

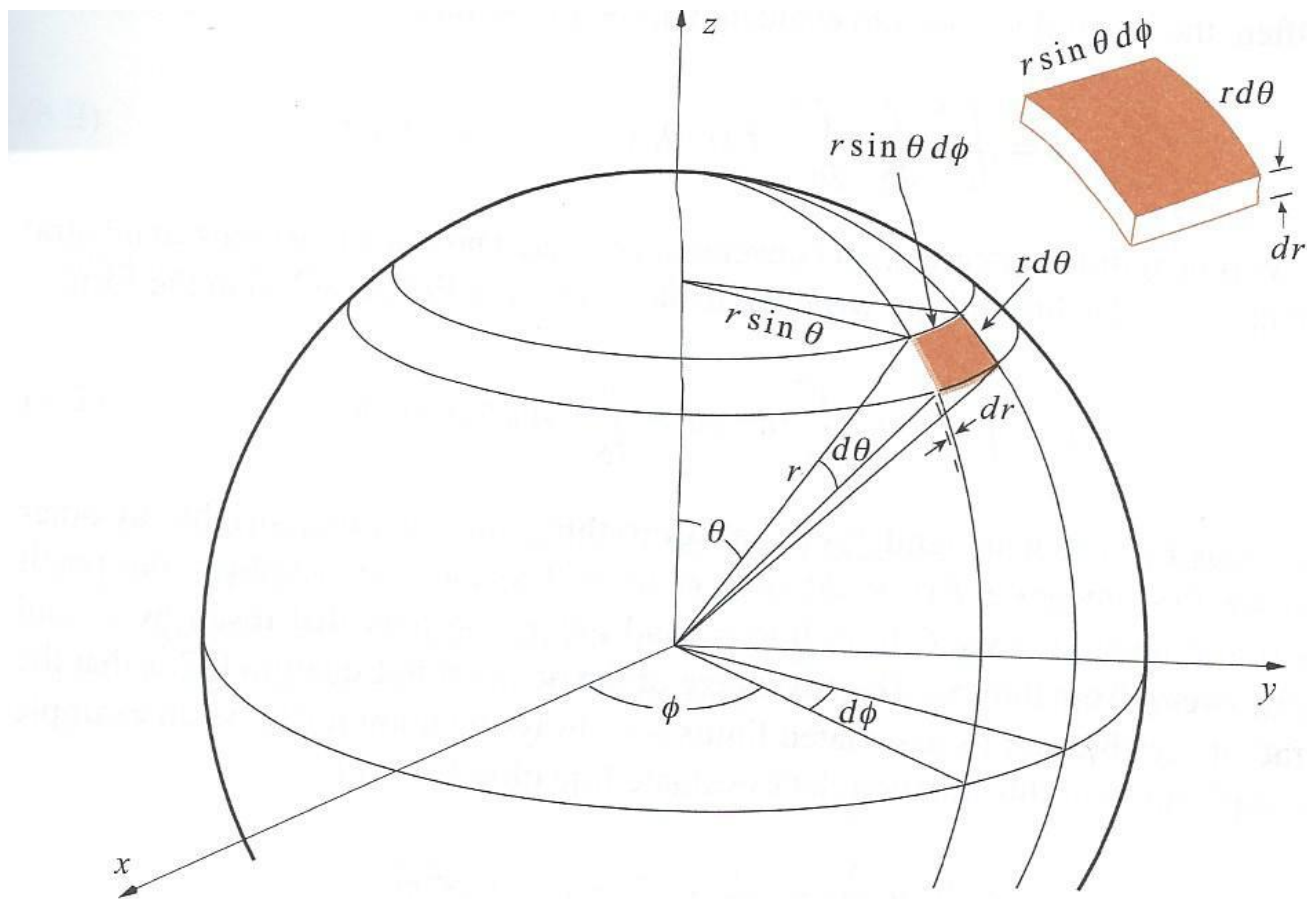


FIGURE E.2

A geometrical construction of the differential volume element in spherical coordinates.

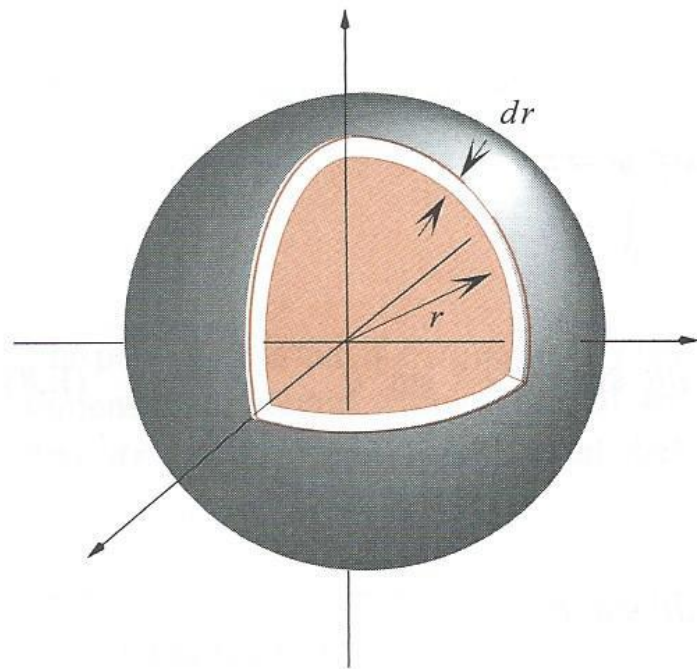


FIGURE E.3

A spherical shell of radius r and thickness dr . The volume of such a shell is $4\pi r^2 dr$, which is its area ($4\pi r^2$) times its thickness (dr).

