method, electronic states, vibrational and rotational states, molecular spectra, and ligand field theory.

The quantum mechanics of atoms and molecules, once the exclusive domain of physicists, has in recent years proliferated into other fields, primarily chemistry and several branches of engineering. In recognition of this wider interest, a full year graduate course in atomic and molecular physics has been taught in the Department of Applied Physics at Stanford University. Attendees consisted of students working in diverse fields such as spectroscopy, magnetic resonance, Mössbauer resonance, quantum electronics, solid state electronics, astrophysics, and biological physics. The present volume is an outgrowth of this course.

Mathematical Background

CHAPTER 1

ANGULAR MOMENTUM

1.1 Orbital Angular Momentum

The orbital angular momentum operator **L** is defined by

$$\mathbf{L} = \frac{1}{\hbar}(\mathbf{r} \times \mathbf{p}) \tag{1.1-1}$$

where **r** is a vector whose components r_i are x, y, z (or x_1, x_2, x_3) and

$$\mathbf{p} = -i\hbar\nabla \tag{1.1-2}$$

is the linear momentum operator; the rectangular components of the gradient operator ∇ are $\partial/\partial x, \partial/\partial y, \partial/\partial z$. Expanding (1.1-1),

$$L_x = \frac{1}{\hbar}(yp_z - zp_y) = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$= i\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right), \tag{1.1-3a}$$

$$L_y = \frac{1}{\hbar}(zp_x - xp_z) = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$= i\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right), \tag{1.1-3b}$$

$$L_z = \frac{1}{\hbar}(xp_y - yp_x) = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$= -i\frac{\partial}{\partial\varphi}. \tag{1.1-3c}$$

In (1.1-3) the angles θ and φ are the polar and azimuth angles, respectively.

The operators L_x, L_y, and L_z are Hermitian, i.e.,

$$L_i^\dagger = L_i \qquad (i = x, y, z), \tag{1.1-4}$$

and, as functions of the coordinates, L_x, L_y, and L_z are pure imaginary operators.

It will often be convenient to use *spherical components* of $\mathbf{L}$; these are defined as

$$L_{+1} = -\frac{1}{\sqrt{2}}(L_x + iL_y) = -\frac{1}{\sqrt{2}} e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right),$$

$$L_{-1} = \frac{1}{\sqrt{2}}(L_x - iL_y) = -\frac{1}{\sqrt{2}} e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial p}\right), \tag{1.1-5}$$

$$L_0 = L_z.$$

The inverse relations are

$$L_x = -\frac{1}{\sqrt{2}}(L_{+1} - L_{-1}), \qquad L_y = \frac{i}{\sqrt{2}}(L_{+1} + L_{-1}), \qquad L_z = L_0. \tag{1.1-6}$$

In contrast to the rectangular components of $\mathbf{L}$, L_{+1} and L_{-1} are *not* Hermitian since

$$L_{+1}^\dagger = -L_{-1}, \qquad L_{-1}^\dagger = -L_{+1}. \tag{1.1-7}$$

The components of $\mathbf{r}$ and $\mathbf{p}$ satisfy certain commutation relations:

$$[r_i, p_j] = i\hbar\,\delta_{ij}, \tag{1.1-8a}$$

$$[r_i, r_j] = [p_i, p_j] = 0, \tag{1.1-8b}$$

$$[r_i, p^2] = 2i\hbar p_i, \tag{1.1-8c}$$

$$[p_i, p^2] = 0 \tag{1.1-8d}$$

in which $r_i, r_j = x, y, z$; $p_i, p_j = p_x, p_y, p_z$, and $p^2 = p_x^2 + p_y^2 + p_z^2$. The definition of $\mathbf{L}$ (1.1-1) together with (1.1-8) imply that

$$[L_x, L_y] = iL_z, \qquad [L_y, L_z] = iL_x, \qquad [L_z, L_x] = iL_y. \tag{1.1-9}$$

