8 | ATOMIC STRUCTURE

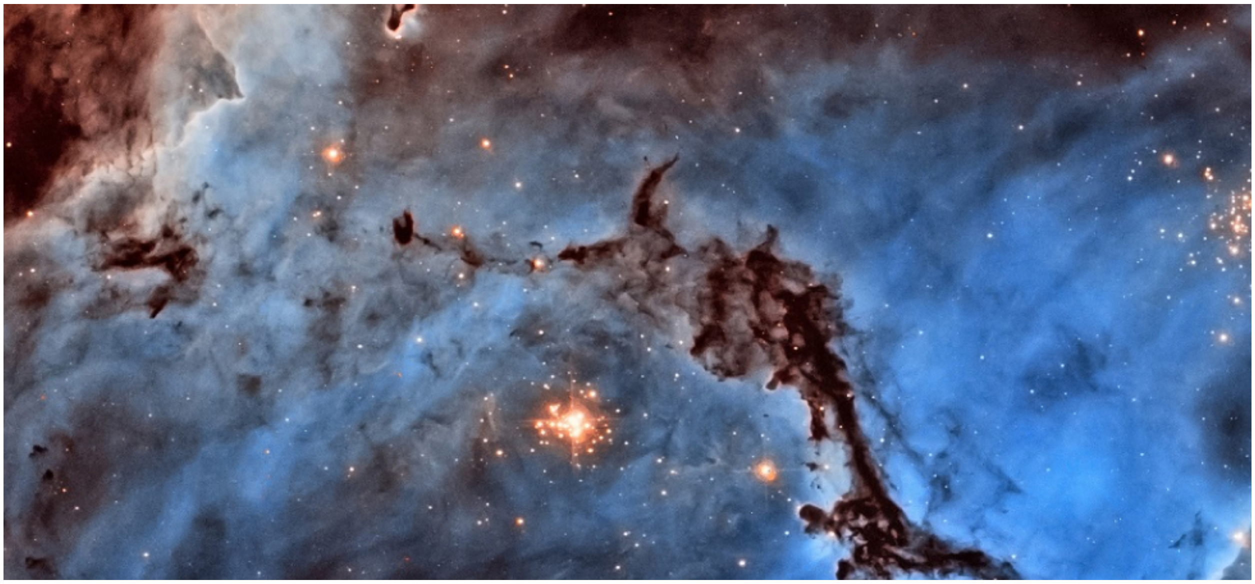


Figure 8.1 NGC1763 is an emission nebula in the Large Magellanic Cloud, which is a satellite galaxy to our Milky Way Galaxy. The colors we see can be explained by applying the ideas of quantum mechanics to atomic structure. (credit: modification of work by NASA, ESA, and Josh Lake)

Chapter Outline

Introduction

In this chapter, we use quantum mechanics to study the structure and properties of atoms. This study introduces ideas and concepts that are necessary to understand more complex systems, such as molecules, crystals, and metals. As we deepen our understanding of atoms, we build on things we already know, such as Rutherford's nuclear model of the atom, Bohr's model of the hydrogen atom, and de Broglie's wave hypothesis.

Figure 8.1 is NGC1763, an emission nebula in the small galaxy known as the Large Magellanic Cloud, which is a satellite of the Milky Way Galaxy. Ultraviolet light from hot stars ionizes the hydrogen atoms in the nebula. As protons and electrons recombine, radiation of different frequencies is emitted. The details of this process can be correctly predicted by quantum mechanics and are examined in this chapter.

8.1 | The Hydrogen Atom

Learning Objectives

By the end of this section, you will be able to:

- Describe the hydrogen atom in terms of wave function, probability density, total energy, and orbital angular momentum
- Identify the physical significance of each of the quantum numbers (n, l, m) of the hydrogen atom
- Distinguish between the Bohr and Schrödinger models of the atom
- Use quantum numbers to calculate important information about the hydrogen atom

The hydrogen atom is the simplest atom in nature and, therefore, a good starting point to study atoms and atomic structure. The hydrogen atom consists of a single negatively charged electron that moves about a positively charged proton (**Figure 8.2**). In Bohr's model, the electron is pulled around the proton in a perfectly circular orbit by an attractive Coulomb force. The proton is approximately 1800 times more massive than the electron, so the proton moves very little in response to the force on the proton by the electron. (This is analogous to the Earth-Sun system, where the Sun moves very little in response to the force exerted on it by Earth.) An explanation of this effect using Newton's laws is given in **Photons and Matter Waves**.

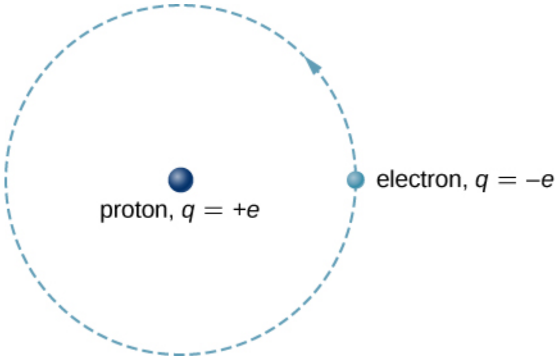


Figure 8.2 A representation of the Bohr model of the hydrogen atom.

With the assumption of a fixed proton, we focus on the motion of the electron.

In the electric field of the proton, the potential energy of the electron is

$$U(r) = -k\frac{e^2}{r}, \tag{8.1}$$

where $k = 1/4\pi\varepsilon_0$ and r is the distance between the electron and the proton. As we saw earlier, the force on an object is equal to the negative of the gradient (or slope) of the potential energy function. For the special case of a hydrogen atom, the force between the electron and proton is an attractive Coulomb force.

Notice that the potential energy function $U(r)$ does not vary in time. As a result, Schrödinger's equation of the hydrogen atom reduces to two simpler equations: one that depends only on space (x, y, z) and another that depends only on time (t). (The separation of a wave function into space- and time-dependent parts for time-independent potential energy functions is discussed in **Quantum Mechanics**.) We are most interested in the space-dependent equation:

$$\frac{-\hbar^2}{2m_e}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) - k\frac{e^2}{r}\psi = E\psi, \tag{8.2}$$

where $\psi = \psi(x, y, z)$ is the three-dimensional wave function of the electron, m_e is the mass of the electron, and E is the total energy of the electron. Recall that the total wave function $\Psi(x, y, z, t),$ is the product of the space-dependent wave function $\psi = \psi(x,\ y,\ z)$ and the time-dependent wave function $\varphi = \varphi(t)$.

In addition to being time-independent, $U(r)$ is also spherically symmetrical. This suggests that we may solve Schrödinger's equation more easily if we express it in terms of the spherical coordinates (r, θ, ϕ) instead of rectangular coordinates $(x,\ y,\ z)$. A spherical coordinate system is shown in **Figure 8.3**. In spherical coordinates, the variable r is the radial coordinate, θ is the polar angle (relative to the vertical z-axis), and ϕ is the azimuthal angle (relative to the x-axis). The relationship between spherical and rectangular coordinates is $x = r\sin\theta\cos\phi,\quad y = r\sin\theta\sin\phi,\quad z = r\cos\theta.$

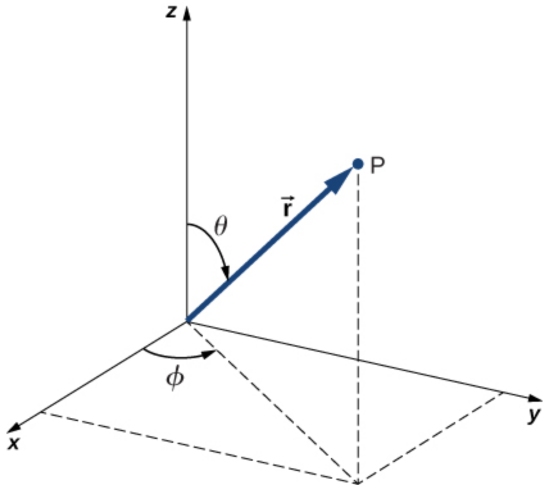


Figure 8.3 The relationship between the spherical and rectangular coordinate systems.

The factor $r\sin\theta$ is the magnitude of a vector formed by the projection of the polar vector onto the xy-plane. Also, the coordinates of x and y are obtained by projecting this vector onto the x- and y-axes, respectively. The inverse transformation gives

$$r = \sqrt{x^2 + y^2 + z^2},\quad \theta = \cos^{-1}\left(\frac{z}{r}\right),\quad \phi = \cos^{-1}\left(\frac{x}{\sqrt{x^2 + y^2}}\right).$$

Schrödinger's wave equation for the hydrogen atom in spherical coordinates is discussed in more advanced courses in modern physics, so we do not consider it in detail here. However, due to the spherical symmetry of $U(r)$, this equation reduces to three simpler equations: one for each of the three coordinates $(r,\ \theta,\ \text{and}\ \phi)$. Solutions to the time-independent wave function are written as a product of three functions:

$$\psi(r,\ \theta,\ \phi) = R(r)\Theta(\theta)\Phi(\phi),$$

where R is the radial function dependent on the radial coordinate r only; Θ is the polar function dependent on the polar coordinate θ only; and Φ is the phi function of ϕ only. Valid solutions to Schrödinger's equation $\psi(r,\ \theta,\ \phi)$ are labeled by the quantum numbers n, l, and m.

n : principal quantum number
l : angular momentum quantum number
m : angular momentum projection quantum number

(The reasons for these names will be explained in the next section.) The radial function R depends only on n and l; the polar function Θ depends only on l and m; and the phi function Φ depends only on m. The dependence of each function on quantum numbers is indicated with subscripts:

$$\psi_{nlm}(r,\ \theta,\ \phi) = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi).$$

Not all sets of quantum numbers $(n,\ l,\ m)$ are possible. For example, the orbital angular quantum number l can never be greater or equal to the principal quantum number $n(l < n)$. Specifically, we have

$$\begin{aligned} n &= 1, 2, 3, \ldots \\ l &= 0, 1, 2, \ldots, (n-1) \\ m &= -l, (-l+1), \ldots, 0, \ldots, (+l-1), \ +l \end{aligned}$$

Notice that for the ground state, $n = 1$, $l = 0$, and $m = 0$. In other words, there is only one quantum state with the wave function for $n = 1$, and it is ψ_{100}. However, for $n = 2$, we have

$$\begin{aligned} &l = 0, \quad m = 0 \\ &l = 1, \quad m = -1, 0, 1. \end{aligned}$$

Therefore, the allowed states for the $n = 2$ state are ψ_{200}, ψ_{21-1}, ψ_{210}, and ψ_{211}. Example wave functions for the hydrogen atom are given in **Table 8.1**. Note that some of these expressions contain the letter *i*, which represents $\sqrt{-1}$. When probabilities are calculated, these complex numbers do not appear in the final answer.

$n = 1, l = 0, m_l = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}} \frac{1}{a_0{}^{3/2}} e^{-r/a_0}$
$n = 2, l = 0, m_l = 0$	$\psi_{200} = \frac{1}{4\sqrt{2\pi}} \frac{1}{a_0{}^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$
$n = 2, l = 1, m_l = -1$	$\psi_{21-1} = \frac{1}{8\sqrt{\pi}} \frac{1}{a_0{}^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta e^{-i\phi}$
$n = 2, l = 1, m_l = 0$	$\psi_{210} = \frac{1}{4\sqrt{2\pi}} \frac{1}{a_0{}^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
$n = 2, l = 1, m_l = 1$	$\psi_{211} = \frac{1}{8\sqrt{\pi}} \frac{1}{a_0{}^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta e^{i\phi}$

Table 8.1 Wave Functions of the Hydrogen Atom

Physical Significance of the Quantum Numbers

Each of the three quantum numbers of the hydrogen atom (*n*, *l*, *m*) is associated with a different physical quantity. The **principal quantum number** *n* is associated with the total energy of the electron, E_n. According to Schrödinger's equation:

$$E_n = -\left(\frac{m_e k^2 e^4}{2^2}\right)\left(\frac{1}{n^2}\right) = -E_0\left(\frac{1}{n^2}\right), \tag{8.3}$$

where $E_0 = -13.6\,\text{eV}$. Notice that this expression is identical to that of Bohr's model. As in the Bohr model, the electron in a particular state of energy does not radiate.

Example 8.1

How Many Possible States?

For the hydrogen atom, how many possible quantum states correspond to the principal number $n = 3$? What are the energies of these states?

Strategy

For a hydrogen atom of a given energy, the number of allowed states depends on its orbital angular momentum. We can count these states for each value of the principal quantum number, $n = 1, 2, 3$. However, the total energy depends on the principal quantum number only, which means that we can use **Equation 8.3** and the number of states counted.

Solution

If $n = 3$, the allowed values of l are 0, 1, and 2. If $l = 0$, $m = 0$ (1 state). If $l = 1$, $m = -1, 0, +1$ (3 states); and if $l = 2$, $m = -2, -1, 0, +1, +2$ (5 states). In total, there are $1 + 3 + 5 = 9$ allowed states. Because the total energy depends only on the principal quantum number, $n = 3$, the energy of each of these states is

$$E_{n3} = -E_0\left(\frac{1}{n^2}\right) = \frac{-13.6\text{ eV}}{9} = -1.51\text{ eV}.$$

Significance

An electron in a hydrogen atom can occupy many different angular momentum states with the very same energy. As the orbital angular momentum increases, the number of the allowed states with the same energy increases.

The **angular momentum orbital quantum number** l is associated with the orbital angular momentum of the electron in a hydrogen atom. Quantum theory tells us that when the hydrogen atom is in the state ψ_{nlm}, the magnitude of its orbital angular momentum is

$$L = \sqrt{l(l+1)}\hbar, \tag{8.4}$$

where

$$l = 0, 1, 2, \ldots, (n-1).$$

This result is slightly different from that found with Bohr's theory, which quantizes angular momentum according to the rule $L = n$, where $n = 1, 2, 3, \ldots.$

Quantum states with different values of orbital angular momentum are distinguished using spectroscopic notation (**Table 8.2**). The designations *s*, *p*, *d*, and *f* result from early historical attempts to classify atomic spectral lines. (The letters stand for sharp, principal, diffuse, and fundamental, respectively.) After *f*, the letters continue alphabetically.

The ground state of hydrogen is designated as the 1*s* state, where "1" indicates the energy level $(n = 1)$ and "*s*" indicates the orbital angular momentum state ($l = 0$). When $n = 2$, l can be either 0 or 1. The $n = 2$, $l = 0$ state is designated "2*s*." The $n = 2$, $l = 1$ state is designated "2*p*." When $n = 3$, l can be 0, 1, or 2, and the states are 3*s*, 3*p*, and 3*d*, respectively. Notation for other quantum states is given in **Table 8.3**.

The **angular momentum projection quantum number** m is associated with the azimuthal angle ϕ (see **Figure 8.3**) and is related to the *z*-component of orbital angular momentum of an electron in a hydrogen atom. This component is given by

$$L_z = m\hbar, \tag{8.5}$$

where

$$m = -l, -l+1, \ldots, 0, \ldots, +l-1, l.$$

The *z*-component of angular momentum is related to the magnitude of angular momentum by

$$L_z = L\cos\theta, \tag{8.6}$$

where θ is the angle between the angular momentum vector and the *z*-axis. Note that the direction of the *z*-axis is determined by experiment—that is, along any direction, the experimenter decides to measure the angular momentum. For example, the *z*-direction might correspond to the direction of an external magnetic field. The relationship between L_z and L is given in **Figure 8.4**.

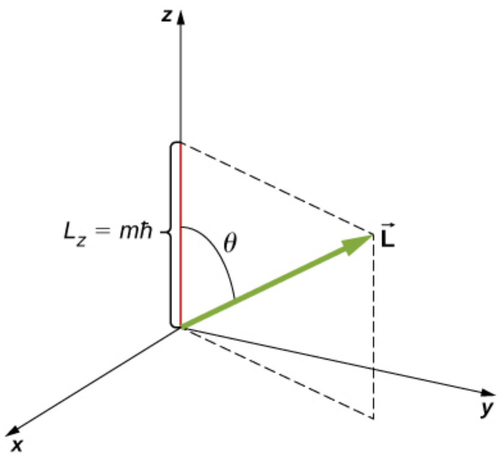


Figure 8.4 The z-component of angular momentum is quantized with its own quantum number m.

Orbital Quantum Number *l*	Angular Momentum	State	Spectroscopic Name
0	0	*s*	Sharp
1	$\sqrt{2}h$	*p*	Principal
2	$\sqrt{6}h$	*d*	Diffuse
3	$\sqrt{12}h$	*f*	Fundamental
4	$\sqrt{20}h$	*g*	
5	$\sqrt{30}h$	*h*	

Table 8.2 Spectroscopic Notation and Orbital Angular Momentum

	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$	$l = 5$
$n = 1$	1*s*					
$n = 2$	2*s*	2*p*				
$n = 3$	3*s*	3*p*	3*d*			
$n = 4$	4*s*	4*p*	4*d*	4*f*		
$n = 5$	5*s*	5*p*	5*d*	5*f*	5*g*	
$n = 6$	6*s*	6*p*	6*d*	6*f*	6*g*	6*h*

Table 8.3 Spectroscopic Description of Quantum States

The quantization of L_z is equivalent to the quantization of θ. Substituting $\sqrt{l(l+1)}\hbar$ for L and m for L_z into this equation, we find

$$m\hbar = \sqrt{l(l+1)}\hbar \cos\theta. \tag{8.7}$$

Thus, the angle θ is quantized with the particular values

$$\theta = \cos^{-1}\left(\frac{m}{\sqrt{l(l+1)}}\right). \tag{8.8}$$

Notice that both the polar angle (θ) and the projection of the angular momentum vector onto an arbitrary z-axis (L_z) are quantized.

The quantization of the polar angle for the $l = 3$ state is shown in **Figure 8.5**. The orbital angular momentum vector lies somewhere on the surface of a cone with an opening angle θ relative to the *z*-axis (unless $m = 0,$ in which case $\theta = 90°$ and the vector points are perpendicular to the *z*-axis).

