Physics 228

Today:
Hydrogen Atom
Zeeman Effect
Electron Spin
Pauli Exclusion Principle
Many Electron Atoms
iClicker

How many degenerate states are there in the $n = 3$ shell? (If you know about the spin of the electron, ignore it.)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$l$</th>
<th>$m_l$</th>
<th>notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1s</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>2s</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0, ±1</td>
<td>2p</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3s</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0, ±1</td>
<td>3p</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>0, ±1, ±2</td>
<td>3d</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>4s</td>
</tr>
</tbody>
</table>

a) 1  
b) 5  
**c) 9**  
d) 12  
e) 14
3D Probability Distributions

These are 2D cuts through the probability densities.
Rotate the image around the z axis for the 3D view.

sphere
sphere + shell
donut
dumbbell

\begin{align*}
sphere & : \quad 1s, m_l = 0 \\
sphere + shell & : \quad 2s, m_l = 0 \\
donut & : \quad 2p, m_l = \pm 1 \\
dumbbell & : \quad 2p, m_l = 0 \\
& \quad 3p, m_l = 0 \\
& \quad 3p, m_l = \pm 1 \\
& \quad 3d, m_l = 0 \\
& \quad 3d, m_l = \pm 1 \\
& \quad 3d, m_l = \pm 2
\end{align*}
Radial Probability Distributions

The radial probability distribution $P(r)$ is the probability that the electron is found in a spherical shell of radius $r$ and thickness $dr$, divided by $dr$. 

![Graph showing radial probability distributions for different $l$ values.](image)

States with $l = 0$

States with $l = 1$

States with $l = 2$ or $l = 3$
What angle does the angular momentum make with the z-axis for the 3d state with $m_l = 0$?

a) There is no 3d state, only 1d or 2d.

b) $|\cos \theta| = 1/\sqrt{2}$

c) $|\sin \theta| = 1/\sqrt{2}$

d) $0^\circ$

e) $90^\circ$
Clicker Question

A potential-energy function is shown. If a quantum-mechanical particle has energy $E < U_0$, it is impossible to find the particle in the region

A) $x < 0$.
B) $0 < x < L$.
C) $x > L$.
D) misleading question — the particle can be found at any $x$.
Shown here is a set of degenerate orbitals belonging to a certain orbital angular momentum quantum number $l$. These orbitals are

- a) s-orbitals
- b) p-orbitals
- c) d-orbitals
- d) f-orbitals
- e) cannot be determined

The degeneracy $2l + 1 = 5$
Thus $l = 2$
Hydrogen Atom in Magnetic Field

• For an object with a magnetic moment $\mu$, there is an interaction energy with the magnetic filed $B$:
  \[ U = -\mu \cdot B. \]

• Classically, an electron orbiting around a proton, encircling an area $A$, corresponds to a circular electric current $I$ , and thus a magnetic moment: $\mu = IA$.

• The current is given by the electron’s charge ($-e$), velocity $v$, and orbital radius: $I = -ev/2\pi r$.

• Thus, the magnitude of the magnetic moment is $\mu = (-ev/2\pi r)(\pi r^2) = -evr/2 = (-e/2m)L$ (L is the angular momentum $rp = rmv$)
  \[ \mu = (-e/2m)L \]
For a magnetic field in $z$-direction, the interaction energy thus becomes $U = (e/2m) \mathbf{L} \cdot \mathbf{B} = (e/2m) L_z B$.

Although this has been derived classically, it is true also in quantum mechanics.

For the H atom, we have $L_z = m_l \hbar$, thus $U = (e\hbar/2m) m_l B$.

