7-5 Total Angular Momentum and the Spin-Orbit Effect

In general an electron in an atom has both orbital angular momentum character by the quantum number l and spin angular momentum characterized by the qua number s. Analogous classical systems that have two kinds of angular momentu Earth, which is spinning about its axis of rotation in addition to revolving abou sun, or a precessing gyroscope, which has angular momentum of precession in tion to its spin. Classically the total angular momentum

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

7.

is an important quantity because the resultant torque on a system equals the ra change of the total angular momentum, and in the case of central forces, the angular momentum is conserved. For a classical system, the magnitude of the angular momentum J can have any value between $L + S$ and $|L - S|$. We already seen that in quantum mechanics, angular momentum is more complic both $\mathbf{L}$ and $\mathbf{S}$ are quantized and their relative directions are restricted. The quant mechanical rules for combining orbital and spin angular momenta or any two ang momenta (such as for two particles) are somewhat difficult to derive, but they are difficult to understand. For the case of orbital and spin angular momenta, the ma tude of the total angular momentum $\mathbf{J}$ is given by

$$|\mathbf{J}| = \sqrt{j(j + 1)}\,\hbar$$

7.

where the *total angular momentum quantum number j* can be either

$$j = l + s \qquad \text{or} \qquad j = |l - s|$$

7.

Fig. 7-16 (*a*) Simplified vector model illustrating the addition of orbital and spin angular momenta. Case shown is for $l = 1$ and $s = \frac{1}{2}$. There are two possible values of the quantum number for the total angular momentum: $j = l + s = \frac{3}{2}$ and $j = l - s = \frac{1}{2}$. (*b*) Vector addition of the orbital and spin angular momenta, also for the case $l = 1$ and $s = \frac{1}{2}$. According to the uncertainty principle the vectors can lie anywhere on the cones, corresponding to the definite values of their z components. Note that there are two ways of forming the states with $j = \frac{3}{2}, m_j = \frac{1}{2}$ and $j = \frac{1}{2}, m_j = \frac{1}{2}$.
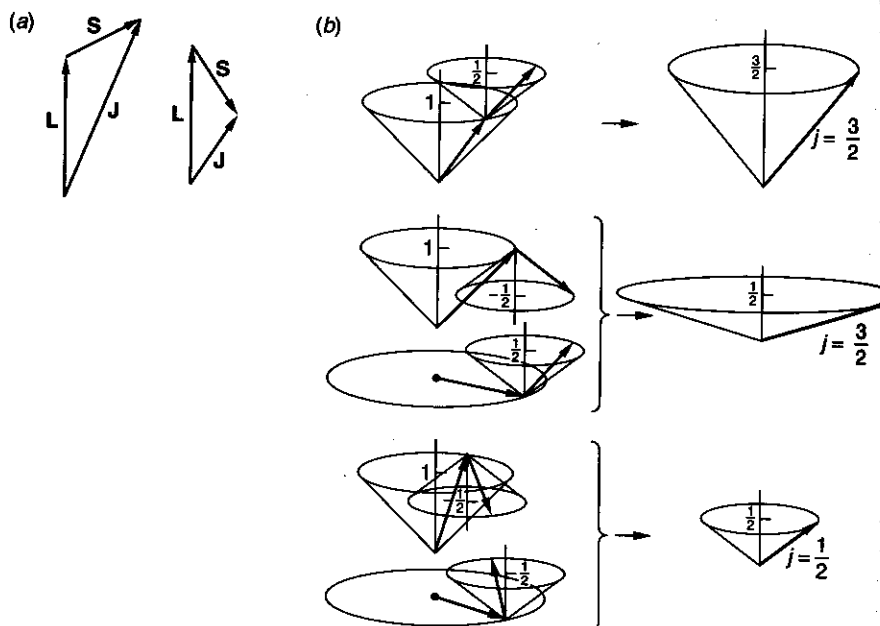
the z component of **J** is given by

$$J_z = m_j \hbar \quad \text{where} \quad m_j = -j, -j + 1, \ldots, j - 1, j \qquad \textbf{7-55}$$