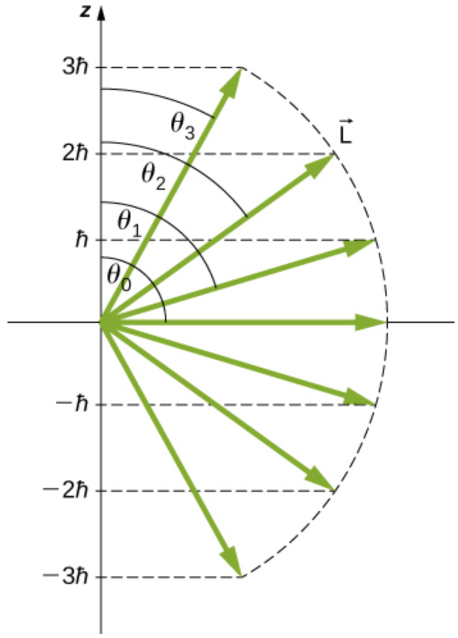


Figure 8.5 The quantization of orbital angular momentum. Each vector lies on the surface of a cone with axis along the *z*-axis.

A detailed study of angular momentum reveals that we cannot know all three components simultaneously. In the previous section, the *z*-component of orbital angular momentum has definite values that depend on the quantum number *m*. This implies that we cannot know both *x*- and *y*-components of angular momentum, L_x and L_y, with certainty. As a result, the precise direction of the orbital angular momentum vector is unknown.

Example 8.2

What Are the Allowed Directions?

Calculate the angles that the angular momentum vector $\vec{\mathbf{L}}$ can make with the *z*-axis for $l = 1$, as shown in **Figure 8.6**.

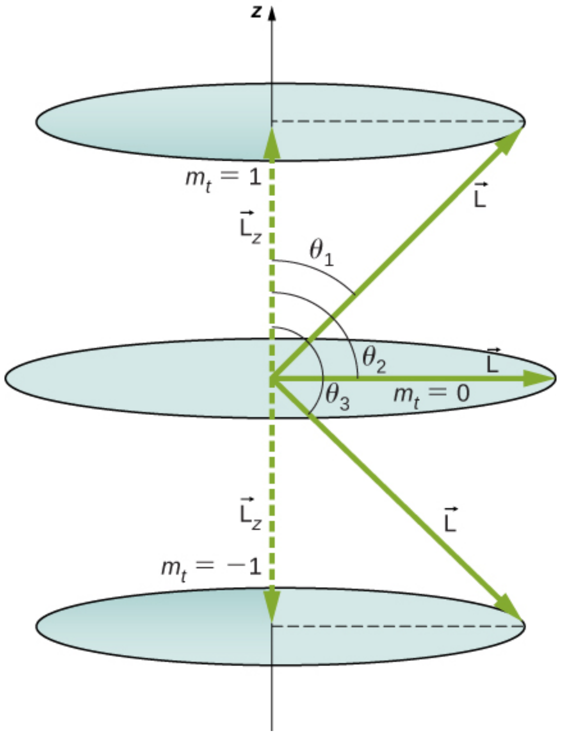


Figure 8.6 The component of a given angular momentum along the *z*-axis (defined by the direction of a magnetic field) can have only certain values. These are shown here for $l = 1$, for which $m = -1,\ 0,\ \text{and} + 1.$ The direction of $\vec{\mathbf{L}}$ is quantized in the sense that it can have only certain angles relative to the *z*-axis.

Strategy

The vectors $\vec{\mathbf{L}}$ and $\vec{\mathbf{L}}_z$ (in the *z*-direction) form a right triangle, where $\vec{\mathbf{L}}$ is the hypotenuse and $\vec{\mathbf{L}}_z$ is the adjacent side. The ratio of L_z to $|\vec{\mathbf{L}}|$ is the cosine of the angle of interest. The magnitudes $L = \left|\vec{\mathbf{L}}\right|$ and L_z are given by

$$L = \sqrt{l(l+1)}\hbar \text{ and } L_z = m\hbar.$$

Solution

We are given $l = 1$, so *ml* can be $+1,\ 0,\ \text{or}\ -1.$ Thus, L has the value given by

$$L = \sqrt{l(l+1)}\hbar = \sqrt{2}\hbar.$$

The quantity L_z can have three values, given by $L_z = m_l \hbar$.

$$L_z = m_l \hbar = \begin{cases} \hbar, & m_l = +1 \\ 0, & m_l = 0 \\ -\hbar, & m_l = -1 \end{cases}$$

As you can see in **Figure 8.6**, $\cos\theta = L_z/L,$ so for $m = +1$, we have

$$\cos\theta_1 = \frac{L_Z}{L} = \frac{\hbar}{\sqrt{2}\hbar} = \frac{1}{\sqrt{2}} = 0.707.$$

Thus,

$$\theta_1 = \cos^{-1} 0.707 = 45.0°.$$

Similarly, for $m = 0$, we find $\cos\theta_2 = 0;$ this gives

$$\theta_2 = \cos^{-1} 0 = 90.0°.$$

Then for $m_l = -1$:

$$\cos\theta_3 = \frac{L_Z}{L} = \frac{-\hbar}{\sqrt{2}\hbar} = -\frac{1}{\sqrt{2}} = -0.707,$$

so that

$$\theta_3 = \cos^{-1}(-0.707) = 135.0°.$$

Significance

The angles are consistent with the figure. Only the angle relative to the *z*-axis is quantized. *L* can point in any direction as long as it makes the proper angle with the *z*-axis. Thus, the angular momentum vectors lie on cones, as illustrated. To see how the correspondence principle holds here, consider that the smallest angle (θ_1 in the example) is for the maximum value of $m_l,$ namely $m_l = l.$ For that smallest angle,

$$\cos\theta = \frac{L_z}{L} = \frac{l}{\sqrt{l(l+1)}},$$

which approaches 1 as *l* becomes very large. If $\cos\theta = 1$, then $\theta = 0°$. Furthermore, for large *l*, there are many values of m_l, so that all angles become possible as *l* gets very large.

8.1 Check Your Understanding Can the magnitude of L_z ever be equal to *L*?

Using the Wave Function to Make Predictions

As we saw earlier, we can use quantum mechanics to make predictions about physical events by the use of probability statements. It is therefore proper to state, "An electron is located within this volume with this probability at this time," but not, "An electron is located at the position (*x*, *y*, *z*) at this time." To determine the probability of finding an electron in a hydrogen atom in a particular region of space, it is necessary to integrate the probability density $|\psi_{nlm}|^2$ over that region:

$$\text{Probability} = \int_{\text{volume}} |\psi_{nlm}|^2 dV, \tag{8.9}$$

where *dV* is an infinitesimal volume element. If this integral is computed for all space, the result is 1, because the probability of the particle to be located *somewhere* is 100% (the normalization condition). In a more advanced course on modern physics, you will find that $|\psi_{nlm}|^2 = \psi^*_{nlm}\psi_{nlm},$ where ψ^*_{nlm} is the complex conjugate. This eliminates the occurrences of $i = \sqrt{-1}$ in the above calculation.

Consider an electron in a state of zero angular momentum ($l = 0$). In this case, the electron's wave function depends only on the radial coordinate *r*. (Refer to the states ψ_{100} and ψ_{200} in **Table 8.1**.) The infinitesimal volume element corresponds to a spherical shell of radius *r* and infinitesimal thickness *dr*, written as

$$dV = 4\pi r^2 dr. \tag{8.10}$$

The probability of finding the electron in the region *r* to $r + dr$ ("at approximately *r*") is

$$P(r)dr = |\psi_{n00}|^2 4\pi r^2 dr. \tag{8.11}$$

Here $P(r)$ is called the **radial probability density function** (a probability per unit length). For an electron in the ground state of hydrogen, the probability of finding an electron in the region r to $r + dr$ is

$$|\psi_{n00}|^2 4\pi r^2 dr = (4/a_0^3)r^2 \exp(-2r/a_0)dr, \tag{8.12}$$

where $a_0 = 0.5$ angstroms. The radial probability density function $P(r)$ is plotted in **Figure 8.7**. The area under the curve between any two radial positions, say r_1 and r_2, gives the probability of finding the electron in that radial range. To find the most probable radial position, we set the first derivative of this function to zero ($dP/dr = 0$) and solve for r. The most probable radial position is not equal to the average or expectation value of the radial position because $|\psi_{n00}|^2$ is not symmetrical about its peak value.

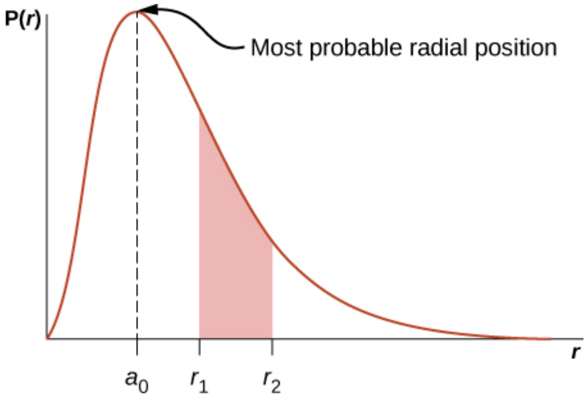


Figure 8.7 The radial probability density function for the ground state of hydrogen.

If the electron has orbital angular momentum ($l \neq 0$), then the wave functions representing the electron depend on the angles θ and ϕ; that is, $\psi_{nlm} = \psi_{nlm}(r, \theta, \phi)$. Atomic orbitals for three states with $n = 2$ and $l = 1$ are shown in **Figure 8.8**. An **atomic orbital** is a region in space that encloses a certain percentage (usually 90%) of the electron probability. (Sometimes atomic orbitals are referred to as "clouds" of probability.) Notice that these distributions are pronounced in certain directions. This directionality is important to chemists when they analyze how atoms are bound together to form molecules.

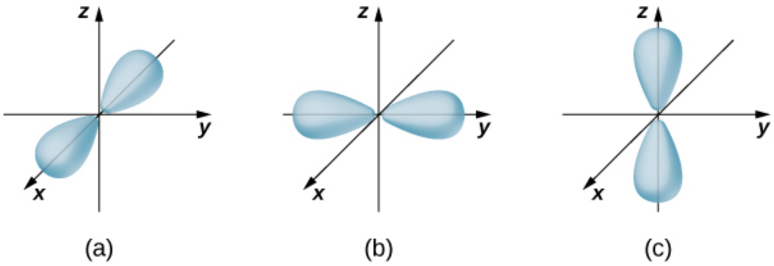


Figure 8.8 The probability density distributions for three states with $n = 2$ and $l = 1$. The distributions are directed along the (a) *x*-axis, (b) *y*-axis, and (c) *z*-axis.

A slightly different representation of the wave function is given in **Figure 8.9**. In this case, light and dark regions indicate locations of relatively high and low probability, respectively. In contrast to the Bohr model of the hydrogen atom, the electron does not move around the proton nucleus in a well-defined path. Indeed, the uncertainty principle makes it impossible to know how the electron gets from one place to another.

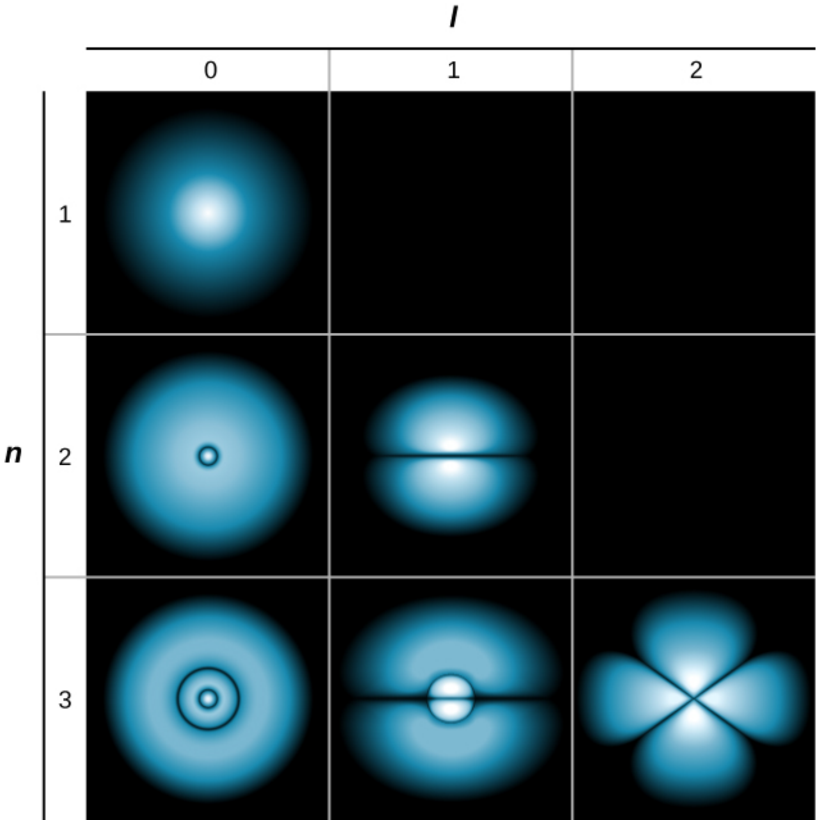


Figure 8.9 Probability clouds for the electron in the ground state and several excited states of hydrogen. The probability of finding the electron is indicated by the shade of color; the lighter the coloring, the greater the chance of finding the electron.

8.2 | Orbital Magnetic Dipole Moment of the Electron

Learning Objectives

By the end of this section, you will be able to:

- Explain why the hydrogen atom has magnetic properties
- Explain why the energy levels of a hydrogen atom associated with orbital angular momentum are split by an external magnetic field
- Use quantum numbers to calculate the magnitude and direction of the orbital magnetic dipole moment of a hydrogen atom

In Bohr's model of the hydrogen atom, the electron moves in a circular orbit around the proton. The electron passes by a particular point on the loop in a certain time, so we can calculate a current $I = Q/t$. An electron that orbits a proton in a hydrogen atom is therefore analogous to current flowing through a circular wire (**Figure 8.10**). In the study of magnetism, we saw that a current-carrying wire produces magnetic fields. It is therefore reasonable to conclude that the hydrogen atom produces a magnetic field and interacts with other magnetic fields.

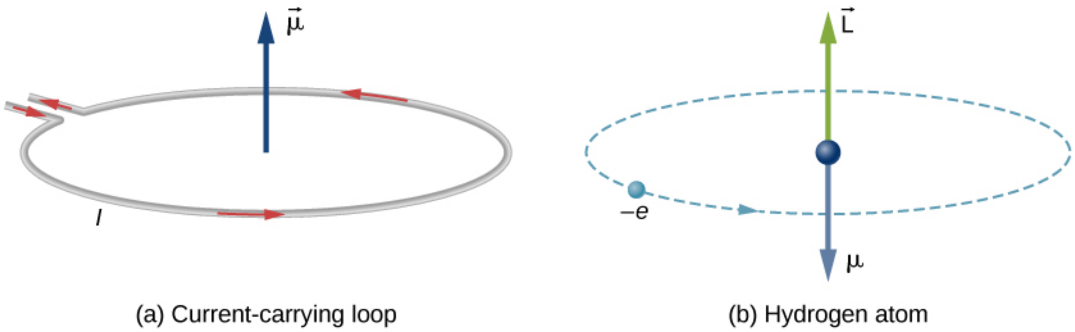


Figure 8.10 (a) Current flowing through a circular wire is analogous to (b) an electron that orbits a proton in a hydrogen atom.

The **orbital magnetic dipole moment** is a measure of the strength of the magnetic field produced by the orbital angular momentum of an electron. From **Force and Torque on a Current Loop (http://cnx.org/content/m58743/latest/#fs-id1171360245659)** , the magnitude of the orbital magnetic dipole moment for a current loop is

$$\mu = IA, \tag{8.13}$$

where I is the current and A is the area of the loop. (For brevity, we refer to this as the magnetic moment.) The current I associated with an electron in orbit about a proton in a hydrogen atom is

$$I = \frac{e}{T}, \tag{8.14}$$

where e is the magnitude of the electron charge and T is its orbital period. If we assume that the electron travels in a perfectly circular orbit, the orbital period is

$$T = \frac{2\pi r}{v}, \tag{8.15}$$

where r is the radius of the orbit and v is the speed of the electron in its orbit. Given that the area of a circle is πr^2, the absolute magnetic moment is

$$\mu = IA = \frac{e}{\left(\frac{2\pi r}{v}\right)}\pi r^2 = \frac{evr}{2}. \tag{8.16}$$

It is helpful to express the magnetic momentum μ in terms of the orbital angular momentum ($\vec{\mathbf{L}} = \vec{\mathbf{r}} \times \vec{\mathbf{p}}$). Because the electron orbits in a circle, the position vector $\vec{\mathbf{r}}$ and the momentum vector $\vec{\mathbf{p}}$ form a right angle. Thus, the magnitude of the orbital angular momentum is

$$L = \left|\vec{\mathbf{L}}\right| = \left|\vec{\mathbf{r}} \times \vec{\mathbf{p}}\right| = rp\sin\theta = rp = rmv. \tag{8.17}$$

Combining these two equations, we have

$$\mu = \left(\frac{e}{2m_e}\right)L. \tag{8.18}$$

In full vector form, this expression is written as

$$\vec{\boldsymbol{\mu}} = -\left(\frac{e}{2m_e}\right)\vec{\boldsymbol{L}}. \tag{8.19}$$

The negative sign appears because the electron has a negative charge. Notice that the direction of the magnetic moment of the electron is antiparallel to the orbital angular momentum, as shown in **Figure 8.10**(b). In the Bohr model of the atom, the relationship between $\vec{\mu}$ and $\vec{\mathbf{L}}$ in **Equation 8.19** is independent of the radius of the orbit.