TABLE 6.2

The first few associated Legendre functions $P_l^{|m|}(x)$

$$P_0^0(x) = 1$$

$$P_1^0(x) = x = \cos \theta$$

$$P_1^1(x) = (1 - x^2)^{1/2} = \sin \theta$$

$$P_2^0(x) = \frac{1}{2}(3x^2 - 1) = \frac{1}{2}(3 \cos^2 \theta - 1)$$

$$P_2^1(x) = 3x(1 - x^2)^{1/2} = 3 \cos \theta \sin \theta$$

$$P_2^2(x) = 3(1 - x^2) = 3 \sin^2 \theta$$

$$P_3^0(x) = \frac{1}{2}(5x^3 - 3x) = \frac{1}{2}(5 \cos^3 \theta - 3 \cos \theta)$$

$$P_3^1(x) = \frac{3}{2}(5x^2 - 1)(1 - x^2)^{1/2} = \frac{3}{2}(5 \cos^2 \theta - 1) \sin \theta$$

$$P_3^2(x) = 15x(1 - x^2) = 15 \cos \theta \sin^2 \theta$$

$$P_3^3(x) = 15(1 - x^2)^{3/2} = 15 \sin^3 \theta$$

TABLE 6.3

The first few spherical harmonics.

$$Y_0^0 = \frac{1}{(4\pi)^{1/2}}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$$

$$Y_1^1 = \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{i\phi}$$

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{-i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$$

$$Y_2^1 = \left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{i\phi}$$

$$Y_2^{-1} = \left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{-i\phi}$$

$$Y_2^2 = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{2i\phi}$$

$$Y_2^{-2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{-2i\phi}$$

two quantum numbers n and l and are given by

$$R_{nl}(r) = - \left\{ \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} \left(\frac{2}{na_0} \right)^{l+3/2} r^l e^{-r/na_0} L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right)$$

TABLE 6.4

The first few associated Laguerre polynomials.

$n = 1,$	$l = 0$	$L_1^1(x) = -1$
$n = 2,$	$l = 0$	$L_2^1(x) = -2!(2 - x)$
	$l = 1$	$L_3^3(x) = -3!$
$n = 3,$	$l = 0$	$L_3^1(x) = -3!(3 - 3x + \frac{1}{2}x^2)$
	$l = 1$	$L_4^3(x) = -4!(4 - x)$
	$l = 2$	$L_5^5(x) = -5!$
$n = 4,$	$l = 0$	$L_4^1(x) = -4!(4 - 6x + 2x^2 - \frac{1}{6}x^3)$
	$l = 1$	$L_5^3(x) = -5!(10 - 5x + \frac{1}{2}x^2)$
	$l = 2$	$L_6^5(x) = -6!(6 - x)$
	$l = 3$	$L_7^7(x) = -7!$

TABLE 6.5

The complete hydrogenlike atomic wave functions for $n = 1, 2$, and 3 . The quantity Z is the atomic number of the nucleus, and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{200} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{210} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{21\pm 1} = \frac{1}{\sqrt{64\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta e^{\pm i\phi}$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{310} = \frac{1}{81} \left(\frac{2}{\pi} \right)^{1/2} \left(\frac{Z}{a_0} \right)^{3/2} (6\sigma - \sigma^2) e^{-\sigma/3} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (6\sigma - \sigma^2) e^{-\sigma/3} \sin \theta e^{\pm i\phi}$
	$l = 2,$	$m = 0$	$\psi_{320} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{32\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta e^{\pm i\phi}$
	$l = 2,$	$m = \pm 2$	$\psi_{32\pm 2} = \frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta e^{\pm 2i\phi}$

TABLE 6.6

The complete hydrogenlike atomic wave functions expressed as real functions for $n = 1, 2$, and 3. The quantity Z is the atomic number of the nucleus and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \cos \phi$
			$\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \sin \phi$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{3s} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \cos \phi$
			$\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \sin \phi$
	$l = 2,$	$m = 0$	$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{3d_{xy}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \cos \phi$
			$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \sin \phi$
	$l = 2,$	$m = \pm 2$	$\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \cos 2\phi$
			$\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \sin 2\phi$

