**3-dimensional Hydrogen atom**

Bohr model:
- Considered only circular orbits
- Found 1 quantum number \( n \)
- Energy \( E_n = -\frac{13.6}{n^2} \text{eV} \), orbit radius \( r_n = \frac{n^2}{\alpha_o} \)

From 3-D particle in box, expect that:
- H atom should have more quantum numbers
- Expect different types of motion w/ same energy

Modified Bohr model

- Different orbit shapes
- \( L = r \times p \)
- These orbits have same energy, but different angular momenta:
  - (Large angular momentum)
  - (Small angular momentum)
  - Rank the angular momenta from largest to smallest:
    - a) A, B, C
    - b) C, B, A
    - c) B, C, A
    - d) B, A, C
    - e) C, A, B

**Angular momentum is quantized: orbital quantum number \( \ell \)**

Angular momentum quantized \( |\mathbf{L}| = \hbar \sqrt{(\ell + 1)} \), \( \ell \) is the orbital quantum number

For a particular \( n \), \( \ell \) has values 0, 1, 2, ... \( n-1 \)
- \( \ell = 0 \), most elliptical
- \( \ell = n-1 \), most circular

For hydrogen atom, all have same energy

**Orbital magnetic dipole moment**

- Angular momentum \( \mathbf{L} \)
- Perpendicular to orbital plane

Orbiting electron produces a current loop

Current loop produces magnetic dipole moment \( \mathbf{\mu} \) along \( \mathbf{L} \)

\( |\mathbf{\mu}| = \mu_0 |\mathbf{L}| \hbar / 2 \)

\( \mu_0 = \frac{e \hbar}{2m} = 0.927 \times 10^{-23} \text{A} \cdot \text{m}^2 \)
3D Hydrogen atom so far...

Each orbit \((n,l)\) has
- Same energy: \(E_n = -13.6/n^2\ eV\)
- Different orbit shape (angular momentum): \(L = \hbar \sqrt{(l+\frac{1}{2})}\)
- Different magnetic moment: \(\mu = \mu_0 \frac{L}{\hbar}\)

Orbital mag. quantum number \(m_\ell\)
- Directions of ‘orbital bar magnet’ quantized.
- Orbital magnetic quantum number
  - \(m_\ell\) ranges from \(-l\) to \(l\) in integer steps \((2l+1)\) different values
  - Determines \(z\)-component of \(L\): \(L_z = m_\ell \hbar\)
  - Also determines angle of \(L\)
  
\[
L_z = L \cos \theta = m_\ell \hbar
\]

For example: \(l=1\) gives 3 states:

Question

- For a quantum state with \(l=2\), how many different orientations of the orbital magnetic dipole moment are there?
  
  A. 1
  B. 2
  C. 3
  D. 4
  E. 5

Summary of quantum numbers

<table>
<thead>
<tr>
<th>Quantum Number</th>
<th>Name</th>
<th>Allowed Values</th>
<th>Number of Allowed States</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n)</td>
<td>Principal quantum number</td>
<td>1, 2, 3, ...</td>
<td>(n) number</td>
</tr>
<tr>
<td>(\ell)</td>
<td>Orbital quantum number</td>
<td>0, 1, 2, ..., (n-1)</td>
<td>(n) - (\ell)</td>
</tr>
<tr>
<td>(m_\ell)</td>
<td>Orbital magnetic quantum number</td>
<td>0, ..., (2\ell + 1)</td>
<td>(2\ell + 1)</td>
</tr>
</tbody>
</table>

For hydrogen atom:
- \(n\) describes energy of orbit
- \(\ell\) describes the magnitude of orbital angular momentum
- \(m_\ell\) describes the angle of the orbital angular momentum

Hydrogen wavefunctions

- Radial probability
- Angular not shown

For given \(n\), probability peaks at same place

Idea of “atomic shell”