The magnetic moment μ can also be expressed in terms of the orbital angular quantum number l. Combining **Equation**

8.18 and **Equation 8.15**, the magnitude of the magnetic moment is

$$\mu = \left(\frac{e}{2m_e}\right)L = \left(\frac{e}{2m_e}\right)\sqrt{l(l+1)}\hbar = \mu_B\sqrt{l(l+1)}. \tag{8.20}$$

The z-component of the magnetic moment is

$$\mu_z = -\left(\frac{e}{2m_e}\right)L_z = -\left(\frac{e}{2m_e}\right)m\hbar = -\mu_B m. \tag{8.21}$$

The quantity μ_B is a fundamental unit of magnetism called the **Bohr magneton**, which has the value 9.3×10^{-24} joule/tesla (J/T) or 5.8×10^{-5} eV/T. Quantization of the magnetic moment is the result of quantization of the orbital angular momentum.

As we will see in the next section, the total magnetic dipole moment of the hydrogen atom is due to both the orbital motion of the electron and its intrinsic spin. For now, we ignore the effect of electron spin.

Example 8.3

Orbital Magnetic Dipole Moment

What is the magnitude of the orbital dipole magnetic moment μ of an electron in the hydrogen atom in the (a) *s* state, (b) *p* state, and (c) *d* state? (Assume that the spin of the electron is zero.)

Strategy

The magnetic momentum of the electron is related to its orbital angular momentum L. For the hydrogen atom, this quantity is related to the orbital angular quantum number l. The states are given in spectroscopic notation, which relates a letter (*s*, *p*, *d*, etc.) to a quantum number.

Solution

The magnitude of the magnetic moment is given in **Equation 8.20**:

$$\mu = \left(\frac{e}{2m_e}\right)L = \left(\frac{e}{2m_e}\right)\sqrt{l(l+1)}\hbar = \mu_B\sqrt{l(l+1)}.$$

a. For the *s* state, $l = 0$ so we have $\mu = 0$ and $\mu_z = 0$.

b. For the *p* state, $l = 1$ and we have

$$\mu = \mu_B\sqrt{1(1+1)} = \sqrt{2}\mu_B$$
$$\mu_z = -\mu_B m, \text{ where } m = (-1, 0, 1), \text{ so}$$
$$\mu_z = \mu_B, 0, -\mu_B.$$

c. For the *d* state, $l = 2$ and we obtain

$$\mu = \mu_B\sqrt{2(2+1)} = \sqrt{6}\mu_B$$
$$\mu_z = -\mu_B m, \text{ where } m = (-2, -1, 0, 1, 2), \text{ so}$$
$$\mu_z = 2\mu_B, \mu_B, 0, -\mu_B, -2\mu_B.$$

Significance

In the *s* state, there is no orbital angular momentum and therefore no magnetic moment. This does not mean that the electron is at rest, just that the overall motion of the electron does not produce a magnetic field. In the *p* state, the electron has a magnetic moment with three possible values for the *z*-component of this magnetic moment; this means that magnetic moment can point in three different polar directions—each antiparallel to the orbital angular momentum vector. In the *d* state, the electron has a magnetic moment with five possible values for the *z*-component of this magnetic moment. In this case, the magnetic moment can point in five different polar directions.

A hydrogen atom has a magnetic field, so we expect the hydrogen atom to interact with an external magnetic field—such as the push and pull between two bar magnets. From **Force and Torque on a Current Loop (http://cnx.org/content/m58743/latest/#fs-id1171360288680)** , we know that when a current loop interacts with an external magnetic field $\vec{\mathbf{B}}$, it experiences a torque given by

$$\vec{\tau} = I\left(\vec{\mathbf{A}} \times \vec{\mathbf{B}}\right) = \vec{\boldsymbol{\mu}} \times \vec{\mathbf{B}}, \tag{8.22}$$

where I is the current, $\vec{\mathbf{A}}$ is the area of the loop, $\vec{\boldsymbol{\mu}}$ is the magnetic moment, and $\vec{\mathbf{B}}$ is the external magnetic field. This torque acts to rotate the magnetic moment vector of the hydrogen atom to align with the external magnetic field. Because mechanical work is done by the external magnetic field on the hydrogen atom, we can talk about energy transformations in the atom. The potential energy of the hydrogen atom associated with this magnetic interaction is given by **Equation 8.23**:

$$U = -\vec{\boldsymbol{\mu}} \cdot \vec{\boldsymbol{B}}. \tag{8.23}$$

If the magnetic moment is antiparallel to the external magnetic field, the potential energy is large, but if the magnetic moment is parallel to the field, the potential energy is small. Work done on the hydrogen atom to rotate the atom's magnetic moment vector in the direction of the external magnetic field is therefore associated with a drop in potential energy. The energy of the system is conserved, however, because a drop in potential energy produces radiation (the emission of a photon). These energy transitions are quantized because the magnetic moment can point in only certain directions.

If the external magnetic field points in the positive *z*-direction, the potential energy associated with the orbital magnetic dipole moment is

$$U(\theta) = -\mu B \cos\theta = -\mu_z B = -(-\mu_{\mathrm{B}} m)B = m\mu_{\mathrm{B}} B, \tag{8.24}$$

where μ_B is the Bohr magneton and m is the angular momentum projection quantum number (or **magnetic orbital quantum number**), which has the values

$$m = -l, -l+1, \ldots, 0, \ldots, l-1, l. \tag{8.25}$$

For example, in the $l = 1$ electron state, the total energy of the electron is split into three distinct energy levels corresponding to $U = -\mu_{\mathrm{B}} B, 0, \mu_{\mathrm{B}} B$.

The splitting of energy levels by an external magnetic field is called the **Zeeman effect**. Ignoring the effects of electron spin, transitions from the $l = 1$ state to a common lower energy state produce three closely spaced spectral lines (**Figure 8.11**, left column). Likewise, transitions from the $l = 2$ state produce five closely spaced spectral lines (right column). The separation of these lines is proportional to the strength of the external magnetic field. This effect has many applications. For example, the splitting of lines in the hydrogen spectrum of the Sun is used to determine the strength of the Sun's magnetic field. Many such magnetic field measurements can be used to make a map of the magnetic activity at the Sun's surface called a **magnetogram** (**Figure 8.12**).

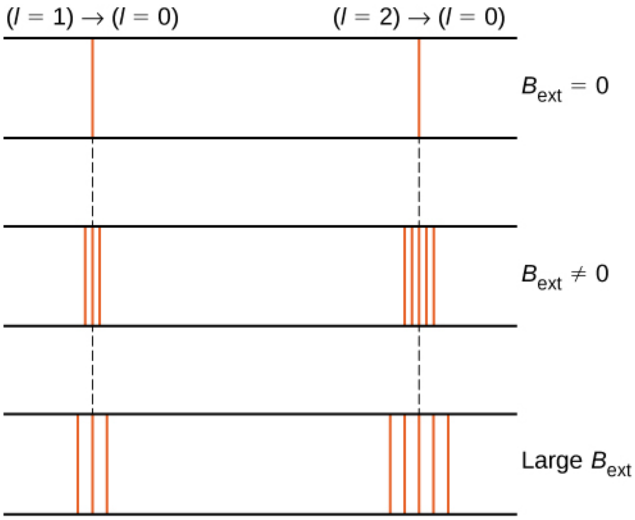


Figure 8.11 The Zeeman effect refers to the splitting of spectral lines by an external magnetic field. In the left column, the energy splitting occurs due to transitions from the state $(n = 2,\ l = 1)$ to a lower energy state; and in the right column, energy splitting occurs due to transitions from the state $(n = 2, l = 2)$ to a lower-energy state. The separation of these lines is proportional to the strength of the external magnetic field.

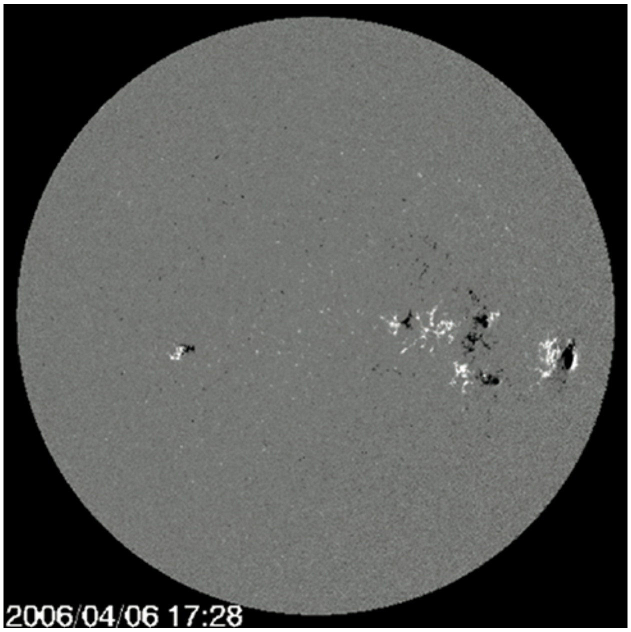


Figure 8.12 A magnetogram of the Sun. The bright and dark spots show significant magnetic activity at the surface of the Sun. (credit: NASA, SDO)

8.3 | Electron Spin

Learning Objectives

By the end of this section, you will be able to:

- Express the state of an electron in a hydrogen atom in terms of five quantum numbers
- Use quantum numbers to calculate the magnitude and direction of the spin and magnetic moment of an electron
- Explain the fine and hyperfine structure of the hydrogen spectrum in terms of magnetic interactions inside the hydrogen atom

In this section, we consider the effects of electron spin. Spin introduces two additional quantum numbers to our model of the hydrogen atom. Both were discovered by looking at the fine structure of atomic spectra. Spin is a fundamental characteristic of all particles, not just electrons, and is analogous to the intrinsic spin of extended bodies about their own axes, such as the daily rotation of Earth.

Spin is quantized in the same manner as orbital angular momentum. It has been found that the magnitude of the intrinsic spin angular momentum S of an electron is given by

$$S = \sqrt{s(s+1)}\hbar, \tag{8.26}$$

where s is defined to be the **spin quantum number**. This is similar to the quantization of L given in **Equation 8.4**, except that the only value allowed for s for an electron is $s = 1/2.$ The electron is said to be a “spin-half particle.” The **spin projection quantum number** m_s is associated with the *z*-components of spin, expressed by

$$S_z = m_s\hbar. \tag{8.27}$$

In general, the allowed quantum numbers are

$$m_s = -s, \ -s+1, \ \ldots, \ 0, \ \ldots, \ +s-1, \ s. \tag{8.28}$$

For the special case of an electron ($s = 1/2$),

$$m_s = -\frac{1}{2}, \frac{1}{2}. \tag{8.29}$$

Directions of intrinsic spin are quantized, just as they were for orbital angular momentum. The $m_s = -1/2$ state is called the “spin-down” state and has a *z*-component of spin, $s_z = -1/2$; the $m_s = +1/2$ state is called the “spin-up” state and has a *z*-component of spin, $s_z = +1/2.$ These states are shown in **Figure 8.13**.

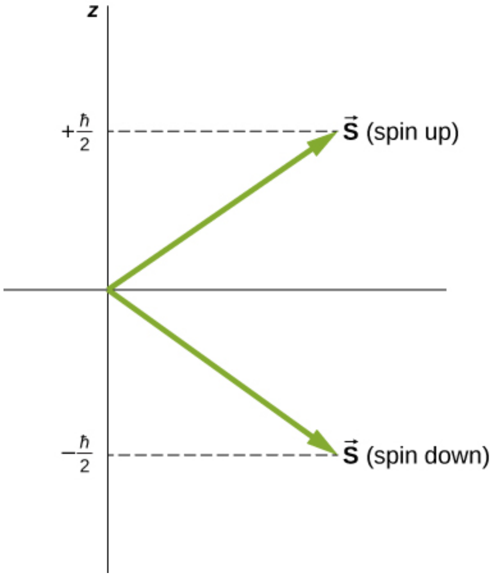


Figure 8.13 The two possible states of electron spin.

The intrinsic magnetic dipole moment of an electron μ_e can also be expressed in terms of the spin quantum number. In analogy to the orbital angular momentum, the magnitude of the electron magnetic moment is

$$\mu_s = \left(\frac{e}{2m_e}\right)S. \tag{8.30}$$

According to the special theory of relativity, this value is low by a factor of 2. Thus, in vector form, the spin magnetic moment is

$$\vec{\boldsymbol{\mu}} = \left(\frac{e}{m_e}\right)\vec{\mathbf{S}}\,. \tag{8.31}$$

The *z*-component of the magnetic moment is

$$\mu_z = -\left(\frac{e}{m_e}\right)S_z = -\left(\frac{e}{m_e}\right)m_s\,\hbar. \tag{8.32}$$

The spin projection quantum number has just two values $(m_s = \pm 1/2)$, so the *z*-component of the magnetic moment also has just two values:

$$\mu_z = \pm\left(\frac{e}{2m_e}\right) = \pm\mu_{\mathrm{B}}\,\hbar, \tag{8.33}$$

where μ_{B} is one Bohr magneton. An electron is magnetic, so we expect the electron to interact with other magnetic fields. We consider two special cases: the interaction of a free electron with an external (nonuniform) magnetic field, and an electron in a hydrogen atom with a magnetic field produced by the orbital angular momentum of the electron.

Example 8.4

Electron Spin and Radiation

A hydrogen atom in the ground state is placed in an external uniform magnetic field ($B = 1.5\ \mathrm{T}$). Determine the frequency of radiation produced in a transition between the spin-up and spin-down states of the electron.

Strategy

The spin projection quantum number is $m_s = \pm 1/2$, so the *z*-component of the magnetic moment is

$$\mu_z = \pm\left(\frac{e}{2m_e}\right) = \pm\mu_{\rm B}\hbar.$$

The potential energy associated with the interaction between the electron magnetic moment and the external magnetic field is

$$U = -\mu_z B = \mp\mu_{\rm B} B.$$

The frequency of light emitted is proportional to the energy (ΔE) difference between these two states.

Solution

The energy difference between these states is $\Delta E = 2\mu_{\rm B} B$, so the frequency of radiation produced is

$$f = \frac{\Delta E}{h} = \frac{2\mu_B B}{h} = \frac{2\left(5.79\times\frac{10^{-5}\ \text{eV}}{\text{T}}\right)(1.5\text{T})}{4.136\times10^{-15}\ \text{eV}\cdot\text{s}} = 4.2\times10^{10}\frac{\text{cycles}}{\text{s}}.$$

Significance

The electron magnetic moment couples with the external magnetic field. The energy of this system is different whether the electron is aligned or not with the proton. The frequency of radiation produced by a transition between these states is proportional to the energy difference. If we double the strength of the magnetic field, holding all other things constant, the frequency of the radiation doubles and its wavelength is cut in half.

In a hydrogen atom, the electron magnetic moment can interact with the magnetic field produced by the orbital angular momentum of the electron, a phenomenon called **spin-orbit coupling**. The orbital angular momentum ($\vec{L}$), orbital magnetic moment ($\vec{\mu}$), spin angular momentum ($\vec{S}$), and spin magnetic moment ($\vec{\mu}_s$) vectors are shown together in **Figure 8.14**.

Just as the energy levels of a hydrogen atom can be split by an *external* magnetic field, so too are the energy levels of a hydrogen atom split by *internal* magnetic fields of the atom. If the magnetic moment of the electron and orbital magnetic moment of the electron are antiparallel, the potential energy from the magnetic interaction is relatively high, but when these moments are parallel, the potential energy is relatively small. Transition from each of these two states to a lower-energy level results in the emission of a photon of slightly different frequency. That is, the spin-orbit coupling “splits” the spectral line expected from a spin-less electron. The **fine structure** of the hydrogen spectrum is explained by spin-orbit coupling.

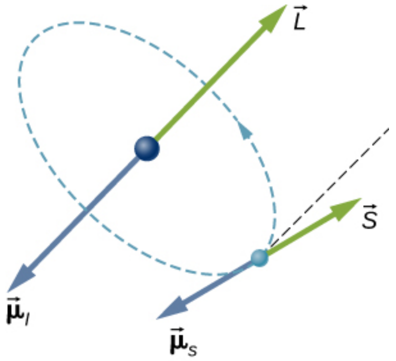


Figure 8.14 Spin-orbit coupling is the interaction of an electron’s spin magnetic moment $\vec{\mu}_s$ with its orbital magnetic moment $\vec{\mu}_l$.

The Stern-Gerlach experiment provides experimental evidence that electrons have spin angular momentum. The experiment passes a stream of silver (Ag) atoms through an external, nonuniform magnetic field. The Ag atom has an orbital angular momentum of zero and contains a single unpaired electron in the outer shell. Therefore, the total angular momentum of the Ag atom is due entirely to the spin of the outer electron ($s = 1/2$) . Due to electron spin, the Ag atoms act as tiny magnets as they pass through the magnetic field. These “magnets” have two possible orientations, which correspond to the spin-up and -down states of the electron. The magnetic field diverts the spin up atoms in one direction and the spin-down atoms in another direction. This produces two distinct bands on a screen (**Figure 8.15**).

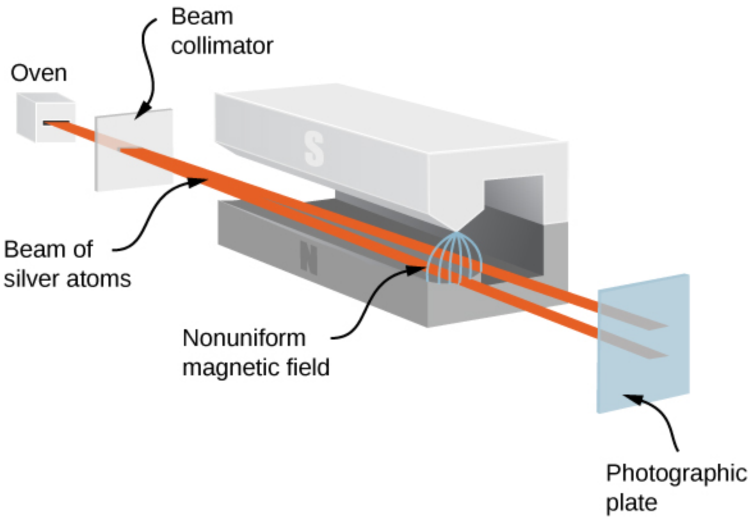


Figure 8.15 In the Stern-Gerlach experiment, an external, nonuniform magnetic field diverts a beam of electrons in two different directions. This result is due to the quantization of spin angular momentum.