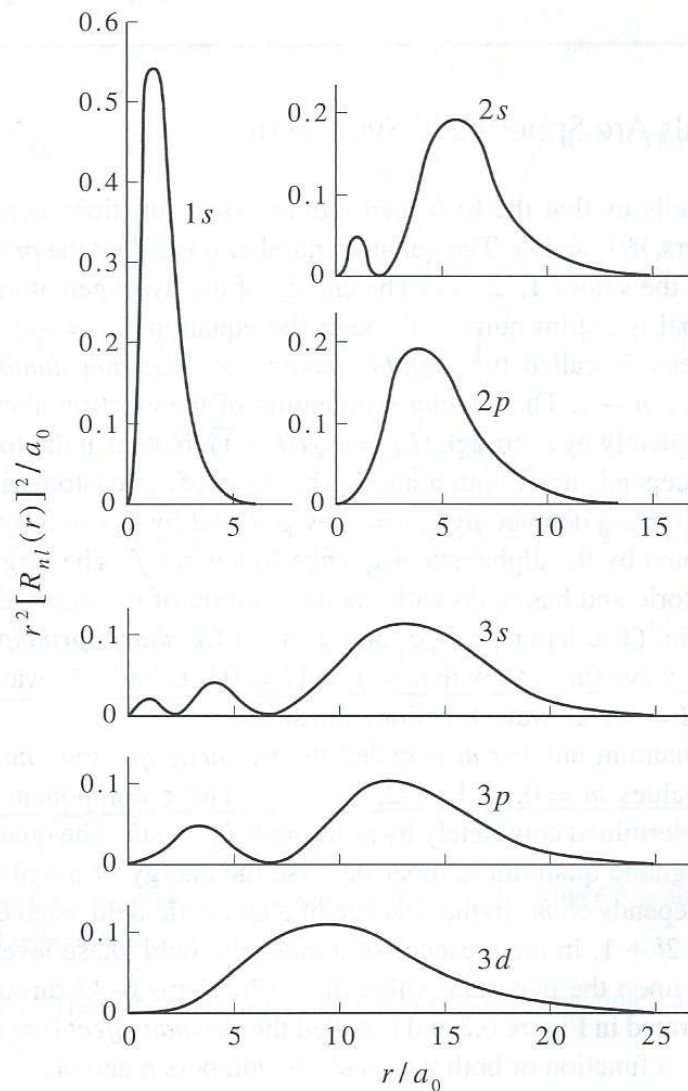


FIGURE 6.3

The probability densities $r^2[R_{nl}(r)]^2$ associated with the radial parts of the hydrogen atomic wave functions.

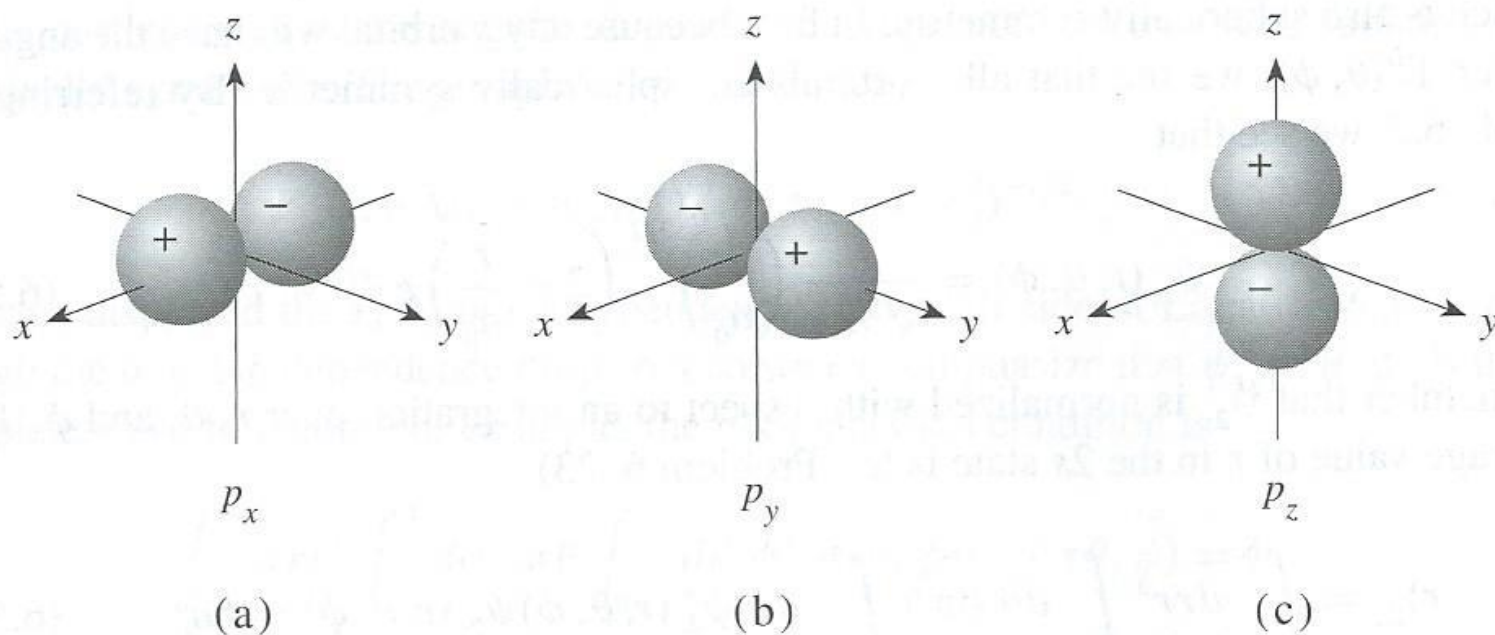


FIGURE 6.4

Three-dimensional polar plots of the angular part of the real representation of the hydrogen atomic wave functions for $l = 1$ (see Equations 6.62 for real representations of p_x and p_y .)