These may be written in any of the compact forms:

$$[L_i, L_j] = iL_k \qquad (i, j, k \text{ cyclic}), \tag{1.1-10a}$$

$$\mathbf{L} \times \mathbf{L} = i\mathbf{L}, \tag{1.1-10b}$$

$$[L_i, L_j] = i\varepsilon_{ijk} L_k, \tag{1.1-10c}$$

in which ε_{ijk} is the antisymmetric unit tensor of rank 3 defined by

$$\varepsilon_{ijk} = \begin{cases} +1, & i,j,k \text{ in cyclic order,} \\ -1, & i,j,k \text{ not in cyclic order,} \\ 0, & \text{two indices alike.} \end{cases} \tag{1.1-11}$$

The three statements (1.1-10a)–(1.1-10c) are equivalent in all respects. Additional commutator relations among the components of $\mathbf{L}$, $\mathbf{r}$, and $\mathbf{p}$ are

$$[L_i, r_j] = i\varepsilon_{ijk} r_k, \tag{1.1-12a}$$

$$[L_i, p_j] = i\varepsilon_{ijk} p_k, \tag{1.1-12b}$$

$$[L_0, L_{\pm 1}] = \pm L_{\pm 1}, \qquad [L_{+1}, L_{-1}] = -L_0. \tag{1.1-13}$$

Another important operator is L^2, also known as the *total orbital angular momentum operator*. It may be expressed in various equivalent forms:

$$\begin{aligned} L^2 &= L_x^2 + L_y^2 + L_z^2 \\ &= -\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + (1 + \cot^2\theta)\frac{\partial^2}{\partial\varphi^2}\right] \\ &= -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \\ &= -L_{+1}L_{-1} + L_0^2 - L_{-1}L_{+1} \\ &= \sum_q (-1)^q L_q L_{-q} \qquad (q = 1, 0, -1). \end{aligned} \tag{1.1-14}$$

Employing relations (1.1-13) we also have

$$L^2 = -2L_{+1}L_{-1} + L_0(L_0 - 1) = -2L_{-1}L_{+1} + L_0(L_0 + 1). \tag{1.1-15}$$

L^2 commutes with all components of $\mathbf{L}$, i.e.,

$$[L^2, L_\mu] = 0 \tag{1.1-16}$$

where L_μ refers to either rectangular components (L_x, L_y, L_z) or spherical components (L_{+1}, L_0, L_{-1}) of $\mathbf{L}$.

1.2 Spherical Harmonics and Related Functions

The spherical harmonics $Y_{lm}(\theta, \varphi)$ are defined by

$$Y_{lm}(\theta, \varphi) = \sqrt{(-1)^{m+|m|}}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-|m|)!}{(l+|m|)!}}\,P_l^{|m|}(\cos\theta)e^{im\varphi} \tag{1.2-1}$$

TABLE 1.1

Spherical Harmonics[a]