According to classical predictions, the angular momentum (and, therefore, the magnetic moment) of the Ag atom can point in any direction, so one expects, instead, a continuous smudge on the screen. The resulting two bands of the Stern-Gerlach experiment provide startling support for the ideas of quantum mechanics.

Visit **PhET Explorations: Stern-Gerlach Experiment (https://openstaxcollege.org/l/21sterngerlach)** to learn more about the Stern-Gerlach experiment.

8.2 Check Your Understanding If the Stern-Gerlach experiment yielded four distinct bands instead of two, what might be concluded about the spin quantum number of the charged particle?

Just like an electron, a proton is spin 1/2 and has a magnetic moment. (According to nuclear theory, this moment is due to the orbital motion of quarks within the proton.) The **hyperfine structure** of the hydrogen spectrum is explained by the interaction between the magnetic moment of the proton and the magnetic moment of the electron, an interaction known as spin-spin coupling. The energy of the electron-proton system is different depending on whether or not the moments are aligned. Transitions between these states (**spin-flip transitions**) result in the emission of a photon with a wavelength of $\lambda \approx 21\text{ cm}$ (in the radio range). The 21-cm line in atomic spectroscopy is a “fingerprint” of hydrogen gas. Astronomers exploit this spectral line to map the spiral arms of galaxies, which are composed mostly of hydrogen (**Figure 8.16**).

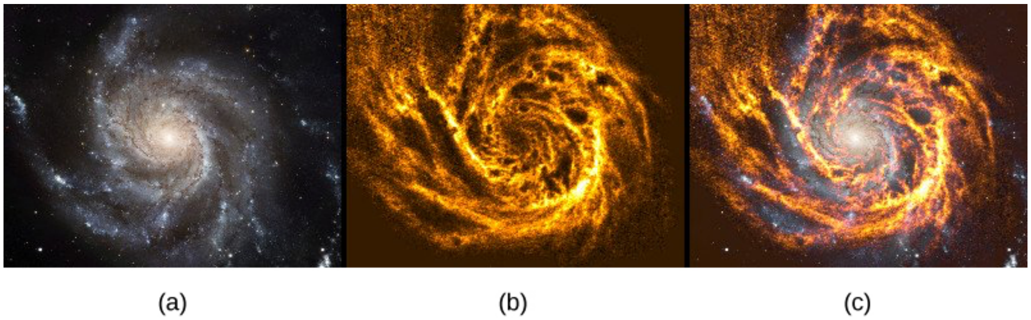

(a) (b) (c)

Figure 8.16 The magnetic interaction between the electron and proton in the hydrogen atom is used to map the spiral arms of the Pinwheel Galaxy (NGC 5457). (a) The galaxy seen in visible light; (b) the galaxy seen in 21-cm hydrogen radiation; (c) the composite image of (a) and (b). Notice how the hydrogen emission penetrates dust in the galaxy to show the spiral arms very clearly, whereas the galactic nucleus shows up better in visible light (credit a: modification of work by ESA & NASA; credit b: modification of work by Fabian Walter).

A complete specification of the state of an electron in a hydrogen atom requires five quantum numbers: n, l, m, s, and m_s. The names, symbols, and allowed values of these quantum numbers are summarized in **Table 8.4**.

Name	Symbol	Allowed values
Principal quantum number	n	1, 2, 3, …
Angular momentum	l	0, 1, 2, … $n - 1$
Angular momentum projection	m	$0, \ \pm 1, \ \pm 2, ... \pm l$
Spin	s	1/2 (electrons)
Spin projection	m_s	$-½, \ +½$

Table 8.4 Summary of Quantum Numbers of an Electron in a Hydrogen Atom

Note that the intrinsic quantum numbers introduced in this section (s and m_s) are valid for many particles, not just electrons. For example, quarks within an atomic nucleus are also spin-half particles. As we will see later, quantum numbers help to classify subatomic particles and enter into scientific models that attempt to explain how the universe works.

8.4 | The Exclusion Principle and the Periodic Table

Learning Objectives

By the end of this section, you will be able to:

- Explain the importance of Pauli's exclusion principle to an understanding of atomic structure and molecular bonding
- Explain the structure of the periodic table in terms of the total energy, orbital angular momentum, and spin of individual electrons in an atom
- Describe the electron configuration of atoms in the periodic table

So far, we have studied only hydrogen, the simplest chemical element. We have found that an electron in the hydrogen atom can be completely specified by five quantum numbers:

n : principal quantum number **(8.34)**
l : angular momentum quantum number
m : angular momentum projection quantum number
s : spin quantum number
m_s : spin projection quantum number

To construct the ground state of a neutral multi-electron atom, imagine starting with a nucleus of charge Ze (that is, a nucleus of atomic number Z) and then adding Z electrons one by one. Assume that each electron moves in a spherically symmetrical electric field produced by the nucleus and all other electrons of the atom. The assumption is valid because the electrons are distributed randomly around the nucleus and produce an average electric field (and potential) that is spherically symmetrical. The electric potential $U(r)$ for each electron does not follow the simple $-1/r$ form because of interactions between electrons, but it turns out that we can still label each individual electron state by quantum numbers, (n, l, m, s, m_s). (The spin quantum number s is the same for all electrons, so it will not be used in this section.)

The structure and chemical properties of atoms are explained in part by **Pauli's exclusion principle**: No two electrons in an atom can have the same values for all four quantum numbers (n, l, m, m_s). This principle is related to two properties of electrons: All electrons are identical ("when you've seen one electron, you've seen them all") and they have half-integral spin $(s = 1/2)$. Sample sets of quantum numbers for the electrons in an atom are given in **Table 8.5**. Consistent with Pauli's exclusion principle, no two rows of the table have the exact same set of quantum numbers.

n	***l***	***m***	m_s	**Subshell symbol**	**No. of electrons: subshell**	**No. of electrons: shell**
1	0	0	½	1*s*	2	2
1	0	0	–½			
2	0	0	½	2*s*	2	8
2	0	0	–½			
2	1	–1	½	2*p*	6	
2	1	–1	–½			
2	1	0	½			
2	1	0	–½			
2	1	1	½			
2	1	1	–½			
3	0	0	½	3*s*	2	18
3	0	0	–½			
3	1	–1	½	3*p*	6	
3	1	–1	–½			
3	1	0	½			
3	1	0	–½			
3	1	1	½			
3	1	1	–½			
3	2	–2	½	3*d*	10	
3	2	–2	–½			
3	2	–1	½			

Table 8.5 Electron States of Atoms Because of Pauli's exclusion principle, no two electrons in an atom have the same set of four quantum numbers.

n	l	m	m_s	Subshell symbol	No. of electrons: subshell	No. of electrons: shell
3	2	–1	–½			
3	2	0	½			
3	2	0	–½			
3	2	1	½			
3	2	1	–½			
3	2	2	½			
3	2	2	–½			

Table 8.5 Electron States of Atoms Because of Pauli's exclusion principle, no two electrons in an atom have the same set of four quantum numbers.

Electrons with the same principal quantum number *n* are said to be in the same shell, and those that have the same value of *l* are said to occupy the same subshell. An electron in the $n = 1$ state of a hydrogen atom is denoted 1*s*, where the first digit indicates the shell $(n = 1)$ and the letter indicates the subshell $(s,\ p,\ d,\ f\ldots$ correspond to $l = 0,\ 1,\ 2,\ 3\ldots).$ Two electrons in the $n = 1$ state are denoted as $1s^2,$ where the superscript indicates the number of electrons. An electron in the $n = 2$ state with $l = 1$ is denoted 2*p*. The combination of two electrons in the $n = 2$ and $l = 0$ state, and three electrons in the $n = 2$ and $l = 1$ state is written as $2s^2 2p^3,$ and so on. This representation of the electron state is called the **electron configuration** of the atom. The electron configurations for several atoms are given in Table 8.6. Electrons in the outer shell of an atom are called **valence electrons**. Chemical bonding between atoms in a molecule are explained by the transfer and sharing of valence electrons.

Element	Electron Configuration	Spin Alignment
H	$1s^1$	$(\uparrow)$
He	$1s^2$	$(\uparrow\downarrow)$
Li	$1s^2 2s^1$	$(\uparrow)$
Be	$1s^2 2s^2$	$(\uparrow\downarrow)$
B	$1s^2 2s^2 2p^1$	$(\uparrow\downarrow)(\uparrow)$
C	$1s^2 2s^2 2p^2$	$(\uparrow\downarrow)(\uparrow)(\uparrow)$
N	$1s^2 2s^2 2p^3$	$(\uparrow\downarrow)(\uparrow)(\uparrow)(\uparrow)$
O	$1s^2 2s^2 2p^4$	$(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow)(\uparrow)$
F	$1s^2 2s^2 2p^5$	$(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow)$
Ne	$1s^2 2s^2 2p^6$	$(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)$
Na	$1s^2 2s^2 2p^6 3s^1$	$(\uparrow)$

Table 8.6 Electron Configurations of Electrons in an Atom The symbol $(\uparrow)$ indicates an unpaired electron in the outer shell, whereas the symbol $(\uparrow\downarrow)$ indicates a pair of spin-up and -down electrons in an outer shell.

Element	Electron Configuration	Spin Alignment
Mg	$1s^2 2s^2 2p^6 3s^2$	$(\uparrow\downarrow)$
Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	$(\uparrow\downarrow)(\uparrow)$

Table 8.6 Electron Configurations of Electrons in an Atom The symbol $(\uparrow)$ indicates an unpaired electron in the outer shell, whereas the symbol $(\uparrow\downarrow)$ indicates a pair of spin-up and -down electrons in an outer shell.

The maximum number of electrons in a subshell depends on the value of the angular momentum quantum number, *l*. For a given a value *l*, there are $2l + 1$ orbital angular momentum states. However, each of these states can be filled by two electrons (spin up and down, $\uparrow\downarrow$). Thus, the maximum number of electrons in a subshell is

$$N = 2(2l + 1) = 4l + 2. \tag{8.35}$$

In the 2*s* $(l = 0)$ subshell, the maximum number of electrons is 2. In the 2*p* $(l = 1)$ subshell, the maximum number of electrons is 6. Therefore, the total maximum number of electrons in the $n = 2$ shell (including both the $l = 0$ and 1 subshells) is $2 + 6$ or 8. In general, the maximum number of electrons in the *n*th shell is $2n^2$.

Example 8.5

Subshells and Totals for $n = 3$

How many subshells are in the $n = 3$ shell? Identify each subshell and calculate the maximum number of electrons that will fill each. Show that the maximum number of electrons that fill an atom is $2n^2$.

Strategy

Subshells are determined by the value of *l*; thus, we first determine which values of *l* are allowed, and then we apply the equation “maximum number of electrons that can be in a subshell $= 2(2l + 1)$” to find the number of electrons in each subshell.

Solution

Because $n = 3$, we know that *l* can be 0, 1, or 2; thus, there are three possible subshells. In standard notation, they are labeled the 3*s*, 3*p*, and 3*d* subshells. We have already seen that two electrons can be in an *s* state, and six in a *p* state, but let us use the equation “maximum number of electrons that can be in a subshell $= 2(2l + 1)$” to calculate the maximum number in each:

$$\begin{aligned}
&3s \text{ has } l = 0;\ \text{thus, } 2(2l + 1) = 2(0 + 1) = 2 \\
&3p \text{ has } l = 1;\ \text{thus, } 2(2l + 1) = 2(2 + 1) = 6 \\
&3d \text{ has } l = 2;\ \text{thus, } 2(2l + 1) = 2(4 + 1) = 10 \\
&\text{Total} = 18 \\
&(\text{in the } n = 3 \text{ shell}).
\end{aligned}$$

The equation “maximum number of electrons that can be in a shell $= 2n^2$” gives the maximum number in the $n = 3$ shell to be

$$\text{Maximum number of electrons} = 2n^2 = 2(3)^2 = 2(9) = 18.$$

Significance

The total number of electrons in the three possible subshells is thus the same as the formula $2n^2$. In standard (spectroscopic) notation, a filled $n = 3$ shell is denoted as $3s^2 3p^6 3d^{10}$. Shells do not fill in a simple manner. Before the $n = 3$ shell is completely filled, for example, we begin to find electrons in the $n = 4$ shell.

The structure of the periodic table (**Figure 8.17**) can be understood in terms of shells and subshells, and, ultimately, the total energy, orbital angular momentum, and spin of the electrons in the atom. A detailed discussion of the periodic table is left to a chemistry course—we sketch only its basic features here. In this discussion, we assume that the atoms are electrically neutral; that is, they have the same number of electrons and protons. (Recall that the total number of protons in an atomic nucleus is called the atomic number, *Z*.)

First, the periodic table is arranged into columns and rows. The table is read left to right and top to bottom in the order of increasing atomic number *Z*. Atoms that belong to the same column or **chemical group** share many of the same chemical properties. For example, the Li and Na atoms (in the first column) bond to other atoms in a similar way. The first row of the table corresponds to the 1*s* ($l = 0$) shell of an atom.

Consider the hypothetical procedure of adding electrons, one by one, to an atom. For hydrogen (H) (upper left), the 1*s* shell is filled with either a spin up or down electron ($\uparrow$ or $\downarrow$). This lone electron is easily shared with other atoms, so hydrogen is chemically active. For helium (He) (upper right), the 1*s* shell is filled with both a spin up and a spin down ($\uparrow\downarrow$) electron. This "fills" the 1*s* shell, so a helium atom tends not to share electrons with other atoms. The helium atom is said to be chemically inactive, inert, or noble; likewise, helium gas is said to be an inert gas or noble gas.

Build an atom by adding and subtracting protons, neutrons, and electrons. How does the element, charge, and mass change? Visit **PhET Explorations: Build an Atom (https://openstaxcollege.org/l/21buildanatom)** to explore the answers to these questions.

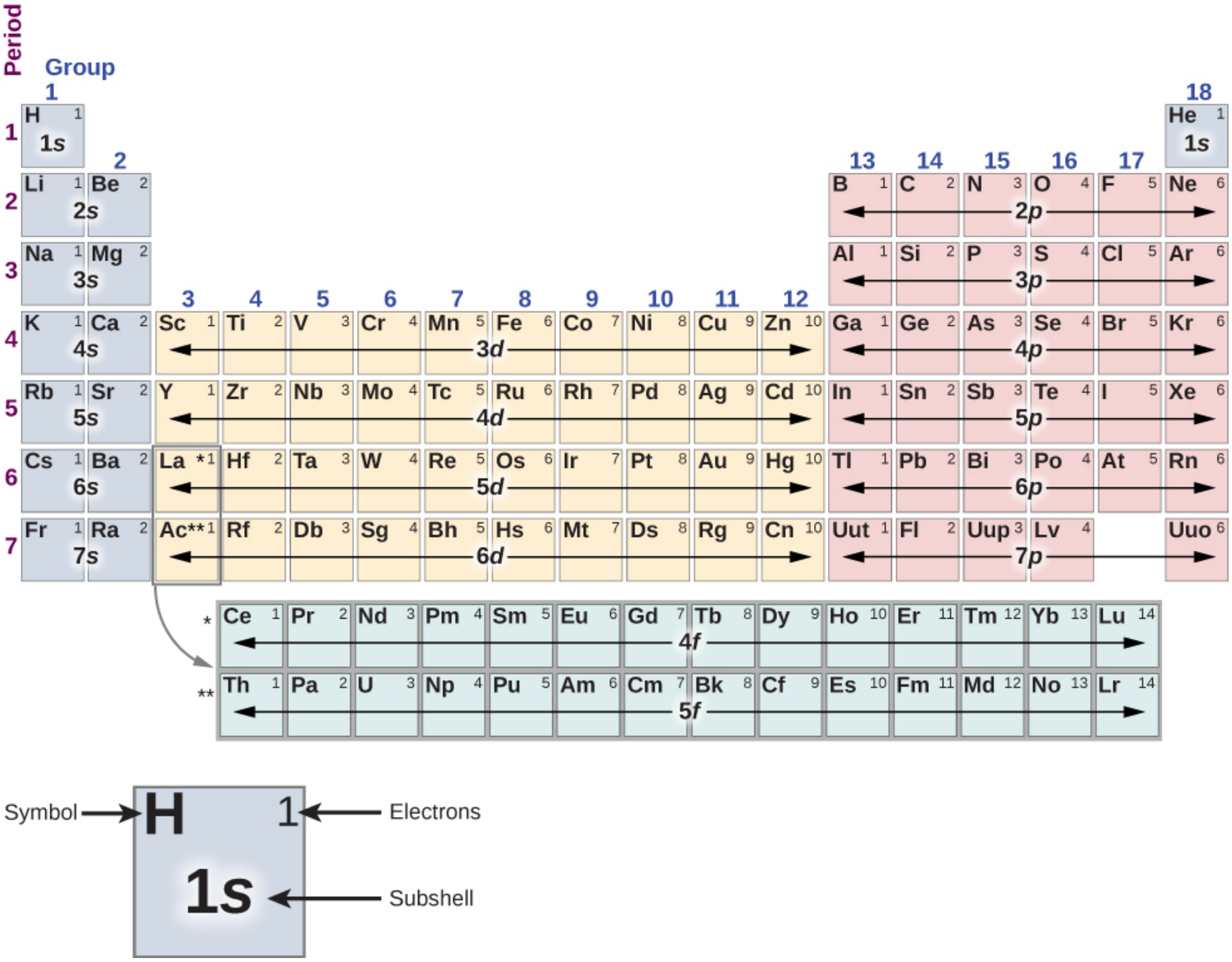


Figure 8.17 The periodic table of elements, showing the structure of shells and subshells.

