr>
<td>Ca</td>
<td></td>
</tr>
<tr>
<td>Sr</td>
<td></td>
</tr>
<tr>
<td>Ba</td>
<td></td>
</tr>
<tr>
<td>Zn</td>
<td></td>
</tr>
<tr>
<td>Cd</td>
<td></td>
</tr>
<tr>
<td>Hg</td>
<td></td>
</tr>
<tr>
<td>He</td>
<td></td>
</tr>
<tr>
<td>Ne</td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td></td>
</tr>
</tbody>
</table>

Wavelength (not scaled)

The first explanations of the emission spectra were empirical (i.e. some old dudes found an equation that worked, but without any explanation behind it).

In 1885 Balmer developed an empirical mathematical relationship between $\nu$ and $n$ for the visible lines of hydrogen emission spectrum.

**Balmer equation**

$$\lambda (\text{nm}) = 364.56 \left( \frac{n^2}{n^2 - 2^2} \right)$$

In 1885 Johann Rydberg developed a generalized but empirical mathematical relationship between $\nu$ and $n$ for all lines of hydrogen emission spectrum! This is freaky!

**Rydberg equation**

$$\frac{1}{\lambda} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

In 1913, scientist Neils Bohr explains the emission spectrum of hydrogen using a quantized planetary model.

1. $e^-$ can only have specific (quantized) energy values (planetary like orbits around nucleus)

2. light emission occurs when $e^-$ moves from a higher energy level to a lower energy level (high $n$ to low $n$)

3. the energy of a level: $E_n = -R_H \left( \frac{1}{n^2} \right)$

4. the difference in energy between any two levels:

$$\Delta E = \hbar\nu = R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

Bohr postulates that light is emitted when an $e^-$ goes from an orbit with a high $n$ value to a lower $n$ value.

The gas is excited by voltage generating light that is dispersed into its component wavelengths by a prism and projected on a screen.
The Bohr model explains all of the emission spectral lines of hydrogen as “quantized jumps” between the various n “energy levels”.

\[
E_{\text{photon}} = h \nu = \Delta E_{\text{atom}} \\
E_{\text{photon}} = E_f - E_i \\
E_f = -R_H \left( \frac{1}{n_f^2} \right) \\
E_i = -R_H \left( \frac{1}{n_i^2} \right) \\
\Delta E = R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)
\]

The Bohr’s model works for hydrogen, but could not explain the emission spectra of other atoms. Classical physics also says that electrons can not accelerate around a nucleus without eventually collapsing into the nucleus (i.e. simple planetary motion of e- around a nucleus fails).

How and why is e- energy quantized and what physics can explain it?

In 1924, Louis DeBroglie reasoned that if light wave could act like a particle then perhaps a particle could act like a wave.

He connects Planck’s Law to Einstein’s energy-mass equivalence equation.

\[
E = h \nu = \frac{hc}{\lambda} = mc^2
\]

Solving for wavelength, substituting \( v = \) velocity for \( c \) and watching our units……..we get the de Broglie equation:

\[
\lambda = \frac{h}{mv}
\]

It says that all particle of mass \( m \), moving at velocity \( v \) have an associated wavelike wavelength!

We only observe wavelike properties of particles when the mass is tiny (electron). Macroscopic objects give de Broglie wavelengths that are too small to be observed.

\[
\lambda = \frac{h}{mv}
\]