The quantity $\mu_B = e\hbar/2m$ is called the Bohr magneton (a quantization unit of magnetic moment):

$$U = m_l \mu_B B$$

We expect atomic energy levels to split into $(2l + 1)$ magnetic sub-levels when a magnetic field is applied (Zeeman effect). Such splitting is indeed observed:
Zeeman effect

$$U = m_l \mu_B B$$

- A magnetic field removes the \((2l+1)\)-fold degeneracy of each \((n, l)\) level.
- The \((2l+1)\) sub-levels have even separations of \(\mu_B B\). Pieter Zeeman discovered this in 1896.
The Stern-Gerlach Experiment

- If the magnetic field is not constant, there will be a force on the atom \( F = - \nabla U = - m_l \mu_B (dB/dz) \).
- An atom beam will separate into \( 2l+1 \) separate bunches if there is a \( B \) field with enough spatial variation.
- This shows the quantization of the \( z \)-component of the magnetic moment, and by inference, the quantization of \( L_z \).
The number of “bunches” should be $2l+1$, therefore odd.

This is observed for some atoms.

However, in other cases an even number is seen.

If we interpret this as angular momentum quantization, we require half-integer angular momentum quantum numbers $j = 1/2, 3/2, \text{etc.}$

The number of sublevels $2j+1$ is then even.
Electron Spin

- This half-integral angular momentum also shows up in the Zeeman effect (called “anomalous Zeeman effect”).
- Half-integral angular momentum is now understood as “spin” of the electron.
- Spin is an intrinsic angular momentum that the electrons always have, irrespective of orbital motion.
- For electrons, the magnitude of the spin angular momentum is
  \[ S = \sqrt{s(s + 1)} \hbar \] with \( s = \frac{1}{2} \) (spin quantum number).
- The \( z \)-component of the spin angular momentum is
  \[ S_z = m_s \hbar \] with \( m_s = \pm \frac{1}{2} \) (spin magnetic quantum number).
- For many particles (electrons, protons, neutrons, …) \( s = \frac{1}{2} \). Such particles are called fermions.
- Other particles have integral spin (\( s = 0 \) for the Higgs boson, \( s = 1 \) for the photon). Such particles are called bosons.
What is the magnitude of the spin angular momentum of an electron?

a) 0
b) \(\hbar\)
c) \(\hbar/2\)
d) \(+\hbar/2\) or \(-\hbar/2\), depending on whether spin is “up” or “down”
e) \(\sqrt[4]\frac{3}{4}\hbar\)

\[S = \sqrt{s(s + 1)}\hbar = \sqrt{\frac{1}{2}\left(\frac{1}{2} + 1\right)}\hbar = \sqrt[4]\frac{3}{4}\hbar\]
Pauli Exclusion Principle

• The Pauli exclusion principle states that each single-particle state (characterized by the four quantum numbers n, l, m_l, m_s) can accommodate no more than one electron.

• As a consequence, as we add electrons to an atom, the inner shells “fill up” first, then the more weakly bound shells will be populated. (“Aufbau principle”).

• The Pauli exclusion principle applies to all half-integer spin particles, i.e., fermions (incl. protons and neutrons).

• There is no such principle for bosons. For example, a large number of photons may occupy the same quantum state in a laser.
Aufbau Principle

Periodic Table of the Elements

Show Dynamic Periodic Table
Cubic Crystal Lattices

(a) Simple cubic (sc)

(b) Face-centered cubic (fcc)

(c) Body-centered cubic (bcc)
Hexagonal Crystal Lattices

(d) Hexagonal close packed (hcp)

(e) Top view, hexagonal close packed
Nearest Neighbors

One important characteristic for these repeating structures is the number of nearest neighbors an atom has. This requires some 3D thinking and visualization.

SC: six (along the cube edges L/R, U/D, F/B).

BCC: eight (from a corner to the centers of the 8 adjacent cubes).

FCC: twelve (from a corner to the centers of the 12 adjacent faces).

(a) Simple cubic (sc)  
(b) Face-centered cubic (fcc)  
(c) Body-centered cubic (bcc)
In a monatomic, simple cubic lattice, how many nearest neighbors does each atom have?

- a) 2
- b) 4
- c) 6
- d) 8
- e) 12