

CHAPTER 7

The Hydrogen Atom

- 7.1 Application of the Schrödinger Equation to the Hydrogen Atom
- 7.2 Solution of the Schrödinger Equation for Hydrogen
- 7.3 Quantum Numbers
- 7.4 Magnetic Effects on Atomic Spectra – The Normal Zeeman Effect
- 7.5 Intrinsic Spin
- 7.6 Energy Levels and Electron Probabilities

The atom of modern physics can be symbolized only through a partial differential equation in an abstract space of many dimensions. All its qualities are inferential; no material properties can be directly attributed to it. An understanding of the atomic world in that primary sensuous fashion...is impossible.

7.1: Application of the Schrödinger Equation to the Hydrogen Atom

- The approximation of the potential energy of the electron-proton system is electrostatic:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

- Rewrite the three-dimensional time-independent Schrödinger Equation.

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x, y, z)} \left[\frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z)}{\partial z^2} \right] = E - V(r)$$

For Hydrogen-like atoms (He⁺ or Li⁺⁺)

- Replace e^2 with Ze^2 (Z is the atomic number).
- Use appropriate reduced mass μ .

Application of the Schrödinger Equation

- The potential (central force) $V(r)$ depends on the distance r between the proton and electron.

$$x = r \sin \theta \cos \phi$$

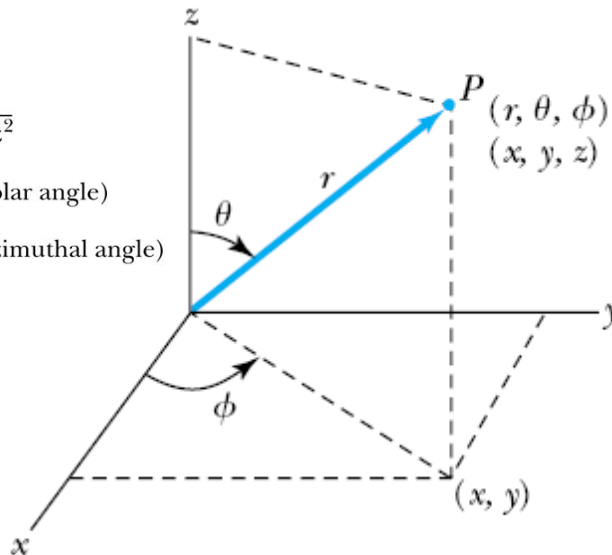
$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

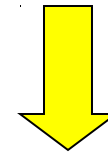
$$\theta = \cos^{-1} \frac{z}{r} \text{ (Polar angle)}$$

$$\phi = \tan^{-1} \frac{y}{x} \text{ (Azimuthal angle)}$$



Transform to spherical polar coordinates because of the radial symmetry.

Insert the Coulomb potential into the transformed Schrödinger equation.



$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) \psi = 0$$

Application of the Schrödinger Equation

- The wave function ψ is a function of r, θ, ϕ
 - Equation is separable.
 - Solution may be a product of three functions.
 - $\psi(r, \theta, \phi) = R(r)f(\theta)g(\phi)$ Equation 7.3
- We can separate Equation 7.3 into three separate differential equations, each depending on one coordinate: $r, \theta,$ or ϕ .

7.2: Solution of the Schrödinger Equation for Hydrogen

- Substitute Eq (7.4) into Eq (7.3) and separate the resulting equation into three equations: $R(r)$, $f(\theta)$, and $g(\phi)$.

Separation of Variables

- The derivatives from Eq (7.4)

$$\frac{\partial \psi}{\partial r} = fg \frac{\partial R}{\partial r} \quad \frac{\partial \psi}{\partial \theta} = Rg \frac{\partial f}{\partial \theta} \quad \frac{\partial^2 \psi}{\partial \phi^2} = Rf \frac{\partial^2 g}{\partial \phi^2}$$

- Substitute them into Eq (7.3)

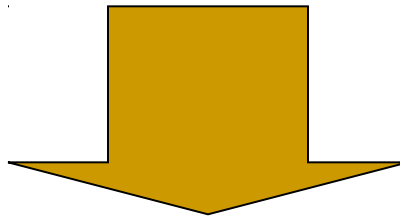
$$\frac{fg}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{Rg}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{Rf}{r^2 \sin^2 \theta} \frac{\partial^2 g}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) Rfg = 0$$

- Multiply both sides of Eq (7.6) by $r^2 \sin^2 \theta / Rfg$

$$-\frac{\sin^2 \theta}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{2\mu}{\hbar^2} r^2 \sin^2 \theta (E - V) - \frac{\sin \theta}{f} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) = \frac{1}{g} \frac{\partial^2 g}{\partial \phi^2}$$

Solution of the Schrödinger Equation

- Only r and θ appear on the left side and only ϕ appears on the right side of Eq (7.7)
- The left side of the equation cannot change as ϕ changes.
- The right side cannot change with either r or θ .



- Each side needs to be equal to a constant for the equation to be true. Set the constant $-m_\ell^2$ equal to the right side of Eq (7.7)

$$\frac{d^2 g}{d\phi^2} = -m_\ell^2 g \quad \text{----- azimuthal equation}$$

- It is convenient to choose a solution to be $e^{im_\ell\phi}$.