The second row corresponds to the 2*s* and 2*p* subshells. For lithium (Li) (upper left), the 1*s* shell is filled with a spin-up *and* spin-down electron ($\uparrow\downarrow$) and the 2*s* shell is filled with either a spin-up or -down electron ($\uparrow$ or $\downarrow$). Its electron configuration is therefore $1s^2 2s^1$ or [He]2*s*, where [He] indicates a helium core. Like hydrogen, the lone electron in the outermost shell is easily shared with other atoms. For beryllium (Be), the 2*s* shell is filled with a spin-up and -down electron ($\uparrow\downarrow$), and has the electron configuration [He] $2s^2$.

Next, we look at the right side of the table. For boron (B), the 1*s* and 2*s* shells are filled and the 2*p* ($l = 1$) shell contains either a spin up or down electron ($\uparrow$ or $\downarrow$). From carbon (C) to neon (N), we the fill the 2*p* shell. The maximum number of electrons in the 2*p* shells is $4l + 2 = 4(2) + 2 = 6$. For neon (Ne), the 1*s* shell is filled with a spin-up and spin-down electron ($\uparrow\downarrow$), and the 2*p* shell is filled with six electrons ($\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow$) . This “fills” the 1*s*, 2*s*, and 2*p* subshells, so like helium, the neon atom tends not to share electrons with other atoms.

The process of electron filling repeats in the third row. However, beginning in the fourth row, the pattern is broken. The actual order of order of electron filling is given by

1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 4*s*, **3*d***, 4*p*, 5*s*, **4*d***, 5*p*, 6*s*, **4*f*, 5*d***, 6*p*, 7*s*,...

Notice that the 3*d*, 4*d*, 4*f*, and 5*d* subshells (in bold) are filled out of order; this occurs because of interactions between electrons in the atom, which so far we have neglected. The **transition metals** are elements in the gap between the first two columns and the last six columns that contain electrons that fill the *d* ($l = 1$) subshell. As expected, these atoms are arranged in $4l + 2 = 4(2) + 2 = 10$ columns. The structure of the periodic table can be understood in terms of the quantization of the total energy (*n*), orbital angular momentum (*l*), and spin (*s*). The first two columns correspond to the *s* ($l = 0$) subshell, the next six columns correspond to the *p* ($l = 1$) subshell, and the gap between these columns corresponds to the d ($l = 2$) subshell.

The periodic table also gives information on molecular bonding. To see this, consider atoms in the left-most column (the so-called alkali metals including: Li, Na, and K). These atoms contain a single electron in the 2*s* subshell, which is easily donated to other atoms. In contrast, atoms in the second-to-right column (the halogens: for example, Cl, F, and Br) are relatively stingy in sharing electrons. These atoms would much rather accept an electron, because they are just one electron shy of a filled shell ("of being noble").

Therefore, if a Na atom is placed in close proximity to a Cl atom, the Na atom freely donates its 2*s* electron and the Cl atom eagerly accepts it. In the process, the Na atom (originally a neutral charge) becomes positively charged and the Cl (originally a neutral charge) becomes negatively charged. Charged atoms are called ions. In this case, the ions are Na^{+} and Cl^{-}, where the superscript indicates charge of the ion. The electric (Coulomb) attraction between these atoms forms a NaCl (salt) molecule. A chemical bond between two ions is called an **ionic bond**. There are many kinds of chemical bonds. For example, in an oxygen molecule O_2 electrons are equally shared between the atoms. The bonding of oxygen atoms is an example of a **covalent bond**.

8.5 | Atomic Spectra and X-rays

Learning Objectives

By the end of this section, you will be able to:

- Describe the absorption and emission of radiation in terms of atomic energy levels and energy differences
- Use quantum numbers to estimate the energy, frequency, and wavelength of photons produced by atomic transitions in multi-electron atoms
- Explain radiation concepts in the context of atomic fluorescence and X-rays

The study of atomic spectra provides most of our knowledge about atoms. In modern science, atomic spectra are used to identify species of atoms in a range of objects, from distant galaxies to blood samples at a crime scene.

The theoretical basis of atomic spectroscopy is the transition of electrons between energy levels in atoms. For example, if an electron in a hydrogen atom makes a transition from the $n = 3$ to the $n = 2$ shell, the atom emits a photon with a wavelength

$$\lambda = \frac{c}{f} = \frac{h \cdot c}{h \cdot f} = \frac{hc}{\Delta E} = \frac{hc}{E_3 - E_2}, \tag{8.36}$$

where $\Delta E = E_3 - E_2$ is energy carried away by the photon and $hc = 1940\,\mathrm{eV} \cdot \mathrm{nm}$. After this radiation passes through a spectrometer, it appears as a sharp spectral line on a screen. The Bohr model of this process is shown in **Figure 8.18**. If the electron later absorbs a photon with energy ΔE, the electron returns to the $n = 3$ shell. (We examined the Bohr model earlier, in **Photons and Matter Waves**.)

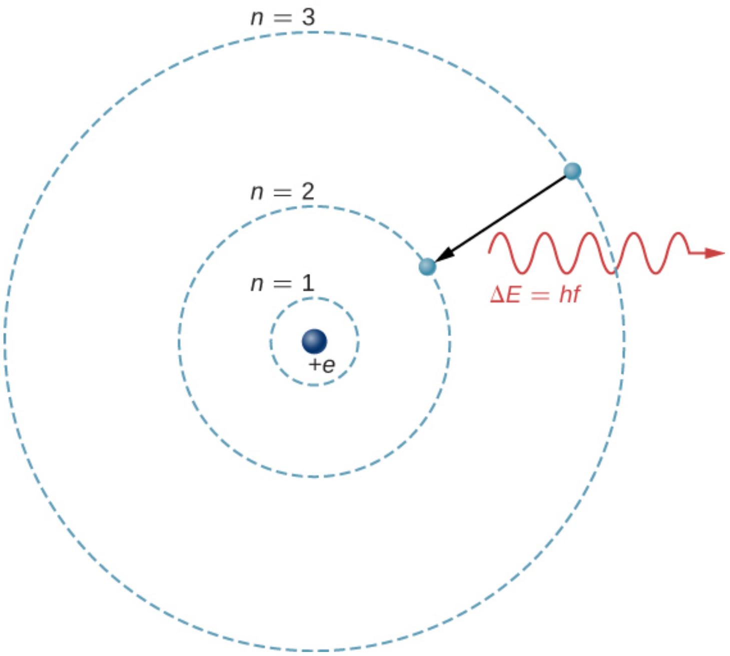


Figure 8.18 An electron transition from the $n = 3$ to the $n = 2$ shell of a hydrogen atom.

To understand atomic transitions in multi-electron atoms, it is necessary to consider many effects, including the Coulomb repulsion between electrons and internal magnetic interactions (spin-orbit and spin-spin couplings). Fortunately, many properties of these systems can be understood by neglecting interactions between electrons and representing each electron by its own single-particle wave function ψ_{nlm}.

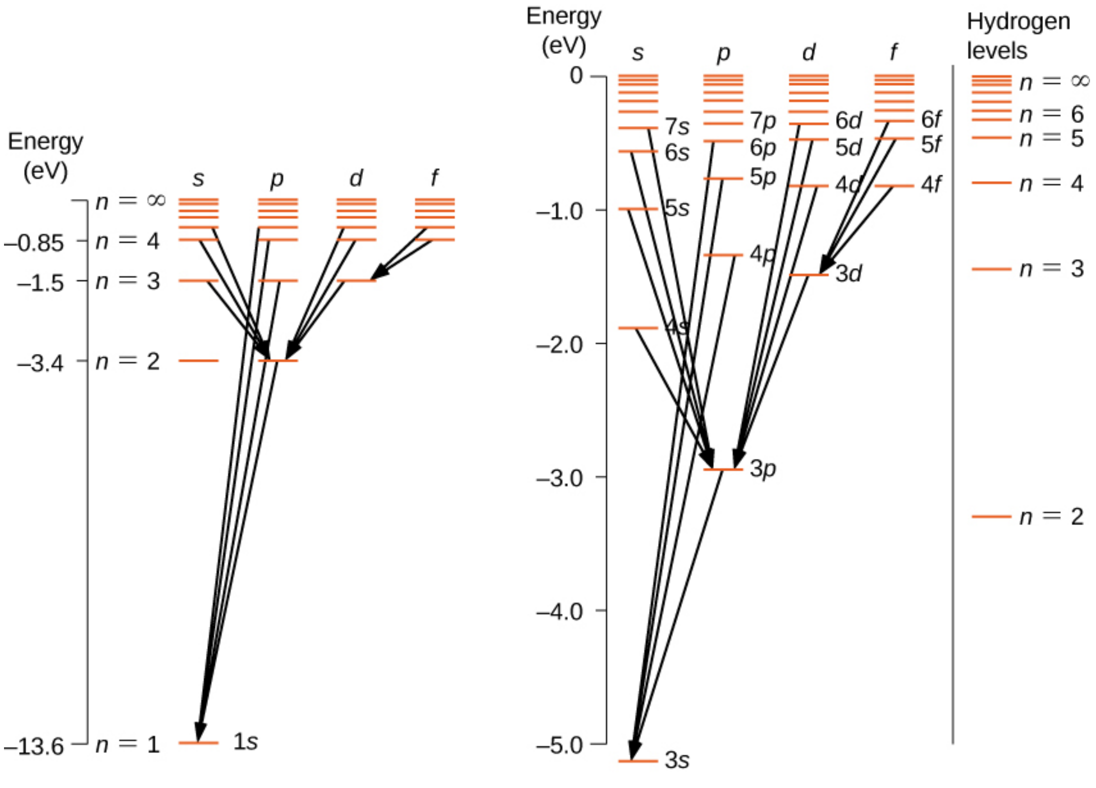
Atomic transitions must obey **selection rules**. These rules follow from principles of quantum mechanics and symmetry. Selection rules classify transitions as either allowed or forbidden. (Forbidden transitions do occur, but the probability of the typical forbidden transition is very small.) For a hydrogen-like atom, atomic transitions that involve electromagnetic interactions (the emission and absorption of photons) obey the following selection rule:

$$\Delta l = \pm 1, \tag{8.37}$$

where l is associated with the magnitude of orbital angular momentum,

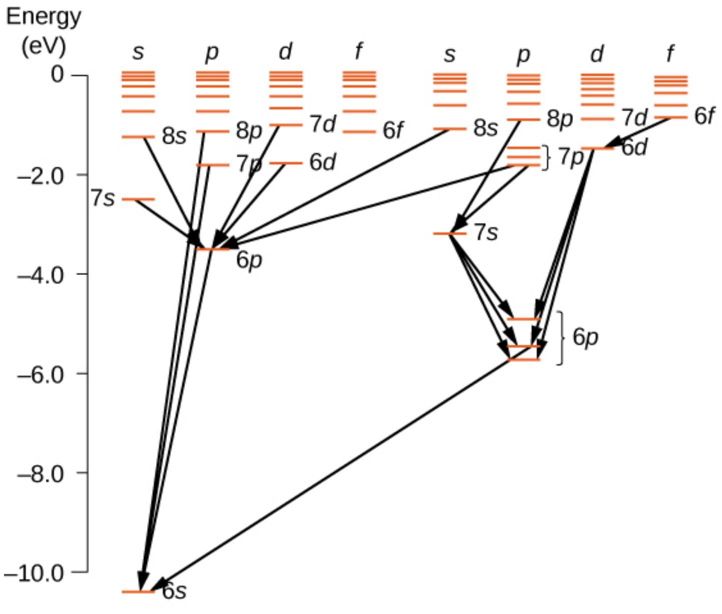
$$L = \sqrt{l(l+1)}\hbar. \tag{8.38}$$

For multi-electron atoms, similar rules apply. To illustrate this rule, consider the observed atomic transitions in hydrogen (H), sodium (Na), and mercury (Hg) (**Figure 8.19**). The horizontal lines in this diagram correspond to atomic energy levels, and the transitions allowed by this selection rule are shown by lines drawn between these levels. The energies of these states are on the order of a few electron volts, and photons emitted in transitions are in the visible range. Technically, atomic transitions can violate the selection rule, but such transitions are uncommon.



(a) Hydrogen

(b) Sodium



(c) Mercury

Figure 8.19 Energy-level diagrams for (a) hydrogen, (b) sodium, and (c) mercury. For comparison, hydrogen energy levels are shown in the sodium diagram.

The hydrogen atom has the simplest energy-level diagram. If we neglect electron spin, all states with the same value of n have the same total energy. However, spin-orbit coupling splits the $n = 2$ states into two angular momentum states (*s* and *p*) of slightly different energies. (These levels are not vertically displaced, because the energy splitting is too small to show up in this diagram.) Likewise, spin-orbit coupling splits the $n = 3$ states into three angular momentum states (*s*, *p*, and *d*).

The energy-level diagram for hydrogen is similar to sodium, because both atoms have one electron in the outer shell. The valence electron of sodium moves in the electric field of a nucleus shielded by electrons in the inner shells, so it does not experience a simple $1/r$ Coulomb potential and its total energy depends on both n and l. Interestingly, mercury has two separate energy-level diagrams; these diagrams correspond to two net spin states of its 6*s* (valence) electrons.

Example 8.6

The Sodium Doublet

The spectrum of sodium is analyzed with a spectrometer. Two closely spaced lines with wavelengths 589.00 nm and 589.59 nm are observed. (a) If the doublet corresponds to the excited (valence) electron that transitions from some excited state down to the 3*s* state, what was the original electron angular momentum? (b) What is the energy difference between these two excited states?

Strategy

Sodium and hydrogen belong to the same column or chemical group of the periodic table, so sodium is "hydrogen-like." The outermost electron in sodium is in the 3*s* ($l = 0$) subshell and can be excited to higher energy levels. As for hydrogen, subsequent transitions to lower energy levels must obey the selection rule:

$$\Delta l = \pm 1.$$

We must first determine the quantum number of the initial state that satisfies the selection rule. Then, we can use this number to determine the magnitude of orbital angular momentum of the initial state.

Solution

a. Allowed transitions must obey the selection rule. If the quantum number of the initial state is $l = 0$, the transition is forbidden because $\Delta l = 0$. If the quantum number of the initial state is $l = 2, 3, 4, \ldots$the transition is forbidden because $\Delta l > 1$. Therefore, the quantum of the initial state must be $l = 1$. The orbital angular momentum of the initial state is

$$L = \sqrt{l(l+1)}\hbar = 1.41\hbar.$$

b. Because the final state for both transitions is the same (3*s*), the difference in energies of the photons is equal to the difference in energies of the two excited states. Using the equation

$$\Delta E = hf = h\left(\frac{c}{\lambda}\right),$$

we have

$$\begin{aligned}\Delta E &= hc\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right)\\ &= \left(4.14 \times 10^{-15}\ \text{eVs}\right)\left(3.00 \times 10^{8}\ \text{m/s}\right) \times \left(\frac{1}{589.00 \times 10^{-9}\ \text{m}} - \frac{1}{589.59 \times 10^{-9}\ \text{m}}\right)\\ &= 2.11 \times 10^{-3}\ \text{eV}.\end{aligned}$$

Significance

To understand the difficulty of measuring this energy difference, we compare this difference with the average energy of the two photons emitted in the transition. Given an average wavelength of 589.30 nm, the average energy of the photons is

$$E = \frac{hc}{\lambda} = \frac{(4.14 \times 10^{-15}\ \text{eVs})(3.00 \times 10^{8}\ \text{m/s})}{589.30 \times 10^{-9}\ \text{m}} = 2.11\ \text{eV}.$$

The energy difference ΔE is about 0.1% (1 part in 1000) of this average energy. However, a sensitive spectrometer can measure the difference.

Atomic Fluorescence

Fluorescence occurs when an electron in an atom is excited several steps above the ground state by the absorption of a high-energy ultraviolet (UV) photon. Once excited, the electron "de-excites" in two ways. The electron can drop back to the ground state, emitting a photon of the same energy that excited it, or it can drop in a series of smaller steps, emitting several low-energy photons. Some of these photons may be in the visible range. Fluorescent dye in clothes can make colors seem brighter in sunlight by converting UV radiation into visible light. Fluorescent lights are more efficient in converting electrical energy into visible light than incandescent filaments (about four times as efficient). **Figure 8.20** shows a scorpion illuminated by a UV lamp. Proteins near the surface of the skin emit a characteristic blue light.

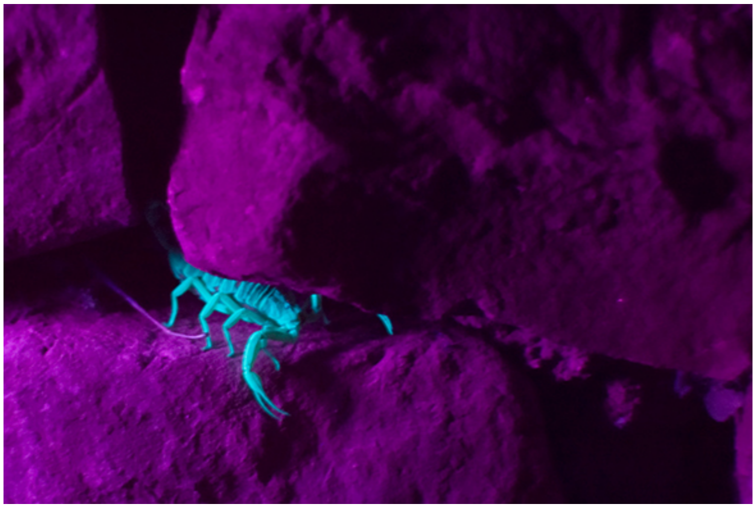


Figure 8.20 A scorpion glows blue under a UV lamp. (credit: Ken Bosma)

X-rays

The study of atomic energy transitions enables us to understand X-rays and X-ray technology. Like all electromagnetic radiation, X-rays are made of photons. X-ray photons are produced when electrons in the outermost shells of an atom drop to the inner shells. (Hydrogen atoms do not emit X-rays, because the electron energy levels are too closely spaced together to permit the emission of high-frequency radiation.) Transitions of this kind are normally forbidden because the lower states are already filled. However, if an inner shell has a vacancy (an inner electron is missing, perhaps from being knocked away by a high-speed electron), an electron from one of the outer shells can drop in energy to fill the vacancy. The energy gap for such a transition is relatively large, so wavelength of the radiated X-ray photon is relatively short.

