Phys 102 – Lecture 26

The quantum numbers and spin
Recall: the Bohr model

Only orbits that fit $n$ e⁻ wavelengths are allowed

**SUCCESSES**

Correct energy quantization & atomic spectra

$$E_n = -\frac{m_e k^2 e^4}{2\hbar^2} \cdot \frac{1}{n^2} \quad n = 1, 2, 3, \ldots$$

**FAILURES**

Radius & momentum quantization violates Heisenberg Uncertainty Principle

$$r_n = \frac{n^2 \hbar^2}{m_e k e^2} \equiv n^2 a_0 \quad \Delta r \cdot \Delta p_r \geq \frac{\hbar}{2}$$

Electron orbits cannot have zero $L$

$$L_n = n\hbar$$

Orbits can hold any number of electrons

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Quantum Mechanical Atom

Schrödinger’s equation determines e\(^{-}\) “wavefunction”

\[
\left(-\frac{\hbar^2}{2m_e} \nabla^2 - \frac{ke^2}{r}\right)\psi(r, \theta, \varphi) = E\psi(r, \theta, \varphi) \quad \Rightarrow \quad \psi_{n, \ell, m_\ell}
\]

3 quantum numbers determine e\(^{-}\) state

“Principal Quantum Number” \( n = 1, 2, 3, \ldots \)

\[
E_n = -\frac{m_e k^2 e^4}{2\hbar^2} \frac{1}{n^2}
\]

Energy

“Orbital Quantum Number” \( \ell = 0, 1, 2, 3 \ldots, n-1 \)

\[
L = \sqrt{\ell(\ell + 1)}\hbar
\]

Magnitude of angular momentum

“Magnetic Quantum Number” \( m_\ell = -\ell, \ldots, 0, +1 \ldots, \ell \)

\[
L_z = m_\ell \hbar
\]

Orientation of angular momentum

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ACT: CheckPoint 3.1 & more

For which state is the angular momentum \textit{required} to be 0?

A. \( n = 3 \)
B. \( n = 2 \)
C. \( n = 1 \)

How many values for \( m_\ell \) are possible for the \( f \) subshell (\( \ell = 3 \))? 

A. 3
B. 5
C. 7
Hydrogen electron orbitals

\[ |\psi_{n,\ell,m_{\ell}}|^2 \propto \text{probability} \]

Shell \( \rightarrow (n, \ell, m_{\ell}) \)

Subshell

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**CheckPoint 2: orbitals**

Orbitals represent probability of electron being at particular location.

- **1s** ($\ell = 0$)
- **2p** ($\ell = 1$)
- **2s** ($\ell = 0$)
- **3s** ($\ell = 0$)

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Angular momentum

What do the quantum numbers $\ell$ and $m_\ell$ represent?

Magnitude of angular momentum vector quantized

$$|\vec{L}| = L = \sqrt{\ell(\ell + 1)} \hbar \quad \ell = 0, 1, 2 \cdots n - 1$$

Only one component of $L$ quantized

$$L_z = m_\ell \hbar \quad m_\ell = -\ell, \cdots -1, 0, 1, \cdots \ell$$

Other components $L_x, L_y$ are not quantized

Classical orbit picture

$\ell = 1$

- $L_z = +\hbar$
- $L_z = 0$
- $L_z = -\hbar$

$\ell = 2$

- $L_z = +2\hbar$
- $L_z = +\hbar$
- $L_z = 0$
- $L_z = -\hbar$
- $L_z = -2\hbar$

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Orbital magnetic dipole

Electron orbit is a current loop and a magnetic dipole

\[ \mu_e = IA = -\frac{e}{2m_e} L \]

Dipole moment is quantized

What happens in a \( B \) field?

\[ U = -\mu_e B \cos \theta = \frac{e\hbar}{2m_e} Bm_\ell \]

Orbitals with different \( L \) have different quantized energies in a \( B \) field

\[ \mu_B \equiv \frac{e\hbar}{2m_e} = 5.8 \times 10^{-5} \text{ eV/T} \]

"Bohr magneton"

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ACT: Hydrogen atom dipole

What is the magnetic dipole moment of hydrogen in its ground state due to the orbital motion of electrons?

\[ \vec{\mu} = -\frac{e}{2m_e} \vec{L} \]

A. \[ \mu_H = -\frac{e\hbar}{2m_e} \]
B. \[ \mu_H = 0 \]
C. \[ \mu_H = +\frac{e\hbar}{2m_e} \]
Calculation: Zeeman effect

Calculate the effect of a 1 T $B$ field on the energy of the 2p ($n = 2$, $\ell = 1$) level.

\[ E_{tot} = E_{n=2} - \mu_e B \cos \theta \]
\[ = E_{n=2} + \frac{e\hbar}{2m_e} B m_\ell \]

For $\ell = 1, m_\ell = -1, 0, +1$

\[ \vec{B} = 0 \]
\[ \vec{B} > 0 \]

- $m_\ell = +1$
- $m_\ell = 0$
- $m_\ell = -1$

Energy level splits into 3, with energy splitting

\[ \Delta E \equiv \frac{e\hbar B}{2m_e} \]

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ACT: Atomic dipole

The H α spectral line is due to e⁻ transition between the $n = 3$, $\ell = 2$ and the $n = 2$, $\ell = 1$ subshells.