Solution of the Schrödinger Equation

- $e^{im_\ell\phi}$ satisfies Eq (7.8) for any value of m_ℓ .
- The solution be single valued in order to have a valid solution for any ϕ , which is
$$g(\phi) = g(\phi + 2\pi)$$
$$g(\phi = 0) = g(\phi = 2\pi) \longrightarrow e^0 = e^{2\pi im_\ell}$$
- m_ℓ to be zero or an integer (positive or negative) for this to be true.
- If Eq (7.8) were positive, the solution would not be realized.
- Set the left side of Eq (7.7) equal to $-m_\ell^2$ and rearrange it.
$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r^2}{\hbar^2} (E - V) = \frac{m_\ell^2}{\sin^2 \theta} - \frac{1}{f \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right)$$
- Everything depends on r on the left side and θ on the right side of the equation.

Solution of the Schrödinger Equation

- Set each side of Eq (7.9) equal to constant $\ell(\ell + 1)$.

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E - V - \frac{\hbar^2 \ell(\ell + 1)}{2\mu r^2} \right] R = 0 \quad \text{----Radial equation}$$

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{df}{d\theta} \right) + \left[\ell(\ell + 1) - \frac{m_\ell^2}{\sin^2 \theta} \right] f = 0 \quad \text{----Angular equation}$$

- Schrödinger equation has been separated into three ordinary second-order differential equations [Eq (7.8), (7.10), and (7.11)], each containing only one variable.

Solution of the Radial Equation

- The radial equation is called the **associated Laguerre equation** and the *solutions* R that satisfy the appropriate boundary conditions are called *associated Laguerre functions*.
- Assume the ground state has $\ell = 0$ and this requires $m_\ell = 0$.

Eq (7.10) becomes

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} (E - V) R = 0$$

- The derivative of $r^2 \frac{dR}{dr}$ yields two terms.

Write those terms and insert Eq (7.1)

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2\mu}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) R = 0$$

Solution of the Radial Equation

- Try a solution $R = Ae^{-r/a_0}$

A is a normalized constant.

a_0 is a constant with the dimension of length.

Take derivatives of R and insert them into Eq (7.13).

$$\left(\frac{1}{a_0^2} + \frac{2\mu}{\hbar^2} E \right) + \left(\frac{2\mu e^2}{4\pi\epsilon_0 \hbar^2} - \frac{2}{a_0} \right) \frac{1}{r} = 0$$

- To satisfy Eq (7.14) for any r is for each of the two expressions in parentheses to be zero.

Set the second parentheses equal to zero and solve for a_0 .

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2}$$

Set the first parentheses equal to zero and solve for E .

$$E = -\frac{\hbar^2}{2\mu a_0^2} = -E_0$$

Both equal to the Bohr result.

Quantum Numbers

- The appropriate boundary conditions to Eq (7.10) and (7.11) leads to the following restrictions on the quantum numbers ℓ and m_ℓ :

- $\ell = 0, 1, 2, 3, \dots$
- $m_\ell = -\ell, -\ell + 1, \dots, -2, -1, 0, 1, 2, \dots, \ell - 1, \ell$
- $|m_\ell| \leq \ell$ and $\ell < 0$.

- The predicted energy level is

$$E_n = -\frac{E_0}{n^2}$$

Hydrogen Atom Radial Wave Functions

- First few radial wave functions $R_{n\ell}$

Table 7.1 Hydrogen Atom Radial Wave Functions

n	ℓ	$R_{n\ell}(r)$
1	0	$\frac{2}{(a_0)^{3/2}} e^{-r/a_0}$
2	0	$\left(2 - \frac{r}{a_0}\right) \frac{e^{-r/2a_0}}{(2a_0)^{3/2}}$
2	1	$\frac{r}{a_0} \frac{e^{-r/2a_0}}{\sqrt{3}(2a_0)^{3/2}}$
3	0	$\frac{1}{(a_0)^{3/2}} \frac{2}{81\sqrt{3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{6}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{30}} \frac{r^2}{a_0^2} e^{-r/3a_0}$

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- Subscripts on R specify the values of n and ℓ .

Solution of the Angular and Azimuthal Equations

- The solutions for Eq (7.8) are $e^{im_\ell\phi}$ or $e^{-im_\ell\phi}$.
- Solutions to the angular and azimuthal equations are linked because both have m_ℓ .
- Group these solutions together into functions.

$$Y(\theta, \phi) = f(\theta)g(\phi) \text{ ---- spherical harmonics}$$

Normalized Spherical Harmonics

Table 7.2 Normalized Spherical Harmonics $Y_{\ell m_{\ell}}(\theta, \phi)$

ℓ	m_{ℓ}	$Y_{\ell m_{\ell}}$
0	0	$\frac{1}{2\sqrt{\pi}}$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}} \cos \theta$
1	± 1	$\mp \frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin \theta e^{\pm i\phi}$
2	0	$\frac{1}{4}\sqrt{\frac{5}{\pi}} (3 \cos^2 \theta - 1)$
2	± 1	$\mp \frac{1}{2}\sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{\pm i\phi}$
2	± 2	$\frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{\pm 2i\phi}$
3	0	$\frac{1}{4}\sqrt{\frac{7}{\pi}} (5 \cos^3 \theta - 3 \cos \theta)$
3	± 1	$\mp \frac{1}{8}\sqrt{\frac{21}{\pi}} \sin \theta (5 \cos^2 \theta - 1) e^{\pm i\phi}$
3	± 2	$\frac{1}{4}\sqrt{\frac{105}{2\pi}} \sin^2 \theta \cos \theta e^{\pm 2i\phi}$
3	± 3	$\mp \frac{1}{8}\sqrt{\frac{35}{\pi}} \sin^3 \theta e^{\pm 3i\phi}$