X-rays can also be produced by bombarding a metal target with high-energy electrons, as shown in **Figure 8.21**. In the figure, electrons are boiled off a filament and accelerated by an electric field into a tungsten target. According to the classical theory of electromagnetism, *any* charged particle that accelerates emits radiation. Thus, when the electron strikes the tungsten target, and suddenly slows down, the electron emits **braking radiation**. (Braking radiation refers to radiation produced by any charged particle that is slowed by a medium.) In this case, braking radiation contains a continuous range of frequencies, because the electrons will collide with the target atoms in slightly different ways.

Braking radiation is not the only type of radiation produced in this interaction. In some cases, an electron collides with another inner-shell electron of a target atom, and knocks the electron out of the atom—billiard ball style. The empty state is filled when an electron in a higher shell drops into the state (drop in energy level) and emits an X-ray photon.

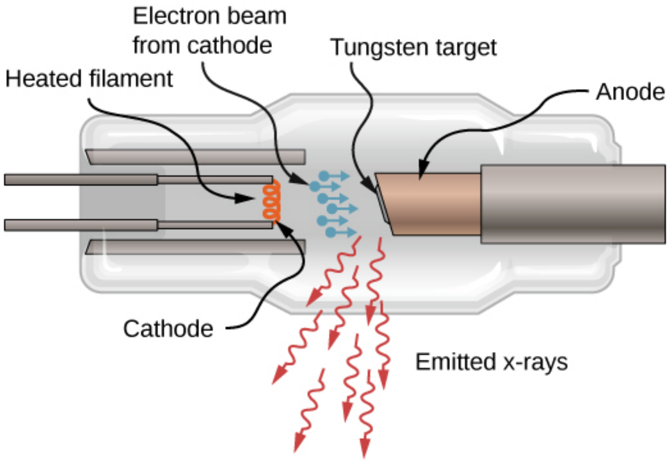


Figure 8.21 A sketch of an X-ray tube. X-rays are emitted from the tungsten target.

Historically, X-ray spectral lines were labeled with letters (*K*, *L*, *M*, *N*, …). These letters correspond to the atomic shells ($n = 1, 2, 3, 4, \ldots$). X-rays produced by a transition from any higher shell to the *K* ($n = 1$) shell are labeled as *K* X-rays. X-rays produced in a transition from the *L* ($n = 2$) shell are called K_α X-rays; X-rays produced in a transition from the *M* ($n = 3$) shell are called K_β X-rays; X-rays produced in a transition from the *N* ($n = 4$) shell are called K_γ X-rays; and so forth. Transitions from higher shells to *L* and *M* shells are labeled similarly. These transitions are represented by an energy-level diagram in **Figure 8.22**.

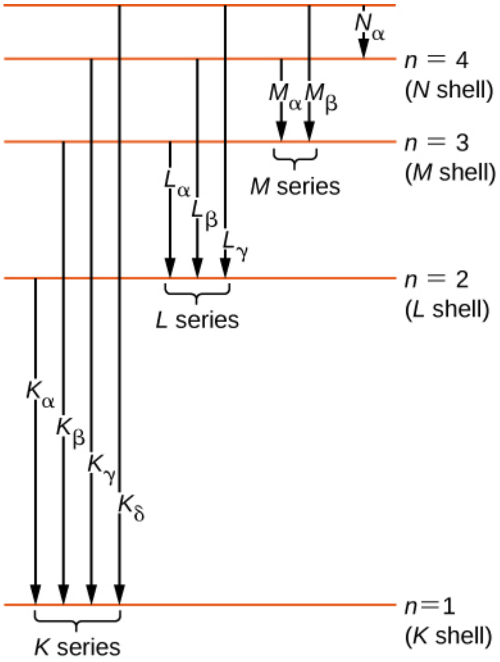


Figure 8.22 X-ray transitions in an atom.

The distribution of X-ray wavelengths produced by striking metal with a beam of electrons is given in **Figure 8.23**. X-ray transitions in the target metal appear as peaks on top of the braking radiation curve. Photon frequencies corresponding to the spikes in the X-ray distribution are called characteristic frequencies, because they can be used to identify the target metal. The sharp cutoff wavelength (just below the K_γ peak) corresponds to an electron that loses all of its energy to a single photon. Radiation of shorter wavelengths is forbidden by the conservation of energy.

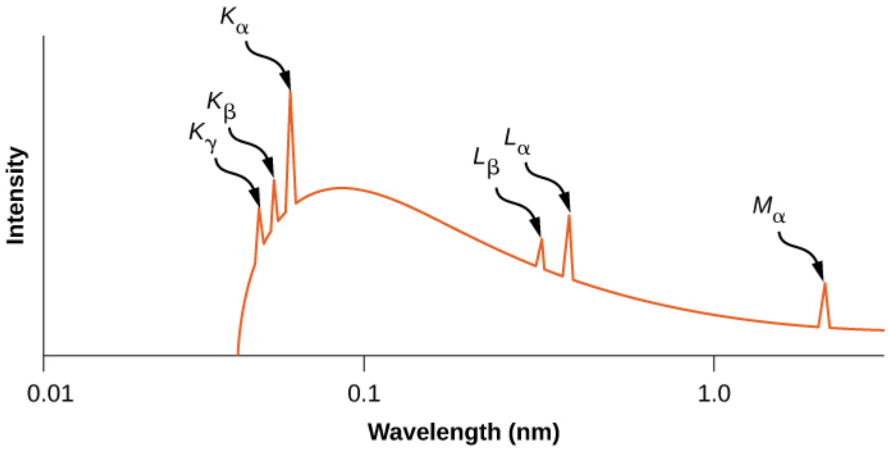


Figure 8.23 X-ray spectrum from a silver target. The peaks correspond to characteristic frequencies of X-rays emitted by silver when struck by an electron beam.

Example 8.7

X-Rays from Aluminum

Estimate the characteristic energy and frequency of the K_α X-ray for aluminum ($Z = 13$).

Strategy

A K_α X-ray is produced by the transition of an electron in the *L* ($n = 2$) shell to the *K* ($n = 1$) shell. An electron in the *L* shell "sees" a charge $Z = 13 - 1 = 12,$ because one electron in the *K* shell shields the nuclear charge. (Recall, two electrons are not in the *K* shell because the other electron state is vacant.) The frequency of the emitted photon can be estimated from the energy difference between the *L* and *K* shells.

Solution

The energy difference between the *L* and *K* shells in a hydrogen atom is 10.2 eV. Assuming that other electrons in the *L* shell or in higher-energy shells do not shield the nuclear charge, the energy difference between the *L* and *K* shells in an atom with $Z = 13$ is approximately

$$\Delta E_{L \to K} \approx (Z-1)^2(10.2\text{ eV}) = (13-1)^2(10.2\text{ eV}) = 1.47 \times 10^3\text{ eV}. \tag{8.39}$$

Based on the relationship $f = (\Delta E_{L \to K})/h$, the frequency of the X-ray is

$$f = \frac{1.47 \times 10^3\text{ eV}}{4.14 \times 10^{-15}\text{ eV} \cdot \text{s}} = 3.55 \times 10^{17}\text{ Hz}.$$

Significance

The wavelength of the typical X-ray is 0.1–10 nm. In this case, the wavelength is:

$$\lambda = \frac{c}{f} = \frac{3.0 \times 10^8\text{ m/s}}{3.55 \times 10^{17}\text{ Hz}} = 8.5 \times 10^{-10} = 0.85\text{ nm}.$$

Hence, the transition $L \to K$ in aluminum produces X-ray radiation.

X-ray production provides an important test of quantum mechanics. According to the Bohr model, the energy of a K_α X-ray depends on the nuclear charge or atomic number, *Z*. If *Z* is large, Coulomb forces in the atom are large, energy differences (ΔE) are large, and, therefore, the energy of radiated photons is large. To illustrate, consider a single electron in a multi-electron atom. Neglecting interactions between the electrons, the allowed energy levels are

$$E_n = -\frac{Z^2(13.6\text{ eV})}{n^2}, \tag{8.40}$$

where $n = 1, 2, \ldots$ and Z is the atomic number of the nucleus. However, an electron in the L ($n = 2$) shell “sees” a charge $Z - 1$, because one electron in the K shell shields the nuclear charge. (Recall that there is only one electron in the K shell because the other electron was “knocked out.”) Therefore, the approximate energies of the electron in the L and K shells are

$$\begin{aligned} E_L &\approx -\frac{(Z-1)^2(13.6\,\text{eV})}{2^2} \\ E_K &\approx -\frac{(Z-1)^2(13.6\,\text{eV})}{1^2}. \end{aligned}$$

The energy carried away by a photon in a transition from the L shell to the K shell is therefore

$$\begin{aligned} \Delta E_{L \to K} &= (Z-1)^2(13.6\,\text{eV})\left(\frac{1}{1^2} - \frac{1}{2^2}\right) \\ &= (Z-1)^2(10.2\,\text{eV}), \end{aligned}$$

where Z is the atomic number. In general, the X-ray photon energy for a transition from an outer shell to the K shell is

$$\Delta E_{L \to K} = hf = \text{constant} \times (Z-1)^2,$$

or

$$(Z-1) = \text{constant}\sqrt{f}, \tag{8.41}$$

where f is the frequency of a K_α X-ray. This equation is **Moseley’s law**. For large values of Z, we have approximately

$$Z \approx \text{constant}\sqrt{f}.$$

This prediction can be checked by measuring f for a variety of metal targets. This model is supported if a plot of Z versus $\sqrt{f}$ data (called a **Moseley plot**) is linear. Comparison of model predictions and experimental results, for both the K and L series, is shown in **Figure 8.24**. The data support the model that X-rays are produced when an outer shell electron drops in energy to fill a vacancy in an inner shell.

8.3 Check Your Understanding X-rays are produced by bombarding a metal target with high-energy electrons. If the target is replaced by another with two times the atomic number, what happens to the frequency of X-rays?

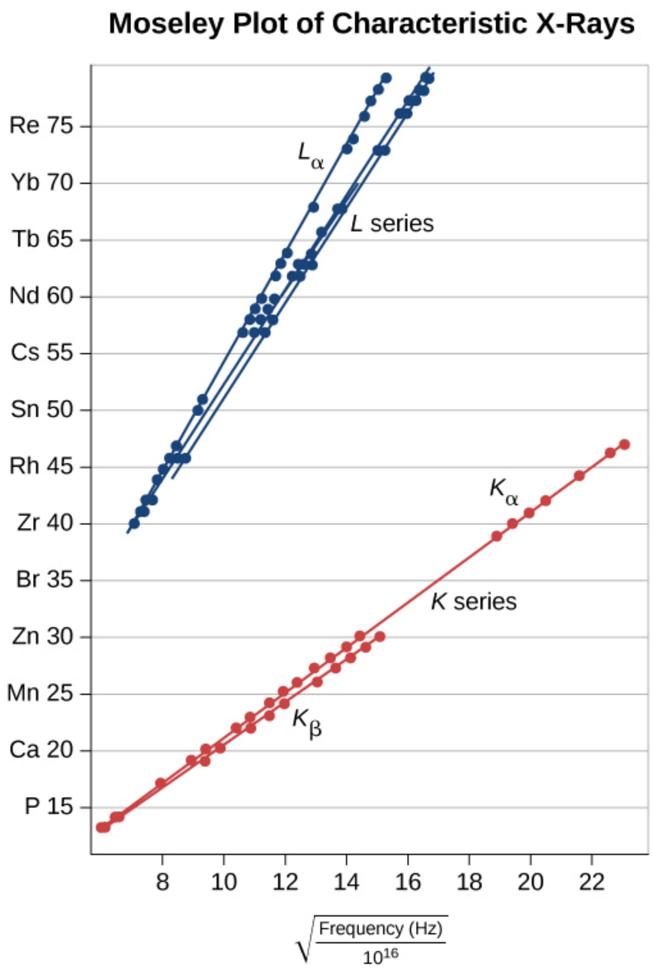


Figure 8.24 A Moseley plot. These data were adapted from Moseley’s original data (H. G. J. Moseley, *Philos. Mag.* (6) 77:703, 1914).

Example 8.8

Characteristic X-Ray Energy

Calculate the approximate energy of a K_α X-ray from a tungsten anode in an X-ray tube.

Strategy

Two electrons occupy a filled *K* shell. A vacancy in this shell would leave one electron, so the effective charge for an electron in the *L* shell would be $Z - 1$ rather than *Z*. For tungsten, $Z = 74,$ so the effective charge is 73.

This number can be used to calculate the energy-level difference between the *L* and *K* shells, and, therefore, the energy carried away by a photon in the transition $L \to K$.

Solution

The effective *Z* is 73, so the K_α X-ray energy is given by

$$E_{K_\alpha} = \Delta E = E_\text{i} - E_\text{f} = E_2 - E_1,$$

where

$$E_1 = -\frac{Z^2}{1^2}E_0 = -\frac{73^2}{1}(13.6\text{ eV}) = -72.5\text{ keV}$$

and

$$E_2 = -\frac{Z^2}{2^2}E_0 = -\frac{73^2}{4}(13.6\,\text{eV}) = -18.1\,\text{keV}.$$

Thus,

$$E_{K_\alpha} = -18.1\,\text{keV} - (-72.5\,\text{keV}) = 54.4\,\text{keV}.$$

Significance

This large photon energy is typical of X-rays. X-ray energies become progressively larger for heavier elements because their energy increases approximately as Z^2. An acceleration voltage of more than 50,000 volts is needed to "knock out" an inner electron from a tungsten atom.

X-ray Technology

X-rays have many applications, such as in medical diagnostics (**Figure 8.25**), inspection of luggage at airports (**Figure 8.26**), and even detection of cracks in crucial aircraft components. The most common X-ray images are due to shadows. Because X-ray photons have high energy, they penetrate materials that are opaque to visible light. The more energy an X-ray photon has, the more material it penetrates. The depth of penetration is related to the density of the material, as well as to the energy of the photon. The denser the material, the fewer X-ray photons get through and the darker the shadow. X-rays are effective at identifying bone breaks and tumors; however, overexposure to X-rays can damage cells in biological organisms.

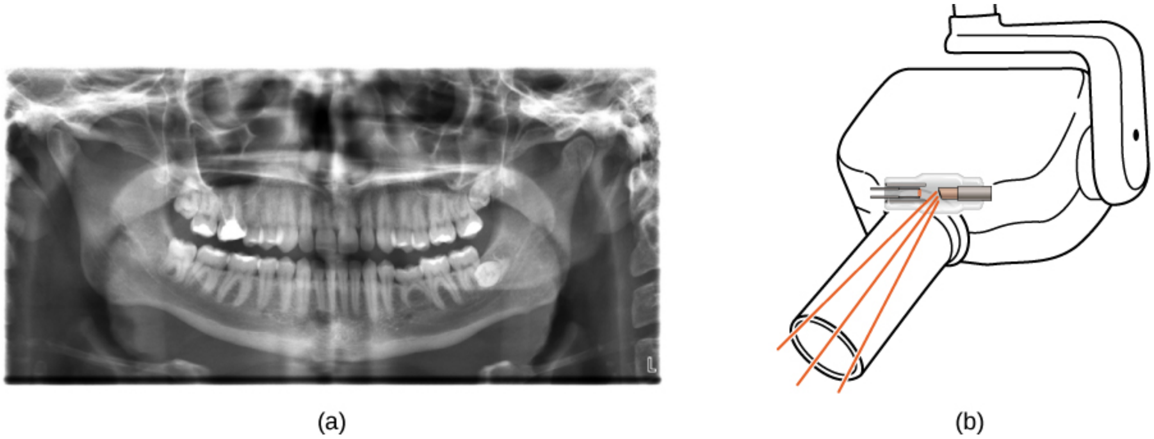


Figure 8.25 (a) An X-ray image of a person's teeth. (b) A typical X-ray machine in a dentist's office produces relatively low-energy radiation to minimize patient exposure. (credit a: modification of work by "Dmitry G"/Wikimedia Commons)

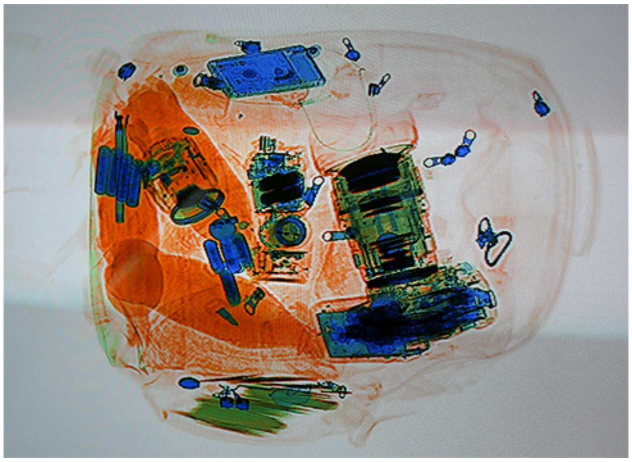


Figure 8.26 An X-ray image of a piece of luggage. The denser the material, the darker the shadow. Object colors relate to material composition—metallic objects show up as blue in this image. (credit: “IDuke”/Wikimedia Commons)

A standard X-ray image provides a two-dimensional view of the object. However, in medical applications, this view does not often provide enough information to draw firm conclusions. For example, in a two-dimensional X-ray image of the body, bones can easily hide soft tissues or organs. The CAT (computed axial tomography) scanner addresses this problem by collecting numerous X-ray images in “slices” throughout the body. Complex computer-image processing of the relative absorption of the X-rays, in different directions, can produce a highly detailed three-dimensional X-ray image of the body.