l	m	$r^l Y_{lm}(x, y, z)$	$Y_{lm}(\theta, \varphi)$
0	0	$\sqrt{\frac{1}{4\pi}}$	$\sqrt{\frac{1}{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}}\, z$	$\sqrt{\frac{3}{4\pi}}\cos\theta$
1	± 1	$\mp\sqrt{\frac{3}{8\pi}}(x \pm iy)$	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$
2	0	$\sqrt{\frac{5}{4\pi}}\sqrt{\frac{1}{4}}(3z^2 - r^2)$	$\sqrt{\frac{5}{4\pi}}\sqrt{\frac{1}{4}}(3\cos^2\theta - 1)$
2	± 1	$\mp\sqrt{\frac{5}{4\pi}}\sqrt{\frac{3}{2}}\, z(x \pm iy)$	$\mp\sqrt{\frac{5}{4\pi}}\sqrt{\frac{3}{2}}\cos\theta\sin\theta\, e^{\pm i\varphi}$
2	± 2	$\sqrt{\frac{5}{4\pi}}\sqrt{\frac{3}{8}}(x \pm iy)^2$	$\sqrt{\frac{5}{4\pi}}\sqrt{\frac{3}{8}}\sin^2\theta\, e^{\pm 2i\varphi}$
3	0	$\sqrt{\frac{7}{4\pi}}\sqrt{\frac{1}{4}}\, z(5z^2 - 3r^2)$	$\sqrt{\frac{7}{4\pi}}\sqrt{\frac{1}{4}}(2\cos^3\theta - 3\cos\theta\sin^2\theta)$
3	± 1	$\mp\sqrt{\frac{7}{4\pi}}\sqrt{\frac{3}{16}}(x \pm iy)(5z^2 - r^2)$	$\mp\sqrt{\frac{7}{4\pi}}\sqrt{\frac{3}{16}}(4\cos^2\theta\sin\theta - \sin^3\theta)e^{\pm i\varphi}$
3	± 2	$\sqrt{\frac{7}{4\pi}}\sqrt{\frac{15}{8}}\, z(x \pm iy)^2$	$\sqrt{\frac{7}{4\pi}}\sqrt{\frac{15}{8}}\cos\theta\sin^2\theta\, e^{\pm 2i\varphi}$
3	± 3	$\mp\sqrt{\frac{7}{4\pi}}\sqrt{\frac{5}{16}}(x \pm iy)^3$	$\mp\sqrt{\frac{7}{4\pi}}\sqrt{\frac{5}{16}}\sin^3\theta\, e^{\pm 3i\varphi}$
4	0	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{1}{64}}(35z^4 - 30z^2r^2 + 3r^4)$	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{1}{64}}(35\cos^4\theta - 30\cos^2\theta + 3)$
4	± 1	$\mp\sqrt{\frac{9}{4\pi}}\sqrt{\frac{5}{16}}(x \pm iy)(7z^3 - 3zr^2)$	$\mp\sqrt{\frac{9}{4\pi}}\sqrt{\frac{5}{16}}\sin\theta(7\cos^3\theta - 3\cos\theta)e^{\pm i\varphi}$
4	± 2	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{5}{32}}(x \pm iy)^2(7z^2 - r^2)$	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{5}{32}}\sin^2\theta(7\cos^2\theta - 1)e^{\pm 2i\varphi}$
4	± 3	$\mp\sqrt{\frac{9}{4\pi}}\sqrt{\frac{35}{16}}\, z(x \pm iy)^3$	$\mp\sqrt{\frac{9}{4\pi}}\sqrt{\frac{35}{16}}\sin^3\theta\cos\theta\, e^{\pm 3i\varphi}$
4	± 4	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{35}{128}}(x \pm iy)^4$	$\sqrt{\frac{9}{4\pi}}\sqrt{\frac{35}{128}}\sin^4\theta\, e^{\pm 4i\varphi}$

[a] In spectroscopic notation, functions that are proportional to Y_{lm} with $l = 0, 1, 2, 3, \ldots$ are called s, p, d, f, ... functions.

with

$$l = 0, 1, 2, \ldots, \tag{1.2-2a}$$

$$m = l, l-1, \ldots, -l, \tag{1.2-2b}$$

and $P_l^{|m|}(\cos\theta)$ an associated Legendre polynomial. The phase convection in (1.2-1) is not universal; the one adopted here is known as the *Condon–Shortley convention*. Some of the commonly used spherical harmonics are listed in Table 1.1; among their properties are:

$$Y_{l\,-m}(\theta, \varphi) = (-1)^m Y^*_{lm}(\theta, \varphi), \tag{1.2-3a}$$

$$Y_{lm}(\pi - \theta, \pi + \varphi) = (-1)^l Y_{lm}(\theta, \varphi). \tag{1.2-3b}$$

The change from (θ, φ) to $(\pi - \theta, \pi + \varphi)$ corresponds to an inversion, that is, a change from (x, y, z) to $(-x, -y, -z)$. From (1.2-3b) it is seen that $Y_{lm}(\theta, \varphi)$ changes sign under inversion when l is an odd integer; when l is even, there is no change in sign. In the former case, $Y_{lm}(\theta, \varphi)$ is said to have *odd parity* and in the latter, *even parity*. The quantity $(-1)^l$, which is equal to $+1$ for l even and -1 for l odd is called the *parity factor*.