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Solution of the Angular and Azimuthal Equations

- The radial wave function R and the spherical harmonics Y determine the probability density for the various quantum states. The total wave function $\psi(r, \theta, \phi)$ depends on n , ℓ , and m_ℓ . The wave function becomes

$$\psi_{nlm_\ell}(r, \theta, \phi) = R_{nl}(r)Y_{\ell m_\ell}(\theta, \phi)$$

7.3: Quantum Numbers

The three quantum numbers:

- n Principal quantum number
- ℓ Orbital angular momentum quantum number
- m_ℓ Magnetic quantum number

The boundary conditions:

- $n = 1, 2, 3, 4, \dots$ Integer
- $\ell = 0, 1, 2, 3, \dots, n - 1$ Integer
- $m_\ell = -\ell, -\ell + 1, \dots, 0, 1, \dots, \ell - 1, \ell$ Integer

The restrictions for quantum numbers:

- $n > 0$
- $\ell < n$
- $|m_\ell| \leq \ell$

Principal Quantum Number n

- It results from the solution of $R(r)$ in Eq (7.4) because $R(r)$ includes the potential energy $V(r)$.

The result for this quantized energy is

$$E_n = \frac{-\mu}{2} \left(\frac{e^2}{4\pi\epsilon_0\hbar} \right)^2 \frac{1}{n^2} = -\frac{E_0}{n^2}$$

- The negative means the energy E indicates that the electron and proton are bound together.

Orbital Angular Momentum Quantum Number ℓ

- It is associated with the $R(r)$ and $f(\theta)$ parts of the wave function.
- Classically, the orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$ with $L = mv_{\text{orbital}}r$.
- ℓ is related to L by
$$L = \sqrt{\ell(\ell + 1)}\hbar$$
- In an $\ell = 0$ state,
$$L = \sqrt{0(1)}\hbar = 0$$



It disagrees with Bohr's semiclassical "planetary" model of electrons orbiting a nucleus $L = n\hbar$.

Orbital Angular Momentum Quantum Number ℓ

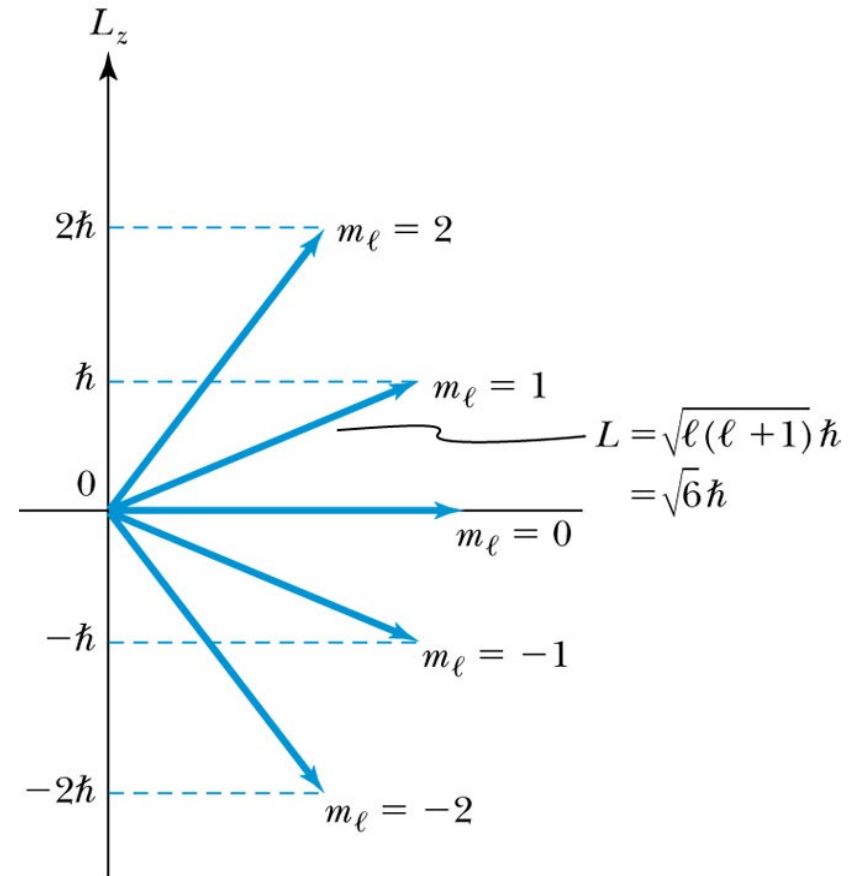
- A certain energy level is **degenerate** with respect to ℓ when the energy is independent of ℓ .
- Use letter names for the various ℓ values.
 - $\ell =$ 0 1 2 3 4 5 ...
 - Letter = *s* *p* *d* *f* *g* *h* ...
- Atomic states are referred to by their n and ℓ .
- A state with $n = 2$ and $\ell = 1$ is called a $2p$ state.
- The boundary conditions require $n > \ell$.