X-rays can also be used to probe the structures of atoms and molecules. Consider X-rays incident on the surface of a crystalline solid. Some X-ray photons reflect at the surface, and others reflect off the “plane” of atoms just below the surface. Interference between these photons, for different angles of incidence, produces a beautiful image on a screen (**Figure 8.27**). The interaction of X-rays with a solid is called X-ray diffraction. The most famous example using X-ray diffraction is the discovery of the double-helix structure of DNA.

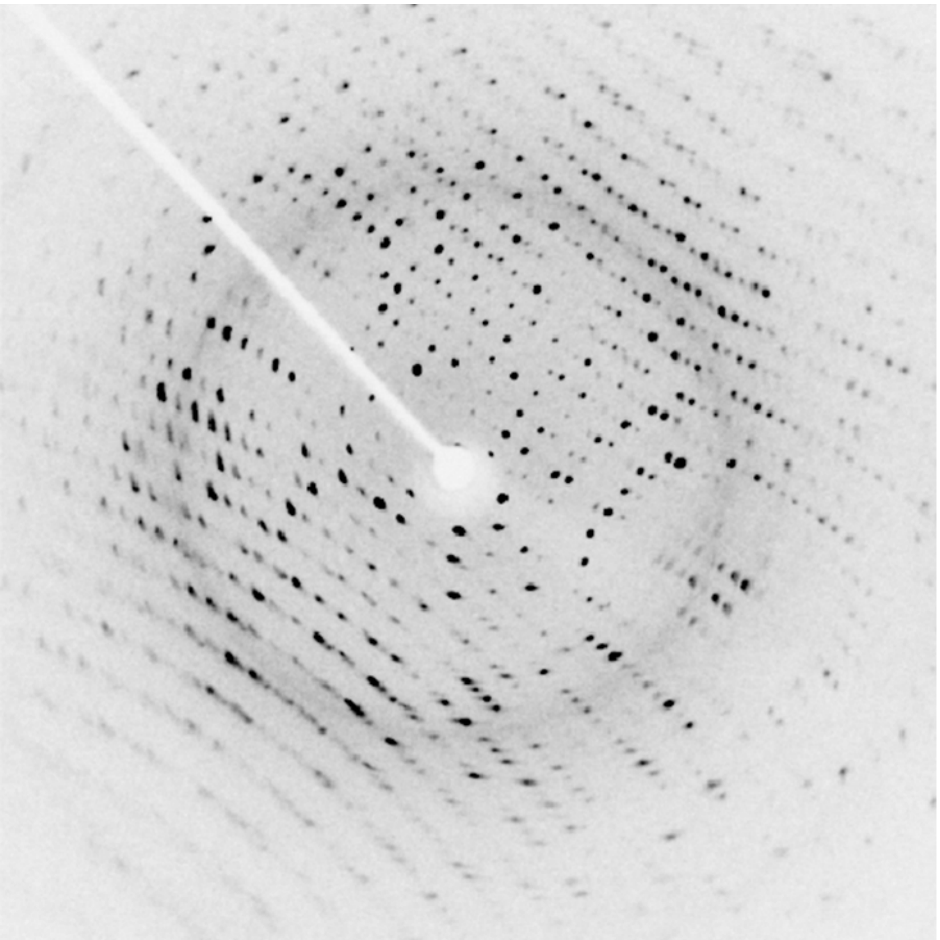


Figure 8.27 X-ray diffraction from the crystal of a protein (hen egg lysozyme) produced this interference pattern. Analysis of the pattern yields information about the structure of the protein. (credit: “Del45”/Wikimedia Commons)

8.6 | Lasers

Learning Objectives

By the end of this section, you will be able to:

- Describe the physical processes necessary to produce laser light
- Explain the difference between coherent and incoherent light
- Describe the application of lasers to a CD and Blu-Ray player

A **laser** is device that emits coherent and monochromatic light. The light is coherent if photons that compose the light are in-phase, and **monochromatic** if the photons have a single frequency (color). When a gas in the laser absorbs radiation, electrons are elevated to different energy levels. Most electrons return immediately to the ground state, but others linger in what is called a **metastable state**. It is possible to place a majority of these atoms in a metastable state, a condition called a **population inversion**.

When a photon of energy disturbs an electron in a metastable state (Figure 8.28), the electron drops to the lower-energy level and emits an addition photon, and the two photons proceed off together. This process is called **stimulated emission**. It occurs with relatively high probability when the energy of the incoming photon is equal to the energy difference between the excited and “de-excited” energy levels of the electron ($\Delta E = hf$). Hence, the incoming photon and the photon produced by de-excitation have the same energy, *hf*. These photons encounter more electrons in the metastable state, and the process repeats. The result is a cascade or chain reaction of similar de-excitations. Laser light is coherent because all light waves in laser light share the same frequency (color) and the same phase (any two points of along a line perpendicular to the direction of motion are on the “same part” of the wave”). A schematic diagram of coherent and incoherent light wave pattern is given in **Figure 8.29**.

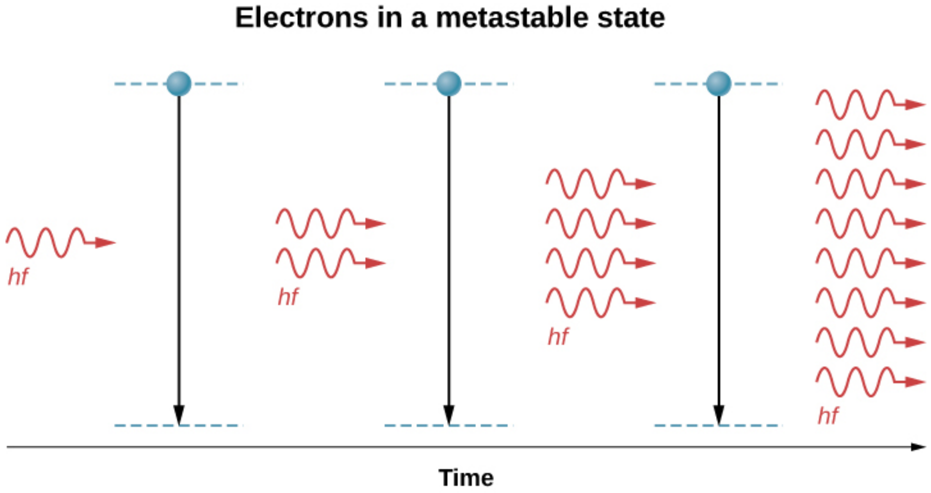


Figure 8.28 The physics of a laser. An incident photon of frequency *f* causes a cascade of photons of the same frequency.

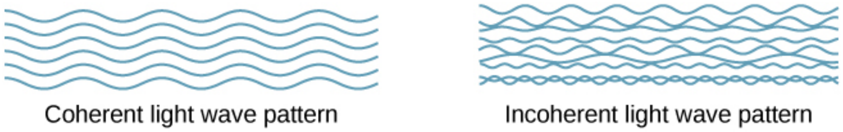


Figure 8.29 A coherent light wave pattern contains light waves of the same frequency and phase. An incoherent light wave pattern contains light waves of different frequencies and phases.

Lasers are used in a wide range of applications, such as in communication (optical fiber phone lines), entertainment (laser light shows), medicine (removing tumors and cauterizing vessels in the retina), and in retail sales (bar code readers). Lasers can also be produced by a large range of materials, including solids (for example, the ruby crystal), gases (helium-gas mixture), and liquids (organic dyes). Recently, a laser was even created using gelatin—an edible laser! Below we discuss two practical applications in detail: CD players and Blu-Ray Players.

CD Player

A CD player reads digital information stored on a compact disc (CD). A CD is 6-inch diameter disc made of plastic that contains small “bumps” and “pits” nears its surface to encode digital or binary data (**Figure 8.30**). The bumps and pits appear along a very thin track that spirals outwards from the center of the disc. The width of the track is smaller than 1/20th the width of a human hair, and the heights of the bumps are even smaller yet.

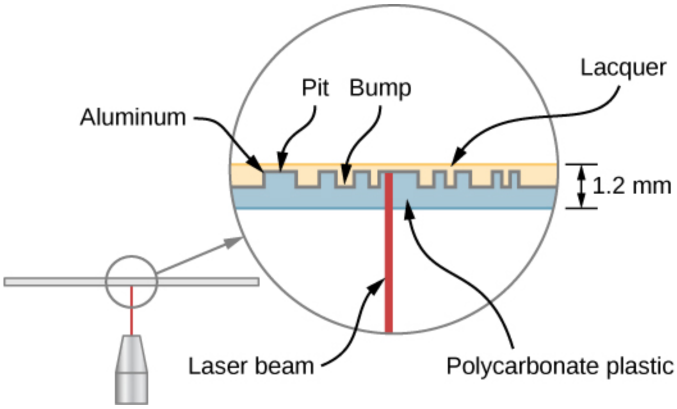


Figure 8.30 A compact disc is a plastic disc that uses bumps near its surface to encode digital information. The surface of the disc contains multiple layers, including a layer of aluminum and one of polycarbonate plastic.

A CD player uses a laser to read this digital information. Laser light is suited to this purpose, because coherent light can be focused onto an incredibly small spot and therefore distinguish between bumps and pits in the CD. After processing by player components (including a diffraction grating, polarizer, and collimator), laser light is focused by a lens onto the CD surface. Light that strikes a bump (“land”) is merely reflected, but light that strikes a “pit” destructively interferes, so no light returns (the details of this process are not important to this discussion). Reflected light is interpreted as a “1” and unreflected light is interpreted as a “0.” The resulting digital signal is converted into an analog signal, and the analog signal is fed into an amplifier that powers a device such as a pair of headphones. The laser system of a CD player is shown in **Figure 8.31**.

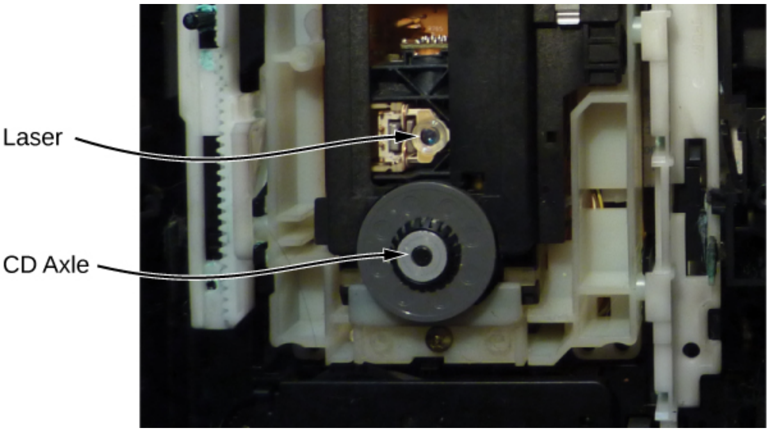


Figure 8.31 A CD player and its laser component.

Blu-Ray Player

Like a CD player, a Blu-Ray player reads digital information (video or audio) stored on a disc, and a laser is used to record this information. The pits on a Blu-Ray disc are much smaller and more closely packed together than for a CD, so much more information can be stored. As a result, the resolving power of the laser must be greater. This is achieved using short wavelength $(\lambda = 405\text{ nm})$ blue laser light—hence, the name “Blu-” Ray. (CDs and DVDs use red laser light.) The different pit sizes and player-hardware configurations of a CD, DVD, and Blu-Ray player are shown in **Figure 8.32**. The pit sizes of a Blu-Ray disk are more than twice as small as the pits on a DVD or CD. Unlike a CD, a Blu-Ray disc store data on a polycarbonate layer, which places the data closer to the lens and avoids readability problems. A hard coating is used to protect the data since it is so close to the surface.

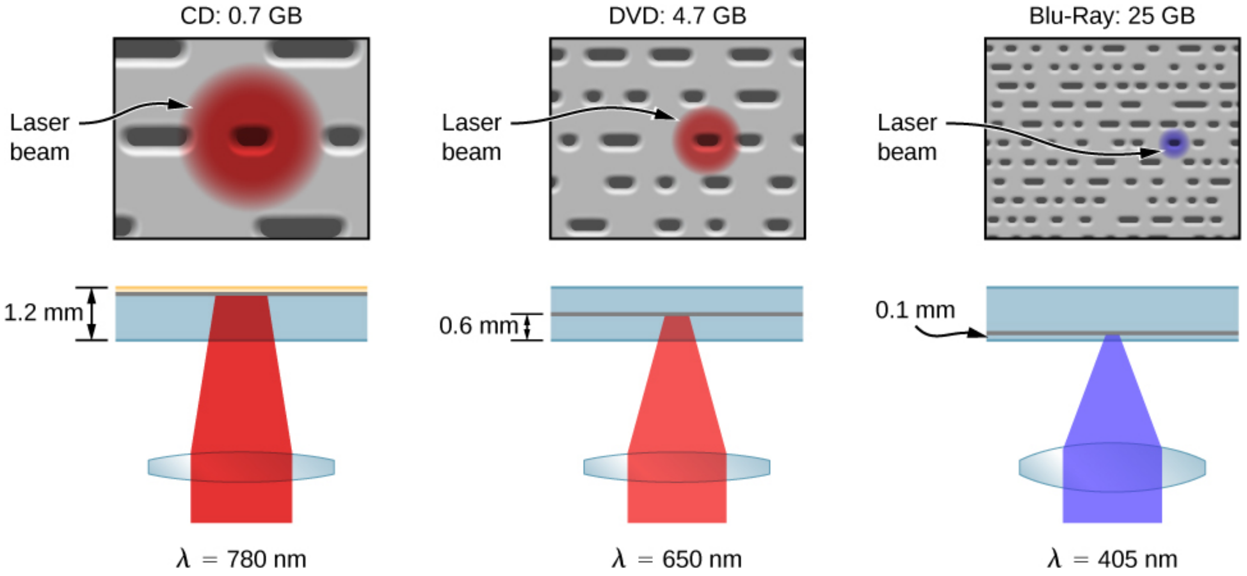


Figure 8.32 Comparison of laser resolution in a CD, DVD, and Blu-Ray Player.

CHAPTER 8 REVIEW

KEY TERMS

angular momentum orbital quantum number (*l*) quantum number associated with the orbital angular momentum of an electron in a hydrogen atom

angular momentum projection quantum number (*m*) quantum number associated with the *z*-component of the orbital angular momentum of an electron in a hydrogen atom

atomic orbital region in space that encloses a certain percentage (usually 90%) of the electron probability

Bohr magneton magnetic moment of an electron, equal to $9.3 \times 10^{-24}\,\text{J/T}$ or $5.8 \times 10^{-5}\,\text{eV/T}$

braking radiation radiation produced by targeting metal with a high-energy electron beam (or radiation produced by the acceleration of any charged particle in a material)

chemical group group of elements in the same column of the periodic table that possess similar chemical properties

coherent light light that consists of photons of the same frequency and phase

covalent bond chemical bond formed by the sharing of electrons between two atoms

electron configuration representation of the state of electrons in an atom, such as $1s^2 2s^1$ for lithium

fine structure detailed structure of atomic spectra produced by spin-orbit coupling

fluorescence radiation produced by the excitation and subsequent, gradual de-excitation of an electron in an atom

hyperfine structure detailed structure of atomic spectra produced by spin-orbit coupling

ionic bond chemical bond formed by the electric attraction between two oppositely charged ions

laser coherent light produced by a cascade of electron de-excitations

magnetic orbital quantum number another term for the angular momentum projection quantum number

magnetogram pictoral representation, or map, of the magnetic activity at the Sun's surface

metastable state state in which an electron "lingers" in an excited state

monochromatic light that consists of photons with the same frequency

Moseley plot plot of the atomic number versus the square root of X-ray frequency

Moseley's law relationship between the atomic number and X-ray photon frequency for X-ray production

orbital magnetic dipole moment measure of the strength of the magnetic field produced by the orbital angular momentum of the electron

Pauli's exclusion principle no two electrons in an atom can have the same values for all four quantum numbers $(n,\, l,\, m,\, m_s)$

population inversion condition in which a majority of atoms contain electrons in a metastable state

principal quantum number (*n*) quantum number associated with the total energy of an electron in a hydrogen atom

radial probability density function function use to determine the probability of a electron to be found in a spatial interval in *r*

selection rules rules that determine whether atomic transitions are allowed or forbidden (rare)

spin projection quantum number (m_s) quantum number associated with the *z*-component of the spin angular momentum of an electron

spin quantum number (*s*) quantum number associated with the spin angular momentum of an electron

spin-flip transitions atomic transitions between states of an electron-proton system in which the magnetic moments are aligned and not aligned

spin-orbit coupling interaction between the electron magnetic moment and the magnetic field produced by the orbital angular momentum of the electron

stimulated emission when a photon of energy triggers an electron in a metastable state to drop in energy emitting an additional photon

transition metal element that is located in the gap between the first two columns and the last six columns of the table of elements that contains electrons that fill the *d* subshell

valence electron electron in the outer shell of an atom that participates in chemical bonding

Zeeman effect splitting of energy levels by an external magnetic field

KEY EQUATIONS

Orbital angular momentum	$L = \sqrt{l(l+1)}\hbar$
z-component of orbital angular momentum	$L_z = m\hbar$
Radial probability density function	$P(r)dr = \left\|\psi_{n00}\right\|^2 4\pi r^2 dr$
Spin angular momentum	$S = \sqrt{s(s+1)}\hbar$
z-component of spin angular momentum	$S_z = m_s\hbar$
Electron spin magnetic moment	$\vec{\boldsymbol{\mu}}_s = \left(\frac{e}{m_e}\right)\vec{\mathbf{S}}$
Electron orbital magnetic dipole moment	$\vec{\boldsymbol{\mu}} = -\left(\frac{e}{2m_e}\right)\vec{\mathbf{L}}$
Potential energy associated with the magnetic interaction between the orbital magnetic dipole moment and an external magnetic field $\vec{\mathbf{B}}$	$U(\theta) = -\mu_z B = m\mu_B B$
Maximum number of electrons in a subshell of a hydrogen atom	$N = 4l + 2$
Selection rule for atomic transitions in a hydrogen-like atom	$\Delta l = \pm 1$
Moseley's law for X-ray production	$(Z-1) = \text{constant}\sqrt{f}$

SUMMARY

8.1 The Hydrogen Atom

- A hydrogen atom can be described in terms of its wave function, probability density, total energy, and orbital angular momentum.
- The state of an electron in a hydrogen atom is specified by its quantum numbers (n, l, m).
- In contrast to the Bohr model of the atom, the Schrödinger model makes predictions based on probability statements.
- The quantum numbers of a hydrogen atom can be used to calculate important information about the atom.