<table>
<thead>
<tr>
<th>Substance</th>
<th>Mass (g)</th>
<th>Speed (m/s)</th>
<th>de Broglie ( \lambda ) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>slow electron</td>
<td>9 x 10^{-28}</td>
<td>1.0</td>
<td>7x10^{-10} \text{ Observable}</td>
</tr>
<tr>
<td>fast electron</td>
<td>9 x 10^{-28}</td>
<td>5.9 x 10^{6}</td>
<td>1x10^{-10}</td>
</tr>
<tr>
<td>alpha particle</td>
<td>6.6 x 10^{-24}</td>
<td>1.5 x 10^{7}</td>
<td>7x10^{-15}</td>
</tr>
<tr>
<td>one-gram mass</td>
<td>1.0</td>
<td>0.01</td>
<td>7x10^{-29}</td>
</tr>
<tr>
<td>baseball</td>
<td>120</td>
<td>25.0</td>
<td>1.2x10^{-34} \text{ Not Observable}</td>
</tr>
<tr>
<td>Earth</td>
<td>6.0 x 10^{27}</td>
<td>3.0x10^{4}</td>
<td>4x10^{-43}</td>
</tr>
</tbody>
</table>

The wave-like properties only manifest when mass is small and high velocity! e- that move at high speeds.

Calculate the wavelength (in nm) of a photon emitted by a hydrogen atom when its electron drops from the \( n = 5 \) state to the \( n = 3 \) state.

\[
E_{\text{photon}} = \Delta E = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \\
E_{\text{photon}} = 2.18 \times 10^{-18} \text{ J} \times (1/25 - 1/9) \\
E_{\text{photon}} = -1.55 \times 10^{-19} \text{ J} \\
E_{\text{photon}} = h \times c / \lambda \\
\lambda = h \times c / E_{\text{photon}} \\
\lambda = 6.63 \times 10^{-34} \text{ (J s)} \times 3.00 \times 10^{8} \text{ (m/s)} / 1.55 \times 10^{-19} \text{ J} \\
\lambda = 1280 \text{ nm}
\]

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\]

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What is the de Broglie wavelength (in meters) of: a) pitched baseball with a mass of 120. g and a speed of 100 mph or 44.7 m/s and b) an electron with a speed of 1.00 x 10^{6} m/s (electron mass = 9.11 x 10^{-31} kg; \( h = 6.626 \times 10^{-34} \text{ kg m}^2/\text{s} \)).

Baseball:

\[
\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ kg m}^2/\text{s}}{(0.120 \text{ kg}) (44.7 \text{ m/s})} = 1.24 \times 10^{-34} \text{ m}
\]

Electron:

\[
\lambda = \frac{6.626 \times 10^{-34} \text{ kg m}^2/\text{s}}{(9.11 \times 10^{-31} \text{ kg})(1.00 \times 10^{6} \text{ m/s})} = 7.27 \times 10^{-10} \text{ m}
\]
Soon after de Broglie’s theory was put forth it was found that e⁻ particles (which were thought to have only particle-like properties) could be made to diffract and interfere just like light waves.

The Heisenburg Uncertainty Principle

The act of measuring where an electron is changes what we measure. We can never know precisely where an electron is only a “probability” of where it may be in space.

\[ \Delta x \Delta p \geq \frac{\hbar}{4\pi} \]

\( \Delta x \) = position uncertainty

\( \Delta p \) = momentum uncertainty \((p = mv)\)

\( \hbar \) = Planck’s constant

A photon of light impinging on an electron would collide with an electron and alter its position or momentum.

Erwin Schrodinger, an Austrian physicist puts forth an equation that describes position and time dependence of an electron in hydrogen. It’s called the “Schrödinger wave equation”.

Schrödinger’s equation is a difficult partial differential equation. It is the framework for all of quantum mechanics!

\[ -\frac{\hbar^2}{8\pi^2m_e} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(x,y,z) - \frac{Ze^2}{r} \Psi(x,y,z) = E\Psi(x,y,z) \]

\( \Psi(x,y,z) \) = wave function

\( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \) = potential energy at x,y,z

\( \frac{Ze^2}{r} \) = how \( \Psi \) changes in space

\( E \) = total quantized energy of the atomic system

1) change of coordinates
2) solve the differential equation

Erwin Schrödinger

Schrodinger’s equation is easier to solve if we transform the x,y,z coordinate system to spherical coordinates: \( r, \theta, \phi \).