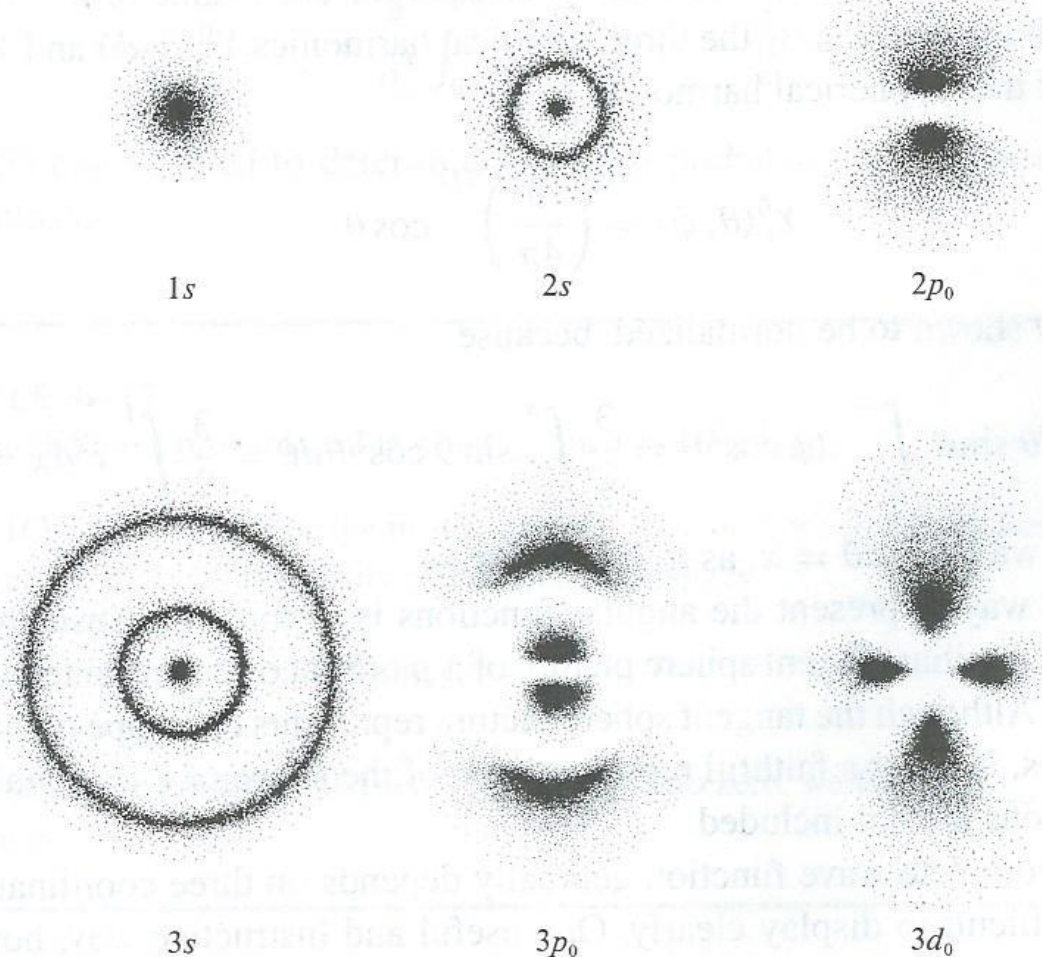
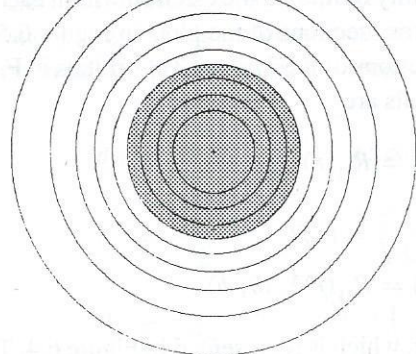
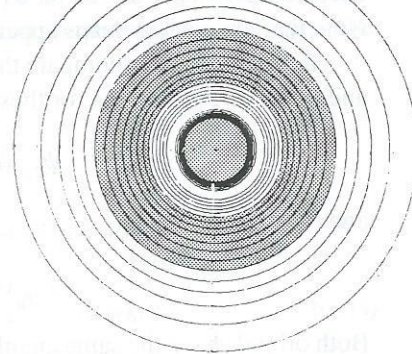


FIGURE 6.5

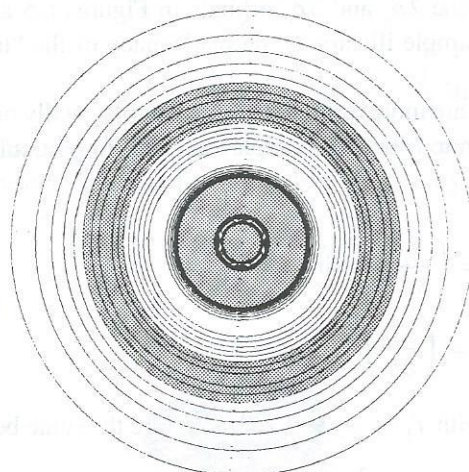
Probability density plots of some hydrogen atomic orbitals. The density of the dots is proportional to the probability of finding the electron in that region.



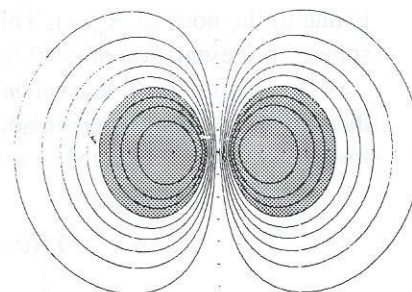
(a) $1s$



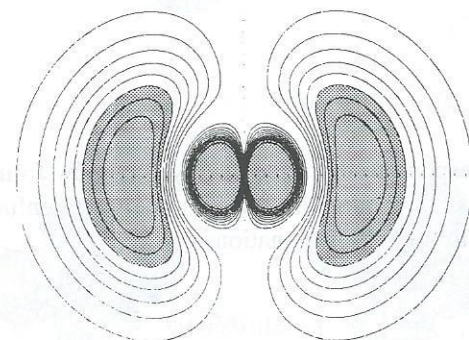
(b) $2s$



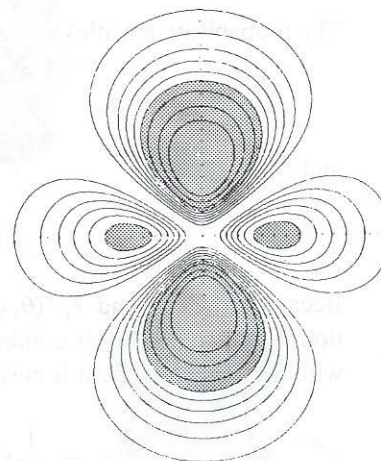
(c) $3s$



(d) $2p_0$



(e) $3p_0$



(f) $3d_0$

FIGURE 6.6

Probability contour maps for the hydrogen atomic orbitals. The nine contours shown in each case enclose the 10%, 20%, ..., 90% probability of finding the electron within each