8.2 Orbital Magnetic Dipole Moment of the Electron

- A hydrogen atom has magnetic properties because the motion of the electron acts as a current loop.
- The energy levels of a hydrogen atom associated with orbital angular momentum are split by an external magnetic field because the orbital angular magnetic moment interacts with the field.
- The quantum numbers of an electron in a hydrogen atom can be used to calculate the magnitude and direction of the

orbital magnetic dipole moment of the atom.

8.3 Electron Spin

- The state of an electron in a hydrogen atom can be expressed in terms of five quantum numbers.
- The spin angular momentum quantum of an electron is $= +½$. The spin angular momentum projection quantum number is $m_s = +½$ or $-½$ (spin up or spin down).
- The fine and hyperfine structures of the hydrogen spectrum are explained by magnetic interactions within the atom.

8.4 The Exclusion Principle and the Periodic Table

- Pauli's exclusion principle states that no two electrons in an atom can have all the same quantum numbers.
- The structure of the periodic table of elements can be explained in terms of the total energy, orbital angular momentum, and spin of electrons in an atom.
- The state of an atom can be expressed by its electron configuration, which describes the shells and subshells that are filled in the atom.

8.5 Atomic Spectra and X-rays

- Radiation is absorbed and emitted by atomic energy-level transitions.
- Quantum numbers can be used to estimate the energy, frequency, and wavelength of photons produced by atomic transitions.
- Atomic fluorescence occurs when an electron in an atom is excited several steps above the ground state by the absorption of a high-energy ultraviolet (UV) photon.
- X-ray photons are produced when a vacancy in an inner shell of an atom is filled by an electron from the outer shell of the atom.
- The frequency of X-ray radiation is related to the atomic number *Z* of an atom.

8.6 Lasers

- Laser light is coherent (monochromatic and "phase linked") light.
- Laser light is produced by population inversion and subsequent de-excitation of electrons in a material (solid, liquid, or gas).
- CD and Blu-Ray players uses lasers to read digital information stored on discs.

CONCEPTUAL QUESTIONS

8.1 The Hydrogen Atom

1. Identify the physical significance of each of the quantum numbers of the hydrogen atom.

2. Describe the ground state of hydrogen in terms of wave function, probability density, and atomic orbitals.

3. Distinguish between Bohr's and Schrödinger's model of the hydrogen atom. In particular, compare the energy and orbital angular momentum of the ground states.

8.2 Orbital Magnetic Dipole Moment of the Electron

4. Explain why spectral lines of the hydrogen atom are split by an external magnetic field. What determines the number and spacing of these lines?

5. A hydrogen atom is placed in a magnetic field. Which of the following quantities are affected? (a) total energy; (b) angular momentum; (c) z-component of angular momentum; (d) polar angle.

6. On what factors does the orbital magnetic dipole moment of an electron depend?

8.3 Electron Spin

7. Explain how a hydrogen atom in the ground state $(l = 0)$ can interact magnetically with an external magnetic field.

8. Compare orbital angular momentum with spin angular momentum of an electron in the hydrogen atom.

9. List all the possible values of s and m_s for an electron. Are there particles for which these values are different?

10. Are the angular momentum vectors $\vec{\mathbf{L}}$ and $\vec{\mathbf{S}}$ necessarily aligned?

11. What is spin-orbit coupling?

8.4 The Exclusion Principle and the Periodic Table

12. What is Pauli's exclusion principle? Explain the importance of this principle for the understanding of atomic structure and molecular bonding.

13. Compare the electron configurations of the elements in the same column of the periodic table.

14. Compare the electron configurations of the elements that belong in the same row of the periodic table of elements.

8.5 Atomic Spectra and X-rays

15. Atomic and molecular spectra are discrete. What does discrete mean, and how are discrete spectra related to the quantization of energy and electron orbits in atoms and molecules?

16. Discuss the process of the absorption of light by matter in terms of the atomic structure of the absorbing medium.

17. NGC1763 is an emission nebula in the Large Magellanic Cloud just outside our Milky Way Galaxy. Ultraviolet light from hot stars ionize the hydrogen atoms in the nebula. As protons and electrons recombine, light in the visible range is emitted. Compare the energies of the photons involved in these two transitions.

18. Why are X-rays emitted only for electron transitions to inner shells? What type of photon is emitted for transitions between outer shells?

19. How do the allowed orbits for electrons in atoms differ from the allowed orbits for planets around the sun?

8.6 Lasers

20. Distinguish between coherent and monochromatic light.

21. Why is a metastable state necessary for the production of laser light?

22. How does light from an incandescent light bulb differ from laser light?

23. How is a Blu-Ray player able to read more information that a CD player?

24. What are the similarities and differences between a CD player and a Blu-Ray player?

PROBLEMS

8.1 The Hydrogen Atom

25. The wave function is evaluated at rectangular coordinates $(x, y, z) = (2, 1, 1)$ in arbitrary units. What are the spherical coordinates of this position?

26. If an atom has an electron in the $n = 5$ state with $m = 3$, what are the possible values of l?

27. What are the possible values of m for an electron in the $n = 4$ state?

28. What, if any, constraints does a value of $m = 1$ place on the other quantum numbers for an electron in an atom?

29. What are the possible values of m for an electron in the $n = 4$ state?

30. (a) How many angles can L make with the z-axis for an $l = 2$ electron? (b) Calculate the value of the smallest angle.

31. The force on an electron is "negative the gradient of the potential energy function." Use this knowledge and **Equation 8.1** to show that the force on the electron in a hydrogen atom is given by Coulomb's force law.

32. What is the total number of states with orbital angular momentum $l = 0$? (Ignore electron spin.)

33. The wave function is evaluated at spherical coordinates $(r, \theta, \phi) = (\sqrt{3}, 45°, 45°)$, where the value of the radial coordinate is given in arbitrary units. What are the rectangular coordinates of this position?

34. Coulomb's force law states that the force between two charged particles is:

$F = k\frac{Qq}{r^2}$. Use this expression to determine the potential energy function.

35. Write an expression for the total number of states with orbital angular momentum *l*.

36. Consider hydrogen in the ground state, ψ_{100}. (a) Use the derivative to determine the radial position for which the probability density, *P*(*r*), is a maximum.

(b) Use the integral concept to determine the average radial position. (This is called the expectation value of the electron's radial position.) Express your answers into terms of the Bohr radius, a_o. Hint: The expectation value is the just average value. (c) Why are these values different?

37. What is the probability that the 1*s* electron of a hydrogen atom is found outside the Bohr radius?

38. How many polar angles are possible for an electron in the $l = 5$ state?

39. What is the maximum number of orbital angular momentum electron states in the $n = 2$ shell of a hydrogen atom? (Ignore electron spin.)

40. What is the maximum number of orbital angular momentum electron states in the $n = 3$ shell of a hydrogen atom? (Ignore electron spin.)

8.2 Orbital Magnetic Dipole Moment of the Electron

41. Find the magnitude of the orbital magnetic dipole moment of the electron in in the 3*p* state. (Express your answer in terms of μ_B.)

42. A current of $I = 2\text{A}$ flows through a square-shaped wire with 2-cm side lengths. What is the magnetic moment of the wire?

43. Estimate the ratio of the electron magnetic moment to the *muon* magnetic moment for the same state of orbital angular momentum. (*Hint:* $m_\mu = 105.7\,\text{MeV}/c^2$)

44. Find the magnitude of the orbital magnetic dipole moment of the electron in in the 4*d* state. (Express your answer in terms of μ_B.)

45. For a 3*d* electron in an external magnetic field of $2.50 \times 10^{-3}\,\text{T}$, find (a) the current associated with the orbital angular momentum, and (b) the maximum torque.

46. An electron in a hydrogen atom is in the $n = 5$, $l = 4$ state. Find the smallest angle the magnetic moment makes with the *z*-axis. (Express your answer in terms of $\mu_{B.}$)

47. Find the minimum torque magnitude $|\vec{\tau}|$ that acts on the orbital magnetic dipole of a 3*p* electron in an external magnetic field of $2.50 \times 10^{-3}\,\text{T}$.

48. An electron in a hydrogen atom is in 3*p* state. Find the smallest angle the magnetic moment makes with the *z*-axis. (Express your answer in terms of μ_B.)

49. Show that $U = -\vec{\mu} \cdot \vec{\mathbf{B}}$.

(*Hint*: An infinitesimal amount of work is done to align the magnetic moment with the external field. This work rotates the magnetic moment vector through an angle $-d\theta$ (toward the positive *z*-direction), where $d\theta$ is a positive angle change.)

8.3 Electron Spin

50. What is the magnitude of the spin momentum of an electron? (Express you answer in terms of $\hbar$.)

51. What are the possible polar orientations of the spin momentum vector for an electron?

52. For $n = 1$, write all the possible sets of quantum numbers (*n*, *l*, *m*, m_s).

53. A hydrogen atom is placed in an external uniform magnetic field ($B = 200\,\text{T}$). Calculate the wavelength of light produced in a transition from a spin up to spin down state.

54. If the magnetic field in the preceding problem is quadrupled, what happens to the wavelength of light produced in a transition from a spin up to spin down state?

55. If the magnetic moment in the preceding problem is doubled, what happens to the frequency of light produced in a transition from a spin-up to spin-down state?

56. For $n = 2$, write all the possible sets of quantum numbers (*n*, *l*, *m*, m_s).

8.4 The Exclusion Principle and the Periodic Table

57. (a) How many electrons can be in the $n = 4$ shell?

(b) What are its subshells, and how many electrons can be in each?

58. (a) What is the minimum value of *l* for a subshell that contains 11 electrons?

(b) If this subshell is in the $n = 5$ shell, what is the spectroscopic notation for this atom?

59. **Unreasonable result.** Which of the following spectroscopic notations are not allowed? (a) $5s^1$ (b) $1d^1$ (c) $4s^3$ (d) $3p^7$ (e) $5g^{15}$. State which rule is violated for each notation that is not allowed.

60. Write the electron configuration for potassium.

61. Write the electron configuration for iron.

62. The valence electron of potassium is excited to a 5*d* state. (a) What is the magnitude of the electron's orbital angular momentum? (b) How many states are possible along a chosen direction?

63. (a) If one subshell of an atom has nine electrons in it, what is the minimum value of *l*? (b) What is the spectroscopic notation for this atom, if this subshell is part of the $n = 3$ shell?

64. Write the electron configuration for magnesium.

65. Write the electron configuration for carbon.

66. The magnitudes of the resultant spins of the electrons of the elements B through Ne when in the ground state are: $\sqrt{3}\hbar/2$, $\sqrt{2}\hbar$, $\sqrt{15}\hbar/2$, $\sqrt{2}\hbar$, $\sqrt{3}\hbar/2$, and 0, respectively. Argue that these spins are consistent with Hund's rule.

8.5 Atomic Spectra and X-rays

67. What is the minimum frequency of a photon required to ionize: (a) a He^+ ion in its ground state? (b) A Li^{2+} ion in its first excited state?

68. The ion Li^{2+} makes an atomic transition from an $n = 4$ state to an $n = 2$ state. (a) What is the energy of the photon emitted during the transition? (b) What is the wavelength of the photon?

69. The red light emitted by a ruby laser has a wavelength of 694.3 nm. What is the difference in energy between the initial state and final state corresponding to the emission of the light?

70. The yellow light from a sodium-vapor street lamp is produced by a transition of sodium atoms from a 3*p* state to a 3*s* state. If the difference in energies of those two states is 2.10 eV, what is the wavelength of the yellow light?

71. Estimate the wavelength of the K_α X-ray from calcium.

72. Estimate the frequency of the K_α X-ray from cesium.

73. X-rays are produced by striking a target with a beam of electrons. Prior to striking the target, the electrons are accelerated by an electric field through a potential energy difference:

$$\Delta U = -e\Delta V,$$

where *e* is the charge of an electron and ΔV is the voltage difference. If $\Delta V = 15{,}000$ volts, what is the minimum wavelength of the emitted radiation?

74. For the preceding problem, what happens to the minimum wavelength if the voltage across the X-ray tube is doubled?

75. Suppose the experiment in the preceding problem is conducted with muons. What happens to the minimum wavelength?

76. An X-ray tube accelerates an electron with an applied voltage of 50 kV toward a metal target. (a) What is the shortest-wavelength X-ray radiation generated at the target? (b) Calculate the photon energy in eV. (c) Explain the relationship of the photon energy to the applied voltage.

77. A color television tube generates some X-rays when its electron beam strikes the screen. What is the shortest wavelength of these X-rays, if a 30.0-kV potential is used to accelerate the electrons? (Note that TVs have shielding to prevent these X-rays from exposing viewers.)

78. An X-ray tube has an applied voltage of 100 kV. (a) What is the most energetic X-ray photon it can produce? Express your answer in electron volts and joules. (b) Find the wavelength of such an X-ray.

79. The maximum characteristic X-ray photon energy comes from the capture of a free electron into a *K* shell vacancy. What is this photon energy in keV for tungsten, assuming that the free electron has no initial kinetic energy?

80. What are the approximate energies of the K_α and K_β X-rays for copper?

81. Compare the X-ray photon wavelengths for copper and gold.

82. The approximate energies of the K_α and K_β X-rays for copper are $E_{K_\alpha} = 8.00\,\text{keV}$ and $E_{K_\beta} = 9.48\,\text{keV}$, respectively. Determine the ratio of X-ray frequencies of gold to copper, then use this value to estimate the corresponding energies of K_α and K_β X-rays for gold.

8.6 Lasers

83. A carbon dioxide laser used in surgery emits infrared radiation with a wavelength of $10.6\,\mu\text{m}$. In 1.00 ms, this laser raised the temperature of $1.00\,\text{cm}^3$ of flesh to $100\,°\text{C}$ and evaporated it. (a) How many photons were required? You may assume that flesh has the same heat of vaporization as water. (b) What was the minimum power output during the flash?

84. An excimer laser used for vision correction emits UV radiation with a wavelength of 193 nm. (a) Calculate the photon energy in eV. (b) These photons are used to evaporate corneal tissue, which is very similar to water in its properties. Calculate the amount of energy needed per molecule of water to make the phase change from liquid to gas. That is, divide the heat of vaporization in kJ/kg by the number of water molecules in a kilogram. (c) Convert this to eV and compare to the photon energy. Discuss the implications.

ADDITIONAL PROBLEMS

85. For a hydrogen atom in an excited state with principal quantum number *n*, show that the smallest angle that the orbital angular momentum vector can make with respect to the *z*-axis is $\theta = \cos^{-1}\left(\sqrt{\frac{n-1}{n}}\right)$.

86. What is the probability that the 1*s* electron of a hydrogen atom is found between $r = 0$ and $r = \infty$?

87. Sketch the potential energy function of an electron in a hydrogen atom. (a) What is the value of this function at $r = 0$? in the limit that $r = \infty$? (b) What is unreasonable or inconsistent with the former result?

88. Find the value of l, the orbital angular momentum quantum number, for the Moon around Earth.

89. Show that the maximum number of orbital angular momentum electron states in the *n*th shell of an atom is n^2. (Ignore electron spin.) (*Hint:* Make a table of the total number of orbital angular momentum states for each shell and find the pattern.)

90. What is the magnitude of an electron magnetic moment?

91. What is the maximum number of electron states in the $n = 5$ shell?

92. A ground-state hydrogen atom is placed in a uniform magnetic field, and a photon is emitted in the transition from a spin-up to spin-down state. The wavelength of the photon is $168\,\mu\text{m}$. What is the strength of the magnetic field?

93. Show that the maximum number of electron states in the *n*th shell of an atom is $2n^2$.

94. The valence electron of chlorine is excited to a 3*p* state. (a) What is the magnitude of the electron's orbital angular momentum? (b) What are possible values for the *z*-component of angular measurement?

95. Which of the following notations are allowed (that is, which violate none of the rules regarding values of quantum numbers)? (a) $1s^1$; (b) $1d^3$; (c) $4s^2$; (d) $3p^7$; (e) $6h^{20}$

96. The ion Be^{3+} makes an atomic transition from an $n = 3$ state to an $n = 2$ state. (a) What is the energy of the photon emitted during the transition? (b) What is the wavelength of the photon?

97. The maximum characteristic X-ray photon energy comes from the capture of a free electron into a *K* shell vacancy. What is this photon frequency for tungsten, assuming that the free electron has no initial kinetic energy?

98. Derive an expression for the ratio of X-ray photon frequency for two elements with atomic numbers Z_1 and Z_2.

99. Compare the X-ray photon wavelengths for copper and silver.

100. (a) What voltage must be applied to an X-ray tube to obtain 0.0100-fm-wavelength X-rays for use in exploring the details of nuclei? (b) What is unreasonable about this result? (c) Which assumptions are unreasonable or inconsistent?

101. A student in a physics laboratory observes a hydrogen spectrum with a diffraction grating for the purpose of measuring the wavelengths of the emitted radiation. In the spectrum, she observes a yellow line and finds its wavelength to be 589 nm. (a) Assuming that this is part of the Balmer series, determine n_i, the principal quantum number of the initial state. (b) What is unreasonable about this result? (c) Which assumptions are unreasonable or inconsistent?