Magnetic Quantum Number m_ℓ

- The angle ϕ is a measure of the rotation about the z axis.
- The solution for $g(\phi)$ specifies that m_ℓ is an integer and related to the z component of L .

$$L_z = m_\ell \hbar$$

- The relationship of L , L_z , ℓ , and m_ℓ for $\ell = 2$.
- $L = \sqrt{\ell(\ell + 1)}\hbar = \sqrt{6}\hbar$ is fixed because L_z is quantized.
- Only certain orientations of \vec{L} are possible and this is called **space quantization**.



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Magnetic Quantum Number m_ℓ

- Quantum mechanics allows \vec{L} to be quantized along only one direction in space. Because of the relation $L^2 = L_x^2 + L_y^2 + L_z^2$ the knowledge of a second component would imply a knowledge of the third component because we know \vec{L} .
- We expect the average of the angular momentum components squared to be $\langle L_x^2 \rangle = \langle L_y^2 \rangle = \langle L_z^2 \rangle$.

$$\langle L^2 \rangle = 3 \langle L_z^2 \rangle = \frac{3}{2\ell + 1} \sum_{m_\ell = -\ell}^{\ell} m_\ell^2 \hbar^2 = \ell(\ell + 1)\hbar^2$$

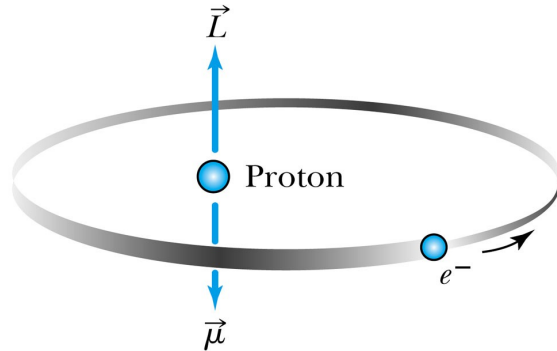
7.4: Magnetic Effects on Atomic Spectra—The Normal Zeeman Effect

- The Dutch physicist Pieter Zeeman showed the spectral lines emitted by atoms in a magnetic field split into multiple energy levels. It is called the **Zeeman effect**.

Anomalous Zeeman effect:

- A spectral line is split into three lines.
- Consider the atom to behave like a small magnet.
- Think of an electron as an orbiting circular current loop of $I = dq / dt$ around the nucleus.
- The current loop has a magnetic moment $\mu = IA$ and the period $T = 2\pi r / v$.
- $\vec{\mu} = -\frac{e}{2m} \vec{L}$ where $L = mvr$ is the magnitude of the orbital angular momentum.

The Normal Zeeman Effect



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- Since there is no magnetic field to align them, $\vec{\mu}$ point in random directions. The dipole has a potential energy

$$V_B = -\vec{\mu} \cdot \vec{B}$$

- The angular momentum is aligned with the magnetic moment, and the torque between $\vec{\mu}$ and \vec{B} causes a precession of $\vec{\mu}$.

$$\mu_z = \frac{e\hbar}{2m} m_\ell = -\mu_B m_\ell$$

Where $\mu_B = e\hbar / 2m$ is called a **Bohr magneton**.

- $\vec{\mu}$ cannot align exactly in the z direction and has only certain allowed quantized orientations.

$$\vec{\mu} = -\mu_B \vec{L} / \hbar$$

The Normal Zeeman Effect

- The potential energy is quantized due to the magnetic quantum number m_ℓ .