$= 0$, the total angular momentum is simply the spin, and $j = s$.) Figure 7-16a is simplified vector model illustrating the two possible combinations $j = l + \frac{1}{2} = \frac{3}{2}$ $j = l - \frac{1}{2} = \frac{1}{2}$ for the case of an electron with $l = 1$. The lengths of the vectors proportional to $[l(l + 1)]^{1/2}$, $[s(s + 1)]^{1/2}$, and $[j(j + 1)]^{1/2}$. The spin and orbital lar momentum vectors are said to be "parallel" when $j = l + s$ and "antiparal-when $j = |l - s|$. A quantum-mechanically more accurate vector addition is in in Figure 7-16b. The quantum number m_j can take on $2j + 1$ possible values teger steps between $-j$ and $+j$, as indicated by Equation 7-55. Equation 7-55 implies that $m_j = m_l + m_s$, since $J_z = L_z + S_z$.

Equation 7-54 is a special case of a more general rule for combining two angular enta which is useful when dealing with more than one particle. For example, are two electrons in the helium atom, each with spin, orbital, and total angular entum. The general rule is:

If $\mathbf{J}_1$ is one angular momentum (orbital, spin, or a combination) and $\mathbf{J}_2$ is another, the resulting total angular momentum $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$ has the value $[j(j + 1)]^{1/2} \hbar$ for its magnitude, where j can be any of the values

$$j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|$$

EXAMPLE 7-2 Addition of Angular Momenta I Two electrons each have zero orbital angular momentum. What are the possible quantum numbers for the total angular momentum of the two-electron system?

handwritten margin notes:
$l = 0$
$L_1 = 0 \qquad S_1 = \frac{1}{2}$
$L_2 = 0 \qquad S_2 = \frac{1}{2}$

Solution
In this case $j_1 = j_2 = \frac{1}{2}$. The general rule then gives two possible results, $j = 1$ and $= 0$. These combinations are commonly called parallel and antiparallel, respectively.

EXAMPLE 7-3 Addition of Angular Momenta II An electron in an atom has orbital angular momentum $\mathbf{L}_1$ with quantum number $l_1 = 2$ and a second electron s orbital angular momentum $\mathbf{L}_2$ with quantum number $l_2 = 3$. What are the pos-le quantum numbers for the total orbital angular momentum $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$?

Solution
nce $l_1 + l_2 = 5$ and $|l_1 - l_2| = 1$, the possible values of l are 5, 4, 3, 2, and 1.

ctroscopic Notation

roscopic notation, a kind of shorthand developed in the early days of spec-py to condense information and simplify the description of transitions between , has since been adopted for general use in atomic, molecular, nuclear, and

particle physics. The notation code appears to be arbitrary,[11] but it is easy to
and, as you will discover, convenient to use. For single electrons we have:

1. For single-electron states the letter code $s\ p\ d\ f\ g\ h$ . . . is used in one-to-o
    correspondence with the values of the orbital angular momentum quantu
    number l: 0 1 2 3 4 5 . . . . For example, an electron with $l = 2$ is said to
    in a d state.

2. The single-electron (Bohr) energy levels are called *shells,* labeled $K\ L\ M$
    O . . . in one-to-one correspondence with the values of the principal qua
    tum number n: 1 2 3 4 5 . . . . For example, an electron with $n = 3$ in
    atom is said to be in the M shell. (This notation is less commonly used.)