The solution to this equation gives rise to function that specify 3 “quantum numbers” associated with an electron’s energy levels that we call orbitals.

The Schrödinger equation gives rise to functions that specify “3-quantum numbers” that completely describe electrons in space. Here they are:

<table>
<thead>
<tr>
<th>( n )</th>
<th>( l )</th>
<th>( m )</th>
<th>( \Psi_{n,m} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>( \Psi_{100} = \frac{1}{\sqrt{\pi}} e^{-r^2} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>( \Psi_{200} = \frac{1}{2\sqrt{\pi}} e^{-r^2} (2r) )</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>( \Psi_{210} = \frac{1}{2\sqrt{\pi}} e^{-r^2} \cos \theta )</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>( \pm 1 )</td>
<td>( \Psi_{211} = \frac{1}{2\sqrt{\pi}} e^{-r^2} \sin \theta )</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>( \Psi_{300} = \frac{1}{24 \sqrt{\pi}} e^{-r^2} (27 - 18r^2 + 2r^4) )</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>( \Psi_{310} = \frac{1}{8 \sqrt{\pi}} e^{-r^2} (12 - 8r^2 + r^4) \cos \theta )</td>
</tr>
</tbody>
</table>

A solution to the Schrödinger wave equation, \( \psi(x,y,z) \) is called an wavefunction or an atomic orbital. It’s a mathematical function that describes an electron in an H atom. It has no physical meaning except when it is squared \( |\psi(x,y,z)|^2 \) (like the square of electric field in light).

Guitar strings (a) can only vibrate at certain wavelengths (frequencies). If we apply this situation to electrons around a nucleus (b) then only certain whole number wavelengths would be allowed—it is quantized. Non-allowed “states” cannot be observed.
What does the Schrödinger Equation Tell Us?

1. The solutions of the Schrödinger equation for the hydrogen atom is a list of functions called "wavefunctions" or "orbitals" that completely describe the spatial location and energy of an electron in a hydrogen atom.

2. Electrons in atoms, elements and molecules exist in discrete quantized "states" that are mathematically described by a "wavefunction" or "orbital".

3. The "wavefunctions" or "orbitals" is specified by 3 quantum numbers n, l, m.

4. The wavefunction $\psi(r, \theta, \phi)$ by itself is not a physically measurable quantity, but the square of the wavefunction is.

Hydrogen atoms are shot through a strong magnet. It is found that the atoms at the collection plate are split into two groups of atoms. The results show that electron spins must be quantized as if they were not one would expect a continuous rectangular patch extending dot to dot (continuous energy as in classical physics).

The wavefunction with its 4-quantum numbers specify all the information we can know about electrons around a nucleus. Chemists call this the "electronic structure of an atom".

What the Quantum Numbers Mean

1. **principal quantum number (n) or SHELL**: Defines the size and energy level of the orbital. 
   
   $n = \{1, 2, 3, 4, \ldots\}$. ($n = 1$ = K shell; $n = 2$ = L shell; $n = 3$ = M shell

2. **angular momentum quantum number (l) or SUBLEVEL**: Defines the "shape" of the orbital or volume in space where the electron is likely to be found. Also called a subshell.

   $l = \{0, 1, 2, 3, \ldots \text{up to a maximum of } n-1\}$ where (0 = s, 1 = p, 2 = d, 3 = f)

3. **magnetic quantum number (m):** Defines the spatial orientation of an orbital of the same energy.

   $m = \{-l, 0, +l\}$

4. **magnetic spin quantum number (m_s):** Defines the orientation of "electron spin".