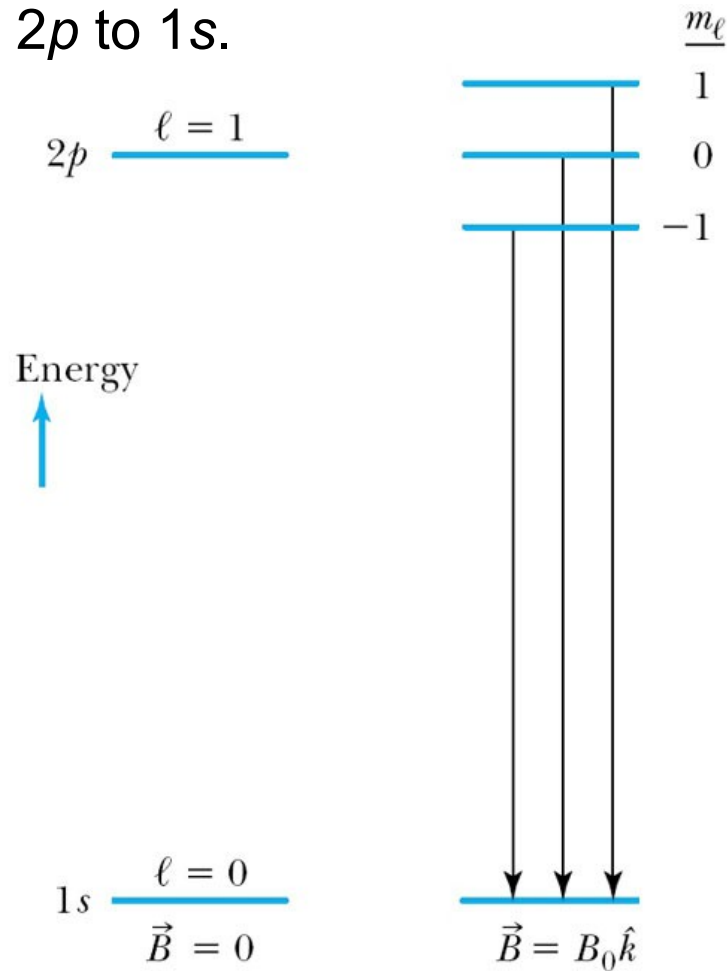
$$V_B = -\mu_z B = +\mu_B m_\ell B$$

- When a magnetic field is applied, the $2p$ level of atomic hydrogen is split into three different energy states with energy difference of $\Delta E = \mu_B B \Delta m_\ell$.

m_ℓ	Energy	$n = 2$	$\ell = 1$	$\vec{B} = 0$	$\ell = 1$	$\vec{B} = B_0 \hat{k}$	$\frac{m_\ell}{1}$		
1	$E_0 + \mu_B B$							$\updownarrow \Delta E = \mu_B B$	1
0	E_0								0
-1	$E_0 - \mu_B B$								$\updownarrow \Delta E$

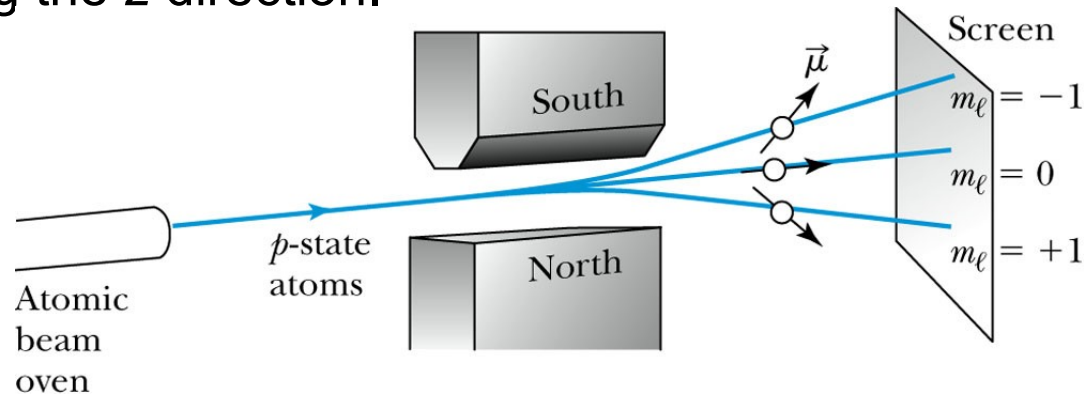
The Normal Zeeman Effect

- A transition from $2p$ to $1s$.



The Normal Zeeman Effect

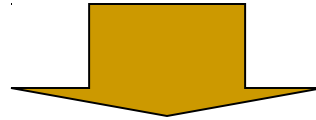
- An atomic beam of particles in the $\ell = 1$ state pass through a magnetic field along the z direction.



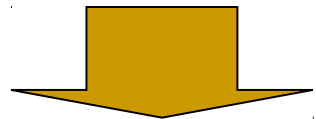
- $V_B = -\mu_z B$
- $F_z = -(dV_B / dz) = \mu_z (dB / dz)$
- The $m_l = +1$ state will be deflected down, the $m_l = -1$ state up, and the $m_l = 0$ state will be undeflected.
- If the space quantization were due to the magnetic quantum number m_l , m_l states is always odd ($2\ell + 1$) and should have produced an odd number of lines.

7.5: Intrinsic Spin

- Samuel Goudsmit and George Uhlenbeck in Holland proposed that *the electron must have an intrinsic angular momentum* and therefore a magnetic moment.



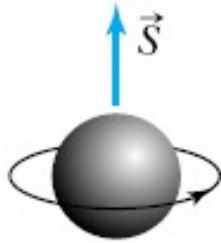
- Paul Ehrenfest showed that the surface of the spinning electron should be moving faster than the speed of light!



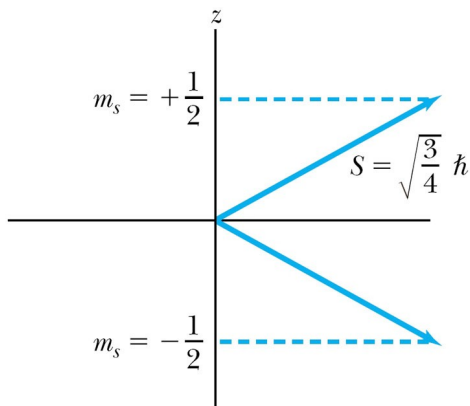
- In order to explain experimental data, Goudsmit and Uhlenbeck proposed that the electron must have an **intrinsic spin quantum number** $s = \frac{1}{2}$.

Intrinsic Spin

- The spinning electron reacts similarly to the orbiting electron in a magnetic field.
- We should try to find L , L_z , ℓ , and m_ℓ .
- The **magnetic spin quantum number** m_s has only two values, $m_s = \pm 1/2$.