For atomic states that may contain one or more particles the notation include
principal quantum number and the angular momenta quantum numbers. The
orbital angular momentum quantum number is denoted by a capital letter in the s
sequence as in rule 1 above, i.e., $S\ P\ D\ F$ . . . correspond to l values 0 1 2 3 .
The value of n is written as a prefix and the value of the total angular momer
quantum number j by a subscript. The magnitude of the total spin quantum numl
appears as a left superscript in the form $2s + 1$.[12] Thus, a state with $l = 1$, a P s
would be written as

$$n^{2s+1}P_j$$

For example, the ground state of hydrogen is written $1^2S_{1/2}$, read "one doubl
one-half." The $n = 2$ state can have $l = 0$ or $l = 1$, so the spectroscopic nota
for these states is $2^2S_{1/2}$, $2^2P_{3/2}$, and $2^2P_{1/2}$. (The principal quantum number
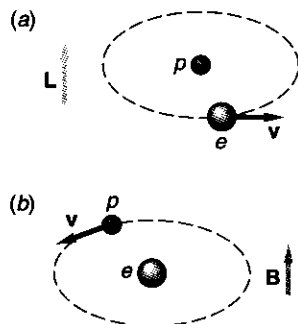spin superscript are sometimes not included if they are not needed in spec
situations.)

(a) An electron
moving about a proton with
angular momentum **L** up.
(b) The magnetic field **B** seen
by the electron due to the
apparent (relative) motion of
the proton is also up. When
the electron spin is parallel
to **L**, the magnetic moment is
antiparallel to **L** and **B**, so
the spin-orbit energy has its
largest value.

Spin-Orbit Coupling

Atomic states with the same n and l values but different j values have slightly d
ferent energies because of the interaction of the spin of the electron with its orbi
motion. This effect is called the *spin-orbit effect.* The resulting splitting of
spectral lines such as the one that results from the splitting of the $2P$ level in
transition $2P \rightarrow 1S$ in hydrogen is called *fine-structure splitting.* We can und
stand the spin-orbit effect qualitatively from a simple Bohr model picture,
shown in Figure 7-17. In this picture, the electron moves in a circular orbit wi
speed v around a fixed proton. In the figure, the orbital angular momentum **L** is
In the frame of reference of the electron, the proton moves in a circle around
thus constituting a circular loop current which produces a magnetic field **B** at
position of the electron. The direction of **B** is also up, parallel to **L**. The potent
energy of a magnetic moment in a magnetic field depends on its orientation and
given by:

$$U = -\mathbf{\mu} \cdot \mathbf{B} = -\mu_z B \qquad \text{7-5}$$

The potential energy is lowest when the magnetic moment is parallel to **B** and high
when it is antiparallel. Since the magnetic moment of the electron is directed opposi
to its spin (because the electron has a negative charge), the spin-orbit energy is high
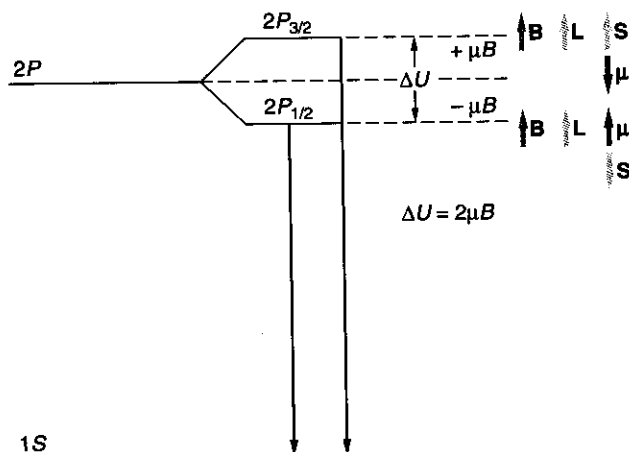
-18 Fine-structure energy-level diagram. On the left, the levels in the absence of a mag-
field are shown. The effect of the magnetic field due to the relative motion of the nucleus
wn on the right. Because of the spin-orbit interaction, the magnetic field splits the 2P
into two energy levels, with the $j = \frac{3}{2}$ level having slightly greater energy than the $j = \frac{1}{2}$
The spectral line due to the transition $2P \rightarrow 1S$ is therefore split into two lines of slightly
ent wavelengths.

