WAVE FUNCTIONS, $\Psi$

- $\Psi$ is a function of the electron’s position in the atom.
- Each $\Psi$ corresponds to an ORBITAL — the region of space within which an electron is found.
- $\Psi$ does NOT describe the exact location of the electron.
- $\Psi^2$ is proportional to the probability of finding an e- at a given location.

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Uncertainty Principle

The last item, the definition of probability rather than absolute location, is a concept that is foreign to us.

A description of the nature of electrons in atoms was proposed by Heisenberg: the uncertainty principle.

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Uncertainty Principle

The principle: One cannot simultaneously define both the position and momentum (= m•v) of an electron (note that momentum and energy both increase with m and v).

In atoms we define e⁻ energy exactly but accept the limitation that we do not know exact position.

QUANTUM NUMBERS

Quantum numbers describing the discrete states of the electron in an atom arise naturally from the mathematics of the Schrödinger equation:

Each orbital is characterized by 3 quantum numbers:

n, l, and ml

Electrons are arranged in shells and subshells.

n → designates a shell
l → designates a subshell within a shell
ml → designates an orbital within a subshell
QUANTUM NUMBERS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Values</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>n (major)</td>
<td>1, 2, 3, ..</td>
<td>Orbital size and energy where $E = -\frac{\hbar c}{n^2}$</td>
</tr>
<tr>
<td>l (angular)</td>
<td>0, 1, 2, .. n-1</td>
<td>Orbital shape or type (subshell)</td>
</tr>
<tr>
<td>$m_l$ (magnetic)</td>
<td>-l..0..+l</td>
<td>Orbital orientation</td>
</tr>
</tbody>
</table>

# of orbitals in subshell = $2l + 1$

Shells and Subshells

When $n = 1$, then $l = 0$ and $m_l = 0$

Therefore, in $n = 1$, there is 1 type of subshell.

- That subshell has a single orbital
  ($m_l$ has a single value $\Rightarrow$ 1 orbital)
- This subshell is labeled $s$
- Each shell has 1 orbital labeled $s$, and it is SPHERICAL in shape.
s Orbitals

See Figure 7.14 and screens 7.12 and 7.13 on the CD-ROM.

1s Orbital

Gives the probability

3s Orbital

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**p Orbitals**

When \( n = 2 \), then \( l = 0 \) or \( 1 \)

Therefore, in \( n = 2 \) shell there are 2 types of orbitals — 2 subshells

For \( l = 0 \) \( m_l = 0 \).
- this is an s subshell

For \( l = 1 \) \( m_l = -1, 0, +1 \)
- this is a p subshell with 3 orbitals

See CD-ROM screens 7.11 and 7.13

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**2p\textsubscript{x} Orbital**  **3p\textsubscript{x} Orbital**

The 3 p orbitals align along the 3 Cartesian axes, \( \perp \) to each other.
When n = 3, what are the values of l?

l = 0, 1, 2

and so there are 3 subshells in the shell.

For l = 0, m_l = 0
→ s subshell with single orbital

For l = 1, m_l = -1, 0, +1
→ p subshell with 3 orbitals

For l = 2, m_l = -2, -1, 0, +1, +2
→ d subshell with 5 orbitals

s orbitals have no planar node (l = 0) and so are spherical.
p orbitals have l = 1, and have 1 planar node and so are “dumbbell” shaped.

This means d orbitals (with l = 2) have 2 planar nodes

See Figure 7.16
When $n = 4$, $l = 0, 1, 2, 3$ so there are 4 subshells in the shell.

For $l = 0$, $m_l = 0$
\[ \rightarrow \text{s subshell with single orbital} \]

For $l = 1$, $m_l = -1, 0, +1$
\[ \rightarrow \text{p subshell with 3 orbitals} \]

For $l = 2$, $m_l = -2, -1, 0, +1, +2$
\[ \rightarrow \text{d subshell with 5 orbitals} \]

For $l = 3$, $m_l = -3, -2, -1, 0, +1, +2, +3$
\[ \rightarrow \text{f subshell with 7 orbitals} \]