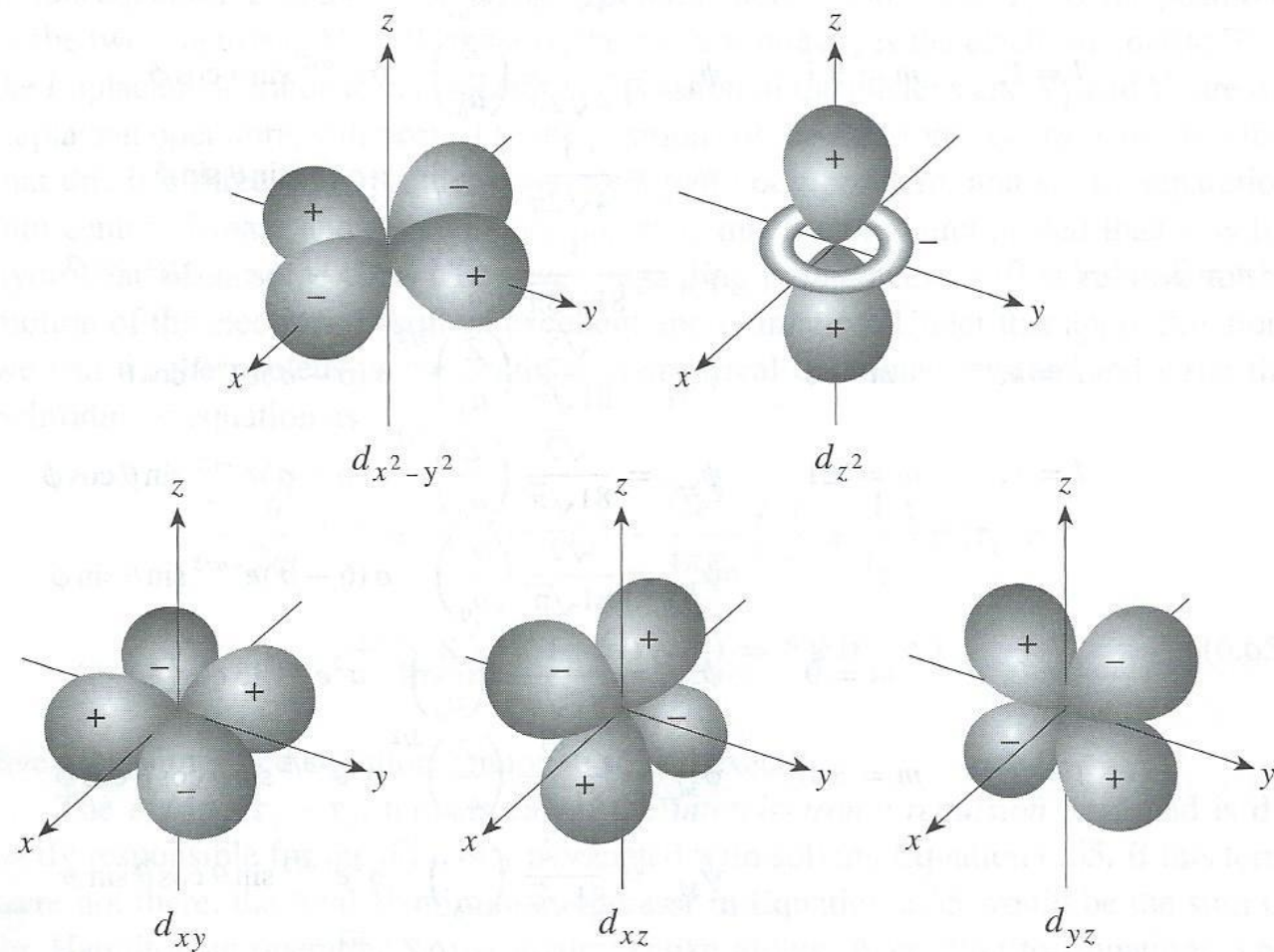


FIGURE 6.7

Three-dimensional plots of the angular part of the real representation of the hydrogen atomic wave functions for $l = 2$. Such plots show the directional character of these orbitals but are not good representations of the shape of these orbitals because the radial functions are not included.

$$d_{z^2} = Y_2^0 = \left(\frac{5}{16\pi} \right)^{1/2} (3 \cos^2 \theta - 1)$$

$$d_{xz} = \frac{1}{\sqrt{2}} (Y_2^1 + Y_2^{-1}) = \left(\frac{15}{4\pi} \right)^{1/2} \sin \theta \cos \theta \cos \phi$$

$$d_{yz} = \frac{1}{\sqrt{2}i} (Y_2^1 - Y_2^{-1}) = \left(\frac{15}{4\pi} \right)^{1/2} \sin \theta \cos \theta \sin \phi$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}} (Y_2^2 + Y_2^{-2}) = \left(\frac{15}{16\pi} \right)^{1/2} \sin^2 \theta \cos 2\phi$$

$$d_{xy} = \frac{1}{\sqrt{2}i} (Y_2^2 - Y_2^{-2}) = \left(\frac{15}{16\pi} \right)^{1/2} \sin^2 \theta \sin 2\phi$$