the spin is parallel to **B** and thus to **L**. The energy of the $2P_{3/2}$ state in hydrogen,
ich **L** and **S** are parallel, is therefore slightly higher than the $2P_{1/2}$ state, in which
d **S** are antiparallel (Figure 7-18).[13] The measured splitting is about 4.5×10^{-5} eV
e $2P_{1/2}$ and $2P_{3/2}$ levels in hydrogen. For other atoms, the fine-structure splitting is
than this. For example, for sodium it is about 2×10^{-3} eV, as will be discussed
ction 7-7.

XAMPLE 7-4 Fine-Structure Splitting The fine-structure splitting of the $2P_{3/2}$ and
$P_{1/2}$ levels in hydrogen is 4.5×10^{-5} eV. From this, estimate the magnetic field that
e 2p electron in hydrogen experiences. Assume **B** is parallel to the z axis.

olution

1. The energy of the 2p electrons is shifted in the presence of a magnetic field
   by an amount given by Equation 7-56:

$$U = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu_z B$$

2. U is positive or negative depending on the relative orientation of $\boldsymbol{\mu}$ and **B**,
   so the total energy difference ΔE between the two levels is:

$$\Delta E = 2U = 2\mu_z B$$

3. Since the magnetic moment of the electron is μ_B, $\mu_z \approx \mu_B$ and:

$$\Delta E \approx 2\mu_B B$$

Ch 15 - Spin - orbit Coupling.

Consider the total angular momentum $J = S + L$ for a particle with Spin $\frac{1}{2}$ (a fermion) and $l=1$.

(orbital angular moment).

We can calculate how the Spin and L add with the Clebsch - Gordan coefficients.

(a) $\langle j_1 m_1 ; j_2 m_2 | j m \rangle =$

$\langle l, m_l ; S, m_s | j m_j \rangle$

(space vectors - products)

$\langle 1 1 ; \frac{1}{2} + \frac{1}{2} |$

$\langle 1 1 ; \frac{1}{2} - \frac{1}{2} |$

$\langle 1 0 ; \frac{1}{2} \frac{1}{2} |$

$\langle 1 0 ; \frac{1}{2} -\frac{1}{2} |$

$\langle 1 -1 ; \frac{1}{2} \frac{1}{2} |$

$\langle 1 -1 ; \frac{1}{2} -\frac{1}{2} |$

$|j, m\rangle$ kets:

$|\frac{3}{2} \frac{1}{2}\rangle$; $|\frac{3}{2} \frac{3}{2}\rangle$

$j = \frac{3}{2}$ $|\frac{3}{2} \frac{1}{2}\rangle$

$(l+s)$ $|\frac{3}{2} -\frac{1}{2}\rangle$

$|\frac{3}{2} -\frac{3}{2}\rangle$

$(l-s)$

$j = \frac{1}{2}$ $|\frac{1}{2} \frac{1}{2}\rangle$

$|\frac{1}{2} -\frac{1}{2}\rangle$

The combinations are already eigenvectors of J_z:

$$J_z |j_1, m_1\rangle \otimes |j_2, m_2\rangle = J_z |j_1 m_1 ; j_2 m_2\rangle = (J_{1z} + J_{2z}) | \qquad \rangle$$

$$= J_{1z} |j_1 m_1\rangle \otimes |j_2 m_2\rangle + |j_1 m_1\rangle \otimes J_{2z} |j_2 m_2\rangle$$

$$= m_1 \hbar |j_1 m_1\rangle \otimes |j_2 m_2\rangle + |j_1 m_1\rangle \otimes m_2 \hbar |j_2 m_2\rangle$$

$$= (m_1 + m_2) \hbar |j_1 m_1\rangle \otimes |j_2 m_2\rangle$$

Also, the total $|j, m\rangle$ ket is an eigenstate: $J_z |j m\rangle = m \hbar |j m\rangle$

So $|j m\rangle$ can only be a linear combination of product vectors with $m_1 + m_2 = m$.