Notation:
- \(s\): \(l=0\)
- \(p\): \(l=1\)
- \(d\): \(l=2\)
- \(f\): \(l=3\)
- \(g\): \(l=4\)

Full hydrogen wave functions:
Surface of constant probability

- Spherically symmetric.
- Probability decreases exponentially with radius.
- Shown here is a surface of constant probability

\[
r = 1, \ \ell = 0, \ m_\ell = 0
\]
**$n=2$: next highest energy**

$n=2, \ell=0, m_{l}=0$

$n=2, \ell=1, m_{l}=0$

$n=2, \ell=1, m_{l}=\pm 1$

*Same energy, but different probabilities*

**$n=3$: two s-states, six p-states and...**

$n=3, \ell=0, m_{l}=0$

$n=3, \ell=1, m_{l}=0$

$n=3, \ell=1, m_{l}=\pm 1$

**...ten d-states**

$n=3, \ell=2, m_{l}=0$

$n=3, \ell=2, m_{l}=\pm 1$

**Electron spin**

New electron property:
Electron acts like a bar magnet with N and S pole.
Magnetic moment fixed...
...but 2 possible orientations of magnet: up and down

Described by spin quantum number $m_{s}$

$S_{z} = m_{s} \hbar$

**Quantum Number Question**

How many different quantum states exist with $n=2$?

A. 1

B. 2

C. 4

D. 8

$\ell = 0 : 2s^{2}$

$m_{l} = 0 : m_{s} = 1/2, -1/2$

2 states

$\ell = 1 : 2p^{6}$

$m_{l} = \pm 1 : m_{s} = 1/2, -1/2$

2 states

$m_{l} = 0 : m_{s} = 1/2, -1/2$

2 states

$m_{l} = -1 : m_{s} = 1/2, -1/2$

2 states

*There are a total of 8 states with n=2*
Question
How many different quantum states are in a 5g (n=5, l =4) sub-shell of an atom?

A. 22
B. 20
C. 18
D. 16
E. 14

zero = 4, so 2(2 \times 4) = 18.
In detail, m_l = -4, -3, -2, -1, 0, 1, 2, 3, 4
and m_s = \pm 1/2 or \mp 1/2 for each.
18 available quantum states for electrons

Other elements: Li has 3 electrons

Electron Configurations

<table>
<thead>
<tr>
<th>Atom</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s^1</td>
</tr>
<tr>
<td>He</td>
<td>1s^2 1s^2</td>
</tr>
<tr>
<td>Li</td>
<td>1s^22s^1</td>
</tr>
<tr>
<td>Be</td>
<td>1s^22s^2 2s^2</td>
</tr>
<tr>
<td>B</td>
<td>1s^22s^22p^1</td>
</tr>
<tr>
<td>Ne</td>
<td>1s^22s^22p^6</td>
</tr>
</tbody>
</table>

(1s shell filled - noble gas)

The periodic table

Atoms in same column have ‘similar’ chemical properties.
Quantum mechanical explanation: similar ‘outer’ electron configurations.

Putting electrons on atom

- Electrons obey Pauli exclusion principle
- Only one electron per quantum state (n, l, m_l, m_s)
- Hydrogen: 1 electron
  one quantum state occupied 
  \( n = 1, l = 0, m_l = 0, m_s = +1/2 \)

- Helium: 2 electrons
  two quantum states occupied 
  \( n = 1, l = 0, m_l = 0, m_s = +1/2 \)

Multi-electron atoms

- Electrons interact with nucleus (like hydrogen)
- Also with other electrons
- Causes energy to depend on

Energy depends only on n

Energy depends on n and l
Excited states of Sodium

- Na level structure
- 11 electrons
  - Ne core = 1s² 2s² 2p⁶ (closed shell)
  - 1 electron outside closed shell
  - Na = [Ne]3s¹
- Outside (11th) electron easily excited to other states.

Optical spectrum

- Optical spectrum of sodium
  - Transitions from high to low energy states
  - Relatively simple
    - 1 electron outside closed shell