The angular parts of the five d orbitals are shown in Figure 6.7. Note that

TABLE 6.6

The complete hydrogenlike atomic wave functions expressed as real functions for $n = 1, 2$, and 3. The quantity Z is the atomic number of the nucleus and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \cos \phi$
			$\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \sin \phi$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{3s} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \cos \phi$
			$\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \sin \phi$
	$l = 2,$	$m = 0$	$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{3d_{xy}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \cos \phi$
			$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \sin \phi$
	$l = 2,$	$m = \pm 2$	$\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \cos 2\phi$
			$\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \sin 2\phi$

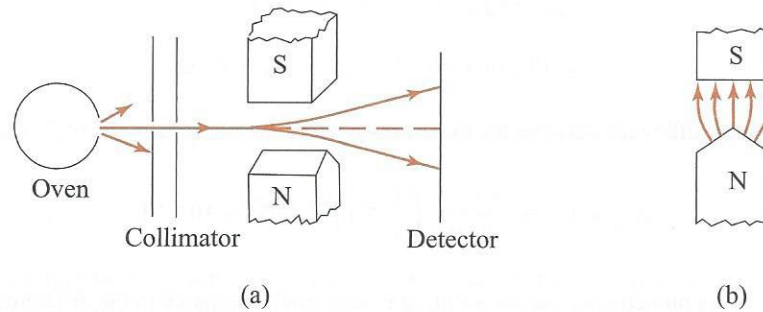


FIGURE 7.10

(a) A schematic diagram of the Stern-Gerlach experiment. (b) A cross-sectional view of the pole pieces of the magnet depicting the inhomogeneous magnetic field that they produce.

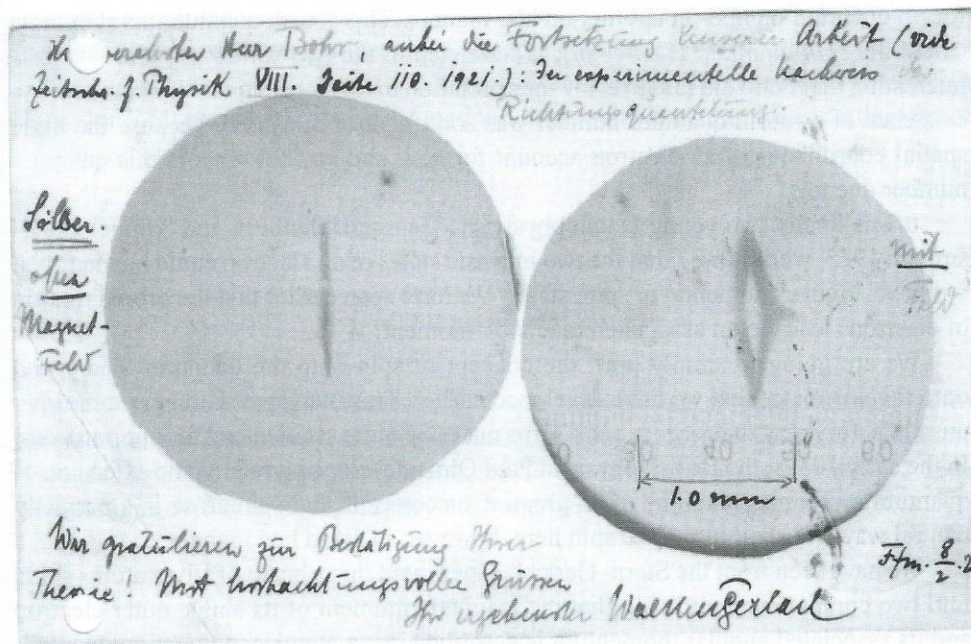


FIGURE 7.11

A postcard from Walther Gerlach to Niels Bohr, dated February 8, 1922. The left side shows the pattern of the beam of silver atoms without a magnetic field, and the right side shows the pattern with the inhomogeneous magnetic field. Reproduced courtesy of Niels Bohr Archive, Copenhagen, Denmark.

TABLE 7.7

A Screen Shot of the First Few Electronic States of Atomic Hydrogen

H I 167 Levels Found (Page 1 of 10)

Data on Landolt levels and level compositions are not available for this ion

Configuration	Term	J	Level (cm ⁻¹)
1s	2S	1/2	0
2p	2P°	1/2	82 258.9206
		3/2	82 259.2865
2s	2S	1/2	82 258.9559
3p	2P°	1/2	97 492.2130
		3/2	97 492.3214
3s	2S	1/2	97 492.2235
3d	2D	3/2	97 492.3212
		5/2	97 492.3574
4p	2P°	1/2	102 823.8505
		3/2	102 823.8962
4s	2S	1/2	102 823.8549
4d	2D	3/2	102 823.8961
		5/2	102 823.9114
4f	2F°	5/2	102 823.9113
		7/2	102 823.9190
5p	2P°	1/2	105 291.6306
		3/2	105 291.6540