   $m_s = \{+1/2 \text{ or } -1/2\}$

Simple Summary of Quantum Numbers

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Permitted Values</th>
<th>Property</th>
</tr>
</thead>
<tbody>
<tr>
<td>principal</td>
<td>n</td>
<td>positive integers (1,2,3,...)</td>
<td>orbital energy (size)</td>
</tr>
<tr>
<td>angular momentum</td>
<td>l</td>
<td>integers from 0 to n-1</td>
<td>orbital shape (0, 1, 2, and 3 correspond to s, p, d, and f orbitals, respectively.)</td>
</tr>
<tr>
<td>magnetic</td>
<td>m_l</td>
<td>integers from -l to 0 to +l</td>
<td>orbital orientation in space</td>
</tr>
<tr>
<td>spin</td>
<td>m_s</td>
<td>+1/2 or -1/2</td>
<td>direction of e^* spin</td>
</tr>
</tbody>
</table>

Allowed Values of Quantum Numbers n, l and m_s

<table>
<thead>
<tr>
<th>When n is</th>
<th>l can be</th>
<th>When l is</th>
<th>m_s can be</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>only 0</td>
<td>0</td>
<td>only 0</td>
</tr>
<tr>
<td>2</td>
<td>0 or 1</td>
<td>0</td>
<td>only 0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>-1, 0, or +1</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0, 1, or 2</td>
<td>1</td>
<td>-1, 0, or +1</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-2, -1, 0, +1, or +2</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0, 1, 2, or 3</td>
<td>0</td>
<td>only 0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>-1, 0, or +1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-2, -1, 0, +1, or +2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-3, -2, -1, 0, +1, +2, or +3</td>
<td></td>
</tr>
</tbody>
</table>
4 quantum numbers will describe each electron in an atom. The order of filling of the orbitals must be remembered using a mnemonic device. We are building toward the electronic configuration of atoms.

A shell describes the n quantum number (n = 1 ⇔ K shell; n = 2 ⇔ L shell and so on).

A subshell refers to a specific n, l quantum number set: a 2s subshell or 2p subshell, or 3s subshell, or 3d subshell. Study the table.

Determining Quantum Numbers from Orbital Diagrams

Write a set of quantum numbers for the third electron and a set for the eighth electron of the F atom.

Use the orbital diagram to find the third and eighth electrons.

SOLUTION:
The third electron is in the 2s orbital. Its quantum numbers are:
\( n = 2 \), \( l = 0 \), \( m_l = 0 \), \( m_s = \pm \frac{1}{2} \)
The eighth electron is in a 2p orbital. Its quantum numbers are:
\( n = 2 \), \( l = 1 \), \( m_l = -1, 0, +1 \), \( m_s = \pm \frac{1}{2} \)

Determining Quantum Numbers for an Energy Level

1) Name the 4 quantum numbers and say what they mean?
2) How many quantum numbers are needed to specify an atomic orbital for an electron?
3) What values of the angular momentum (\( l \)) and magnetic (\( m_l \)) quantum numbers are allowed for a principal quantum number \( n = 3 \) and \( n = 4 \)?
4) How many orbitals are allowed for \( n = 3 \) and \( n = 4 \)?

There are 16 \( m_l \) values and therefore 16 orbitals with \( n = 4 \).

Determining Sublevel Names and Orbital Quantum Numbers

Give the orbital name, possible magnetic quantum numbers, and number of orbitals and number of electrons held in a sublevel with the following quantum numbers:

(a) \( n = 3 \), \( l = 2 \)
(b) \( n = 2 \), \( l = 0 \)
(c) \( n = 5 \), \( l = 1 \)
(d) \( n = 4 \), \( l = 3 \)

SOLUTION:

Determine Quantum Numbers for an Energy Level

1) Name the 4 quantum numbers and say what they mean?
2) How many quantum numbers are needed to specify an atomic orbital for an electron?
3) What values of the angular momentum (\( l \)) and magnetic (\( m_l \)) quantum numbers are allowed for a principal quantum number \( n = 3 \) and \( n = 4 \)?
4) How many orbitals are allowed for \( n = 3 \) and \( n = 4 \)?

**PLAN:** remember \( l \) values can be integers from 0 to \( n-1 \); \( m_l \) can be integers from \(-l\) through 0 to \(+l\).