How many levels should the $n = 3$, $\ell = 2$ state split into in a $B$ field?

A. 1  
B. 3  
C. 5
Intrinsic angular momentum

A beam of H atoms in ground state passes through a $B$ field

$n = 1$, so $\ell = 0$ and expect NO effect from $B$ field

Instead, observe beam split in two!

Since we expect $2\ell + 1$ values for magnetic dipole moment, $e^-$ must have intrinsic angular momentum $\ell = \frac{1}{2}$.

“Spin” $s$

“Stern-Gerlach experiment”
**Spin angular momentum**

Electrons have an intrinsic angular momentum called “spin”

\[
|\vec{S}| = S = \sqrt{s(s+1)}\hbar \quad \text{with } s = \frac{1}{2}
\]

\[
S_z = m_s \hbar \quad m_s = -\frac{1}{2}, +\frac{1}{2}
\]

Spin also generates magnetic dipole moment

\[\vec{\mu}_s = -\frac{e}{2m_e} g\vec{S}\]

with \(g \approx 2\)

\[
U = -\mu_s B \cos \theta = \frac{ge\hbar}{2m_e} Bm_s
\]

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**Magnetic resonance**

$e^-$ in B field absorbs photon with energy equal to splitting of energy levels

\[ m_s = \pm \frac{1}{2} \quad hf = \Delta E \]

“Electron spin resonance”
Typically microwave EM wave

Protons & neutrons also have spin $\frac{1}{2}$

\[ \vec{\mu}_{prot} = \pm \frac{e}{2m_p} g_p \vec{S} \ll \vec{\mu}_s \quad \text{since} \quad m_p \gg m_e \]

“Nuclear magnetic resonance”

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Quantum number summary

“Principal Quantum Number”, \( n = 1, 2, 3, \ldots \)

\[
E_n = -\frac{m_e k^2 e^4}{2\hbar^2} \frac{1}{n^2}
\]

Energy

“Orbital Quantum Number”, \( \ell = 0, 1, 2, \ldots, n-1 \)

\[
L = \sqrt{\ell(\ell + 1)}\hbar
\]

Magnitude of angular momentum

“Magnetic Quantum Number”, \( m_\ell = -\ell, \ldots, -1, 0, +1, \ldots, \ell \)

\[
L_z = m_\ell \hbar
\]

Orientation of angular momentum

“Spin Quantum Number”, \( m_s = -\frac{1}{2}, +\frac{1}{2} \)

\[
S_z = m_s \hbar
\]

Orientation of spin
**Electronic states**

*Pauli Exclusion Principle*: no two $e^-$ can have the same set of quantum numbers

\[ E = n \quad s (\ell = 0) \]
\[ p (\ell = 1) \]

\[ n = 2 \quad m_e = -1 \quad m_e = 0 \quad m_e = +1 \]

\[ m_s = +\frac{1}{2} \quad m_s = -\frac{1}{2} \]
Pauli exclusion & energies determine sequence

\( s (\ell = 0) \)

\( p (\ell = 1) \)

\( d (\ell = 2) \)

\( f (\ell = 3) \)
CheckPoint 3.2

How many electrons can there be in a 5g \((n = 5, \ell = 4)\) sub-shell of an atom?
ACT: Quantum numbers

How many total electron states exist with \( n = 2 \)?

A. 2
B. 4
C. 8
Where would you expect the most magnetic elements to be in the periodic table?

A. Alkali metals ($s, \ell = 1$)
B. Noble gases ($p, \ell = 2$)
C. Rare earth metals ($f, \ell = 4$)
Summary of today’s lecture

• Quantum numbers
  Principal quantum number \( E_n = -\frac{Z^2}{n^2} \times 13.6 \text{ eV} \)
  Orbital quantum number \( L = \sqrt{\ell(\ell + 1)\hbar}, \quad \ell = 0,1,n-1 \)
  Magnetic quantum number \( L_z = m_z\hbar, \quad m_\ell = -\ell,\ldots,0,\ldots,\ell \)

• Spin angular momentum
  \( e^- \) has intrinsic angular momentum \( S_z = m_s\hbar \quad m_s = -\frac{1}{2}, \frac{1}{2} \)

• Magnetic properties
  Orbital & spin angular momentum generate magnetic dipole moment

• Pauli Exclusion Principle
  No two \( e^- \) can have the same quantum numbers