Source: http://physics.nist.gov/PhysRefData/ASD/levels_form.html

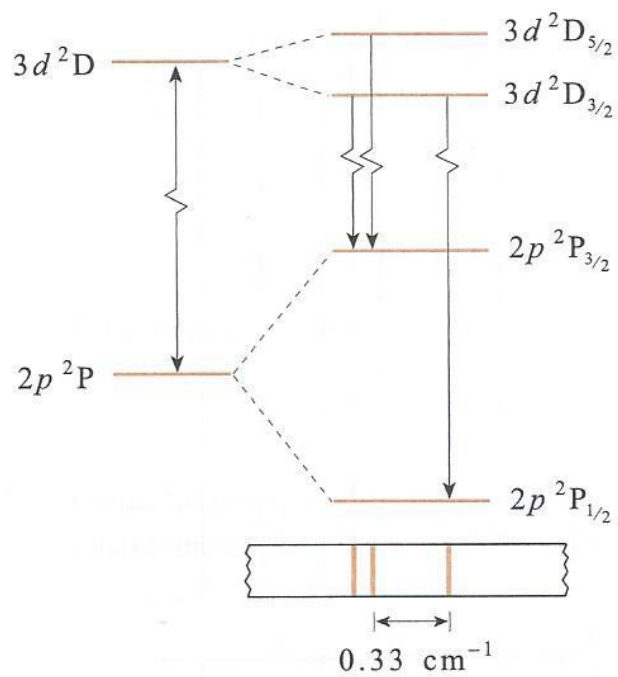


FIGURE 7.12

The fine structure of the spectral line associated with the $3d^2D \rightarrow 2p^2P$ transition in atomic hydrogen.

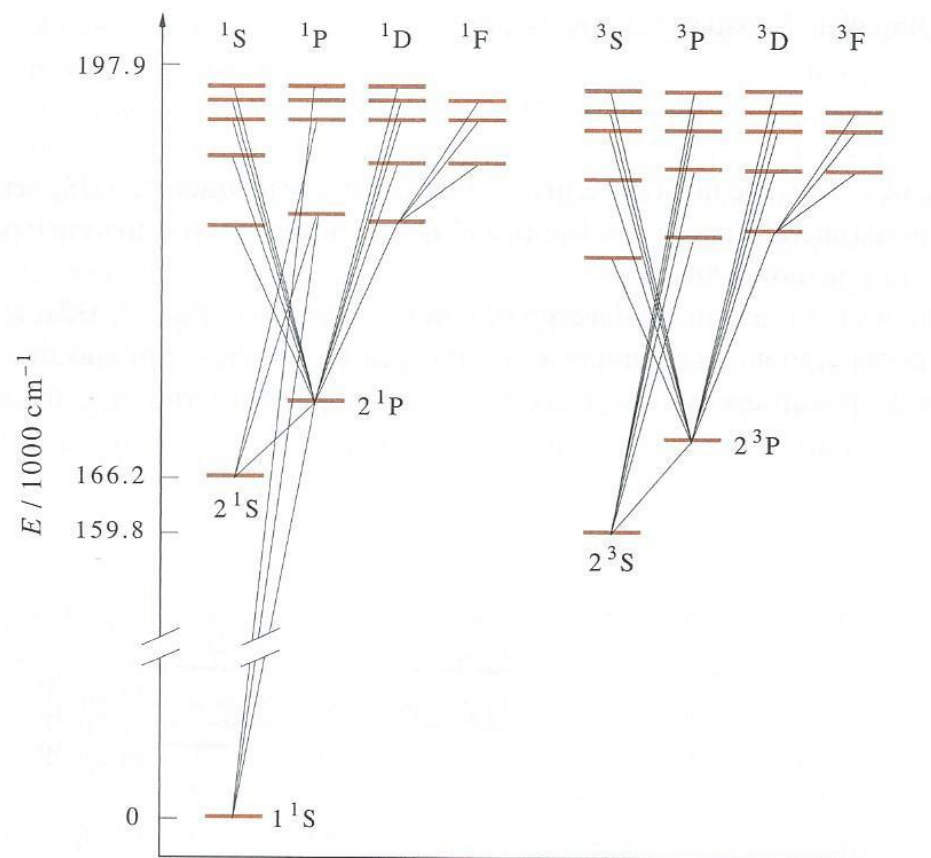


FIGURE 9.10

The energy-level diagram of a helium atom, showing the two separate sets of singlet and triplet states.