**SOLUTION:**
For \( n = 3 \), \( l = 0, 1, 2 \)
For \( n = 4 \), \( l = 0, 1, 2, 3 \)
For \( l = 0 \) \( m_l = 0 \)
For \( l = 1 \) \( m_l = -1, 0, +1 \)
For \( l = 2 \) \( m_l = -2, -1, 0, +1, +2 \)
For \( l = 3 \) \( m_l = -3, -2, -1, 0, +1, +2, +3 \)

There are 9 \( m_l \) values and therefore 9 orbitals with \( n = 3 \).
There are 16 \( m_l \) values and therefore 16 orbitals with \( n = 4 \).
SAMPLE PROBLEM 7.7 Identifying Incorrect Quantum Numbers

Problem What is wrong with each of the following quantum number designations and/or sublevel names?

<table>
<thead>
<tr>
<th>n</th>
<th>l</th>
<th>m_l</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1p</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>-1</td>
<td>4d</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>-2</td>
<td>3p</td>
</tr>
</tbody>
</table>

Solution
(a) A sublevel with n = 1 can have only l = 0, not l = 1. The only possible sublevel name is 1s.
(b) A sublevel with l = 3 is an f sublevel, not a d sublevel. The name should be 4f.
(c) A sublevel with l = 1 can have only m_l of -1, 0, +1, not -2.

FOLLOW-UP PROBLEM 7.7 Supply the missing quantum numbers and sublevel names.

<table>
<thead>
<tr>
<th>n</th>
<th>l</th>
<th>m_l</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>0</td>
<td>4p</td>
<td>n = 4, l = 1</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>2p</td>
<td>n = 2, l = 0, m_l = +1/2</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>3d</td>
<td>n = 3, l = 0, m_l = 0</td>
</tr>
<tr>
<td>?</td>
<td>?</td>
<td>2s</td>
<td>n = 2, l = 0, m_l = +1/2</td>
</tr>
</tbody>
</table>

How many 2p orbitals are there in an atom?

If l = 1, then m_l = -1, 0, or +1

3 orbitals

If two electrons can be placed in one orbital how many electrons can go exist in the 3d subshell?

If l = 2, then m_l = -2, -1, 0, +1, or +2

5 orbitals which can each holding 2 electrons for a total of 10 e⁻ in the subshell

n=3 l = 2

Ψ has no physical meaning or reality (it’s only a function). Ψ² represents the probability function for finding an electron. We can integrate the function to get the total probability of finding an electron.

Ψ = Mathematical Construct

Ψ² = Probability Density

The square of the wavefunction Ψ² is the probability density: a measure of the probability of finding an electron in a region of space.

Probability density at point r in space

Radial probability distribution of points added up in a circular strips of (r + rdr)

s-orbital shape “3-D Boundary Surface Plot” where electron spends 90% of its time

Radial Probability Distribution Plots

Probability Density Plots

Quantum Number Allowed Values Possible Orbitals

<table>
<thead>
<tr>
<th>n</th>
<th>Positive integers</th>
<th>1, 2, 3, 4,...</th>
</tr>
</thead>
<tbody>
<tr>
<td>l</td>
<td>0 up to max of n-1</td>
<td>0, 1, 0, 1,</td>
</tr>
<tr>
<td>m_l</td>
<td>-l,...0...,+l</td>
<td>0, -1, 0, 1,</td>
</tr>
</tbody>
</table>

Orbital Name

Shapes or Boundary Surface Plots

1s 2s 2p 3s 3p 3d
The shape of an orbital is given by the “l” quantum number \( l = \{0,1,2 \text{ up to } n-1\} \). The number of orbitals and its orientation in space is given by the angular momentum quantum number \( m_l \{ -l, \ldots 0, \ldots +l \} \).