The electron's spin will be either “up” or “down” and can never be spinning with its magnetic moment μ_s exactly along the z axis.



The **intrinsic spin angular momentum** vector $|\vec{S}| = \sqrt{s(s+1)}\hbar = \sqrt{3/4}\hbar$.

Intrinsic Spin

- The magnetic moment is $\vec{\mu}_s = -(e/m)\vec{S}$, or $-2\mu_B\vec{S}/\hbar$.
- The coefficient of \vec{S}/\hbar is $-2\mu_B$ as with \vec{L} is a consequence of theory of relativity.

- The **gyromagnetic ratio** (l or s).

- $g_l = 1$ and $g_s = 2$, then

$$\mu_l = -\frac{g_l\mu_B\vec{L}}{\hbar} = -\frac{\mu_B\vec{L}}{\hbar} \quad \text{and} \quad \vec{\mu}_s = -\frac{g_s\mu_B\vec{L}}{\hbar} = -2\frac{\mu_B\vec{L}}{\hbar}$$

- The z component of \vec{S} is $S_z = m_s\hbar = \pm\hbar/2$.

- In $l = 0$ state \longrightarrow no splitting due to $\vec{\mu}_s$.

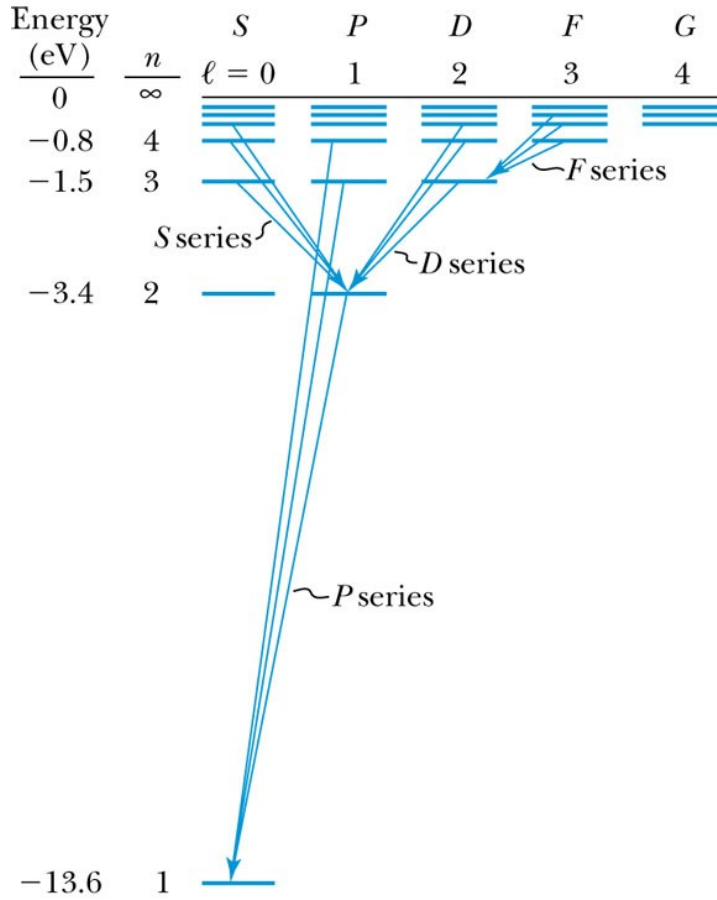
\searrow there is space quantization due to the intrinsic spin.

- Apply m_l and the potential energy becomes

$$V_B = -\vec{\mu}_s \cdot \vec{B} = +\frac{e\hbar}{m}\vec{S} \cdot \vec{B}$$

7.6: Energy Levels and Electron Probabilities

- For hydrogen, the energy level depends on the principle quantum number n .



- In ground state an atom cannot emit radiation. It can absorb electromagnetic radiation, or gain energy through inelastic bombardment by particles.

Selection Rules

- We can use the wave functions to calculate transition probabilities for the electron to change from one state to another.

Allowed transitions:

- Electrons absorbing or emitting photons to change states when $\Delta\ell = \pm 1$.

Forbidden transitions:

- Other transitions possible but occur with much smaller probabilities when $\Delta\ell \neq \pm 1$.

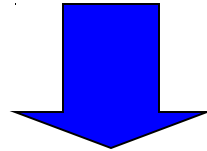
$$\Delta n = \text{anything}$$

$$\Delta\ell = \pm 1$$

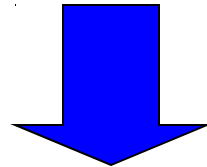
$$\Delta m_\ell = 0, \pm 1$$

Probability Distribution Functions

- We must use wave functions to calculate the probability distributions of the electrons.



- The “position” of the electron is spread over space and is not well defined.



- We may use the radial wave function $R(r)$ to calculate radial probability distributions of the electron.
- The probability of finding the electron in a differential volume element $d\tau$ is $dP = \psi^*(r, \theta, \phi) \psi(r, \theta, \phi) d\tau$.