Start with $|j m\rangle = |\frac{3}{2} \frac{3}{2}\rangle$ $m = m_1 + m_2 = \frac{3}{2}$ if

$m_1 = 1, \; m_2 = \frac{1}{2}$

So $|\frac{3}{2} \frac{3}{2}\rangle = |11; \frac{1}{2} \frac{1}{2}\rangle$

Operate on both sides with $J_- = J_{1-} + J_{2-}$

(12.5.20) $J_\pm |j m\rangle = \hbar\sqrt{(j \mp m)(j \pm m+1)} \; |j, m\pm 1\rangle$

p. 336 $J_- |j m\rangle = \hbar\sqrt{(j+m)(j-m+1)} \; |j, m-1\rangle$

$J_- |\frac{3}{2} \frac{3}{2}\rangle = \hbar\sqrt{(\frac{3}{2}+\frac{3}{2})(\frac{3}{2}-\frac{3}{2}+1)} \; |\frac{3}{2} \frac{1}{2}\rangle = \sqrt{3} \, \hbar |\frac{3}{2} \frac{1}{2}\rangle$

$J_- |11; \frac{1}{2} \frac{1}{2}\rangle = J_{1-} |11\rangle \otimes |\frac{1}{2} \frac{1}{2}\rangle + |11\rangle \otimes J_{2-} |\frac{1}{2} \frac{1}{2}\rangle$

$= \hbar\sqrt{(1+1)(1-1+1)} |10\rangle \otimes |\frac{1}{2} \frac{1}{2}\rangle + |11\rangle \otimes \hbar\sqrt{(\frac{1}{2}+\frac{1}{2})(\frac{1}{2}-\frac{1}{2}+1)} |\frac{1}{2} -\frac{1}{2}\rangle$

$= \hbar\sqrt{2} \, |10\rangle \otimes |\frac{1}{2} \frac{1}{2}\rangle + \hbar |11\rangle \otimes |\frac{1}{2} -\frac{1}{2}\rangle$

$\sqrt{3}\hbar |\frac{3}{2} \frac{1}{2}\rangle = \hbar\sqrt{2} \, |10, \frac{1}{2} \frac{1}{2}\rangle + \hbar |11, \frac{1}{2} -\frac{1}{2}\rangle$

$|\frac{3}{2} \frac{1}{2}\rangle = \sqrt{\frac{2}{3}} \, |10, \frac{1}{2} \frac{1}{2}\rangle + \frac{1}{\sqrt{3}} |11, \frac{1}{2} -\frac{1}{2}\rangle$

$\langle 0, \frac{1}{2} \frac{1}{2} | \frac{3}{2} \frac{1}{2}\rangle = \sqrt{\frac{2}{3}} \langle 10, \frac{1}{2} \frac{1}{2} |10, \frac{1}{2} \frac{1}{2}\rangle + \frac{1}{\sqrt{3}} \langle 10, \frac{1}{2} \frac{1}{2} | 11, \frac{1}{2} -\frac{1}{2}\rangle$

$= \sqrt{\frac{2}{3}} \cdot 1 \qquad + \qquad 0$

these are orthonormal.

Similarly,

$\langle 11, \frac{1}{2} -\frac{1}{2} | \frac{3}{2} \frac{1}{2}\rangle = 0 \qquad + \qquad \frac{1}{\sqrt{3}} \cdot 1$

These are the Clebsch-Gordan coefficients!
The $l=1$, $s=\frac{1}{2}$ state is $\sqrt{\frac{2}{3}}$ made of $\begin{smallmatrix} l, m_l; \; s, m_s \\ 1 \; 0, \; \frac{1}{2} \; \frac{1}{2} \end{smallmatrix}$

and $\frac{1}{\sqrt{3}}$ made of $1 \; 1, \frac{1}{2} -\frac{1}{2}$