- **l = 0**: s orbital
- **l = 1**: p orbital
- **l = 2**: d orbital
- **l = 3**: f orbital

The 3 p \((l = 1)\) orbital Boundary Surface Plots (Shapes)

- Three p-orbitals superimposed

The Five d-orbital \((l = 2)\) Boundary Surface Plots (Shapes)

- Five d-orbitals superimposed

The Seven f-orbital \((l = 3)\) Boundary Surface Plots (Shapes)

The “Aufbau Process” is used to generate the electronic configuration of elements filling the lowest energy orbitals sequentially.

1. Lower energy orbitals fill first.
2. **Hund's Rule**: degenerate (i.e. orbitals with the same energy) orbitals fill one at a time before electrons are paired in an orbital.
3. **Pauli Exclusion Principle**: No two electrons in an atom can have the same 4-quantum numbers.

Electrons fill the lowest energy orbitals first, 2 at a time!

Chemists use *spdf notation* and *orbital box diagrams* to denote or show the “ground state electronic configuration” of elements.

<table>
<thead>
<tr>
<th>Element</th>
<th>spdf Notation</th>
<th>orbital box diagram</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s(^1)</td>
<td><img src="1sDiagram.png" alt="" /></td>
</tr>
<tr>
<td>He</td>
<td>1s(^2)</td>
<td><img src="1s2Diagram.png" alt="" /></td>
</tr>
</tbody>
</table>

An arrow denotes an electron with "spin up" or "spin-down".

Remember, no two electrons can have the same 4-quantum numbers!
Building electronic configuration using Aufbau and Hund

<table>
<thead>
<tr>
<th>Atomic Number/Element</th>
<th>Orbital Box Diagram</th>
<th>Full-electronic configuration</th>
<th>Condensed-electronic configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s</td>
<td>1s</td>
<td>[He]</td>
</tr>
<tr>
<td>He</td>
<td>1s 2s</td>
<td>1s^2</td>
<td>[He]2s^1</td>
</tr>
<tr>
<td>Li</td>
<td>1s 2s</td>
<td>1s^2</td>
<td>[He]2s^1</td>
</tr>
<tr>
<td>Be</td>
<td>1s 2s</td>
<td>1s^2</td>
<td>[He]2s^2</td>
</tr>
</tbody>
</table>

Atomic Number/Element | Orbital Box Diagram | Full-electronic configuration | Condensed-electronic configuration |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>1s 2s 2p</td>
<td>1s^2 2s^2 2p^1</td>
<td>[He]2s^2 2p^1</td>
</tr>
<tr>
<td>C</td>
<td>1s 2s 2p</td>
<td>1s^2 2s^2 2p^2</td>
<td>[He]2s^2 2p^2</td>
</tr>
<tr>
<td>N</td>
<td>1s 2s 2p 3s</td>
<td>1s^2 2s^2 2p^3</td>
<td>[He]2s^2 2p^3</td>
</tr>
<tr>
<td>O</td>
<td>1s 2s 2p 3s 3p</td>
<td>1s^2 2s^2 2p^4</td>
<td>[He]2s^2 2p^4</td>
</tr>
<tr>
<td>F</td>
<td>1s 2s 2p 3s 3p 4s</td>
<td>1s^2 2s^2 2p^5</td>
<td>[He]2s^2 2p^5</td>
</tr>
<tr>
<td>Ne</td>
<td>1s 2s 2p 3s 3p 4s</td>
<td>1s^2 2s^2 2p^6</td>
<td>[He]2s^2 2p^6</td>
</tr>
</tbody>
</table>

*Colored type indicates sublevel to which last electron is added.

Atomic Number/Element | Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only) | Full Electron Configuration | Condensed Electron Configuration |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>19 K</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>20 Ca</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>21 Sc</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>22 Ti</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>23 V</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>24 Cr</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>25 Mn</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>26 Fe</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>27 Co</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
<tr>
<td>28 Ni</td>
<td>4s</td>
<td>[Ar]</td>
<td>[Ar]</td>
</tr>
</tbody>
</table>

*Colored box indicates sublevel to which last electron is added.