Probability Distribution Functions

- The differential volume element in spherical polar coordinates is

$$d\tau = r^2 \sin \theta \, dr \, d\theta \, d\phi$$

Therefore,

$$P(r) \, dr = r^2 R^*(r) R(r) \, dr \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta \int_0^{2\pi} |g(\phi)|^2 \, d\phi$$

- We are only interested in the radial dependence.

$$P(r) \, dr = r^2 |R(r)|^2 \, dr$$

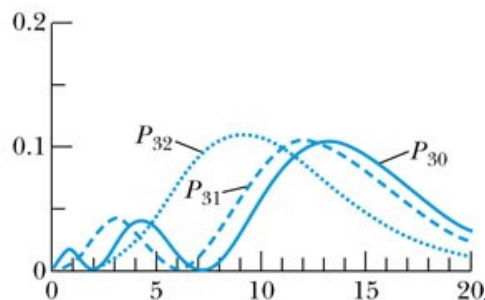
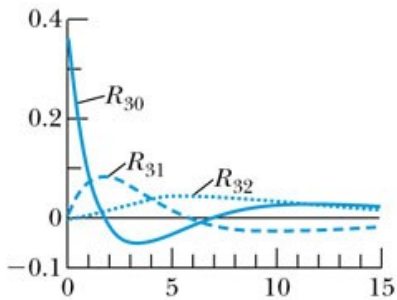
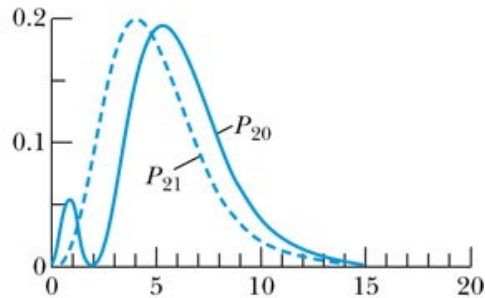
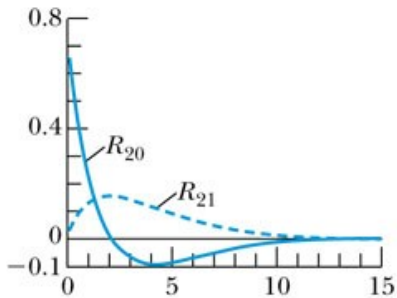
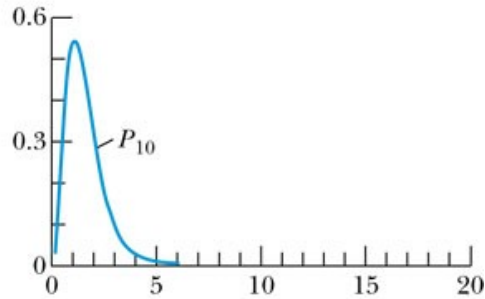
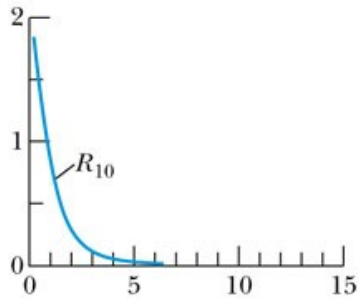
- The radial probability density is $P(r) = r^2 |R(r)|^2$ and it depends only on n and l .

Probability Distribution Functions

Radial wave functions (R_{nl})

Radial probability distribution (P_{nl})

- $R(r)$ and $P(r)$ for the lowest-lying states of the hydrogen atom.



Radius (a_0)

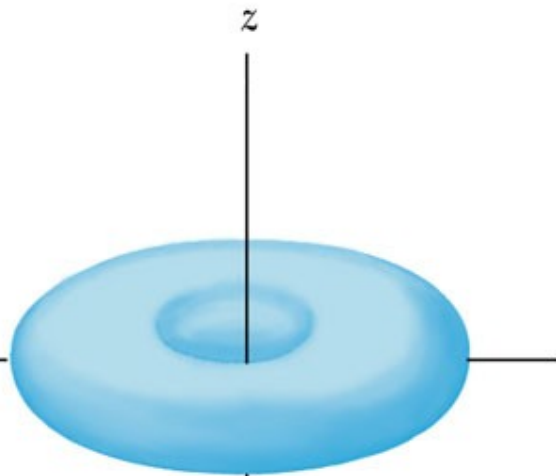
Radius (a_0)

(a)

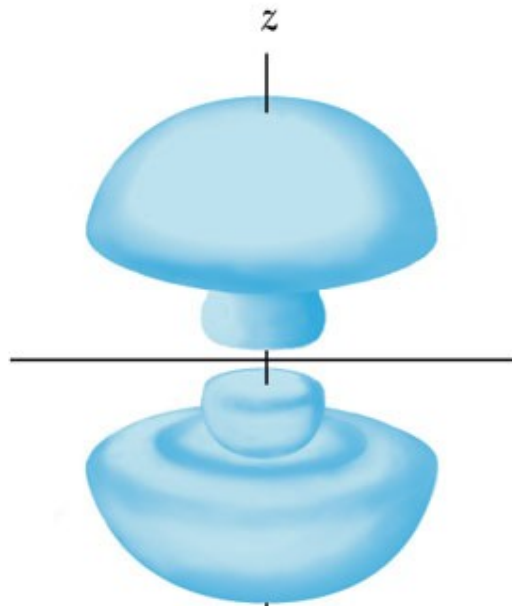
(b)