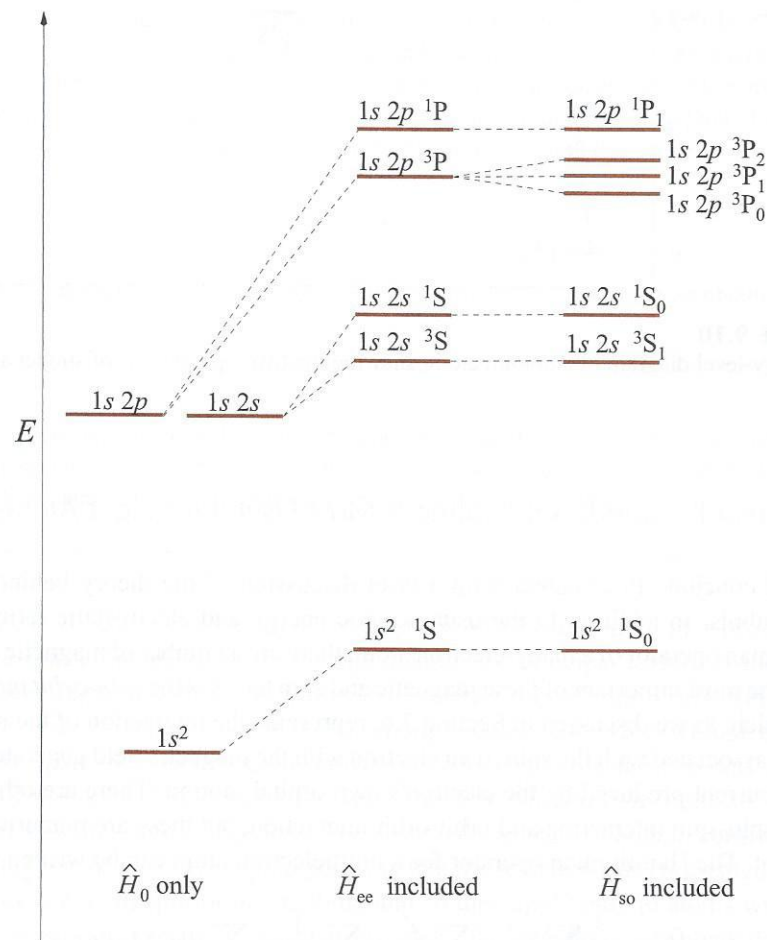


FIGURE 9.11

A schematic diagram of how the energies of the $1s^2$, $1s2s$, and $1s2p$ electron configurations of a helium atom are split by the electron-electron repulsion term and the spin-orbit interaction term. The energies in this figure are not to scale, the splitting due to spin-orbit coupling is much smaller than that due to electron-electron repulsion.

TABLE 9.5

A Screen Shot of the First Few Electronic States of Atomic Sodium^a

Na I 409 Levels Found

Data on Lande factors and level compositions are not available for this ion.

Configuration	Term	J	Level (cm ⁻¹)
2p ⁶ 3s	2S	1/2	0
2p ⁶ 3p	2P°	1/2	16 956.172
		3/2	16 973.368
2p ⁶ 4s	2S	1/2	25 739.991
2p ⁶ 3d	2D	5/2	29 172.839
		3/2	29 172.889
2p ⁶ 4p	2P°	1/2	30 266.99
		3/2	30 272.58
2p ⁶ 5s	2S	1/2	33 200.675
2p ⁶ 4d	2D	5/2	34 548.731
		3/2	34 548.766

a. Source: The NIST website http://physics.nist.gov/PhysRefData/ASD/levels_form.html

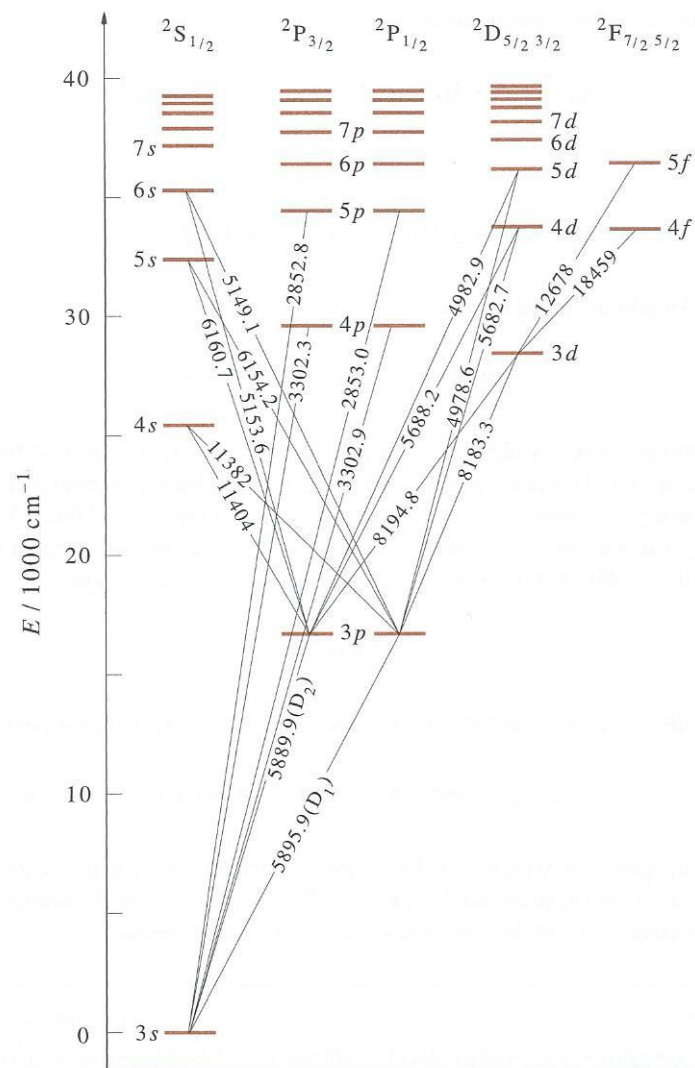


FIGURE 9.9
An energy-level diagram of atomic sodium.

TABLE 9.4

The Possible Term Symbols (Excluding the J Subscript) for Various Electron Configuration for Equivalent Electrons

Electron configuration	Term symbol (excluding the J subscript)
s^1	2S
p^1	2P
p^2, p^4	$^1S, ^1D, ^3P$
p^3	$^2P, ^2D, ^4S$
p^1, p^5	2P
d^1, d^9	2D
d^2, d^8	$^1S, ^1D, ^1G, ^3P, ^3F$
d^3, d^7	$^2P, ^2D$ (twice), $^2F, ^2G, ^2H, ^4P, ^4F$
d^4, d^6	1S (twice), 1D (twice), $^1F, ^1G$ (twice), $^1I, ^3P$ (twice), $^3D, ^3F$ (twice), $^3G, ^3H,$
d^5	$^2S, ^2P, ^2D$ (thrice), 2F (twice), 2G (twice), $^2H, ^2I, ^4P, ^4D, ^4F, ^4G, ^6S$