Probability Distribution Functions

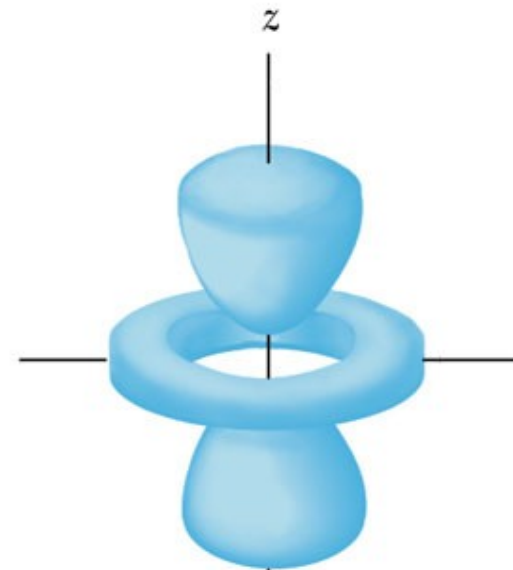
- The probability density for the hydrogen atom for three different electron states.



$$\begin{aligned}n &= 2 \\ \ell &= 1 \\ m_\ell &= \pm 1\end{aligned}$$



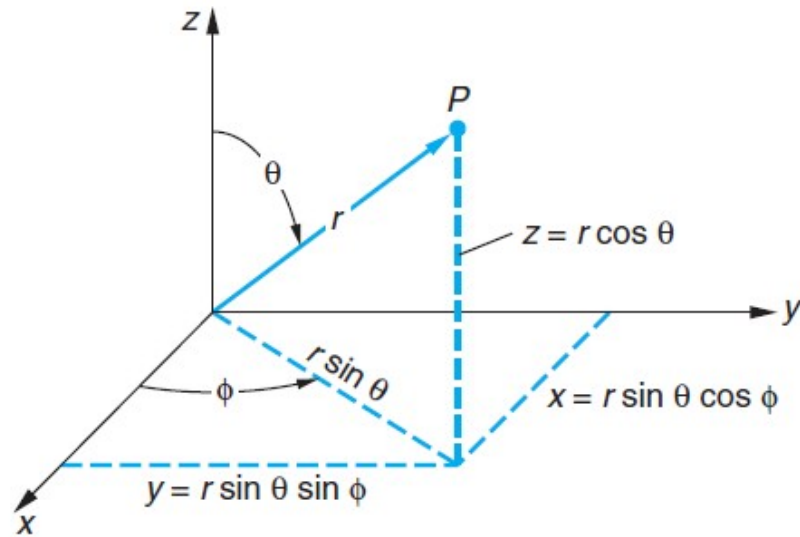
$$\begin{aligned}n &= 3 \\ \ell &= 0 \\ m_\ell &= 0\end{aligned}$$



$$\begin{aligned}n &= 3 \\ \ell &= 2 \\ m_\ell &= 0\end{aligned}$$

TOPIC	RELEVANT EQUATIONS AND REMARKS
1. Schrödinger equation in three dimensions	The equation is solved for the hydrogen atom by separating it into three ordinary differential equations, one for each coordinate r , θ , ϕ . The quantum numbers n , ℓ , and m arise from the boundary conditions to the solutions of these equations.
2. Quantization	
Angular momentum	$ \mathbf{L} = \sqrt{\ell(\ell + 1)}\hbar$ for $\ell = 0, 1, 2, 3, \dots$ 7-22
z component of \mathbf{L}	$L_z = m\hbar$ for $m = 0, \pm 1, \pm 2, \dots, \pm \ell$ 7-23
Energy	$E_n = -\left(\frac{kZe^2}{\hbar}\right)^2 \frac{\mu}{2n^2} = -13.6 \frac{Z^2}{n^2} \text{ eV}$ 7-24
3. Hydrogen wave functions	$\Psi_{n\ell m} = C_{n\ell m} R_{n\ell}(r) Y_{n\ell m}(\theta, \phi)$ where $C_{n\ell m}$ are normalization constants, $R_{n\ell}$ are the radial functions, and $Y_{\ell m}$ are the spherical harmonics.
4. Electron spin	The electron spin is not included in Schrödinger's wave equation.
Magnitude of \mathbf{S}	$ \mathbf{S} = \sqrt{s(s + 1)}\hbar$ $s = \frac{1}{2}$ 7-36
z component of \mathbf{S}	$S_z = m_s \hbar$ $m_s = \pm \frac{1}{2}$
Stern-Gerlach experiment	This was the first direct observation of the electron spin.
5. Spin-orbit coupling	\mathbf{L} and \mathbf{S} add to give the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$, whose magnitude is given by $ \mathbf{J} = \sqrt{j(j + 1)}\hbar$ 7-53 where $j = \ell + s$ or $ \ell - s $. This interaction leads to the fine-structure splitting of the energy levels.
6. Exclusion principle	No more than one electron can occupy a given quantum state specified by a particular set of the single-particle quantum numbers n , ℓ , m_ℓ , and m_s .

Figure 7-2 Geometric relations between spherical (polar) and rectangular coordinates.



Range of variables

Cartesian

$$x, y, z: -\infty \rightarrow +\infty$$

Spherical

$$r: 0 \rightarrow +\infty$$

$$\theta: 0 \rightarrow \pi$$

$$\phi: 0 \rightarrow 2\pi$$