When $\theta = 0$,

$$Y_{lm}(0, \varphi) = \begin{cases} 0 & \text{for } m \neq 0, \\ \sqrt{\dfrac{2l+1}{4\pi}} & \text{for } m = 0. \end{cases} \tag{1.2-4}$$

The spherical harmonics satisfy the orthogonality relation

$$\int Y^*_{lm}(\theta, \varphi) Y_{l'm'}(\theta, \varphi) \sin\theta\, d\theta\, d\varphi \equiv \int Y^*_{lm}(\theta, \varphi) Y_{l'm'}(\theta, \varphi)\, d\Omega = \delta_{ll'}\,\delta_{mm'} \tag{1.2-5}$$

in which $d\Omega = \sin\theta\, d\theta\, d\varphi$ is an element of solid angle. An arbitrary function $f(\theta, \varphi)$, satisfying the usual criteria for expansion in terms of an orthonormal set, may be expanded in terms of spherical harmonics as

$$f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_{lm}(\theta, \varphi), \tag{1.2-6a}$$

$$a_{lm} = \int Y^*_{lm}(\theta, \varphi) f(\theta, \varphi)\, d\Omega. \tag{1.2-6b}$$

It is often desirable to work with real functions constructed as linear combinations of the (complex) spherical harmonics. Several examples are listed in Table 1.2 and are shown in the form of polar diagrams in Fig. 1.1.

Orbital angular momentum operators and spherical harmonics are intimately related. This may be seen from the standpoint of a central force

TABLE 1.2
Real Combinations of Spherical Harmonics

Notation	Cartesian coordinates	Polar coordinates	Spherical harmonics
s	1	1	$\sqrt{4\pi}\,Y_{0\,0}$
p_x	x	$r\sin\theta\cos\varphi$	$\sqrt{\frac{4\pi}{3}}\sqrt{\frac{1}{2}}(-Y_{1\,1}+Y_{1\,-1})r$
p_y	y	$r\sin\theta\sin\varphi$	$\sqrt{\frac{4\pi}{3}}\sqrt{\frac{1}{2}}\,i(Y_{1\,1}+Y_{1\,-1})r$
p_z	z	$r\cos\theta$	$\sqrt{\frac{4\pi}{3}}Y_{1\,0}r$
d_{z^2}	$\frac{1}{2}(3z^2-r^2)$	$\frac{1}{2}r^2(3\cos^2\theta-1)$	$\sqrt{\frac{4\pi}{5}}Y_{2\,0}r^2$
$d_{x^2-y^2}$	$\frac{1}{2}\sqrt{3}(x^2-y^2)$	$\frac{1}{2}\sqrt{3}r^2\sin^2\theta\cos 2\varphi$	$\sqrt{\frac{4\pi}{5}}\sqrt{\frac{1}{2}}(Y_{2\,2}+Y_{2\,-2})r^2$
d_{xy}	$\sqrt{3}xy$	$\sqrt{3}r^2\sin^2\theta\cos\varphi\sin\varphi$	$\sqrt{\frac{4\pi}{5}}\sqrt{\frac{1}{2}}\,i(-Y_{2\,2}+Y_{2\,-2})r^2$
d_{yz}	$\sqrt{3}yz$	$\sqrt{3}r^2\sin\theta\cos\theta\sin\varphi$	$\sqrt{\frac{4\pi}{5}}\sqrt{\frac{1}{2}}\,i(Y_{2\,1}+Y_{2\,-1})r^2$
d_{zx}	$\sqrt{3}zx$	$\sqrt{3}r^2\sin\theta\cos\theta\cos\varphi$	$\sqrt{\frac{4\pi}{5}}\sqrt{\frac{1}{2}}(-Y_{2\,1}+Y_{2\,-1})r^2$

problem. Let the Hamiltonian of a particle of mass m and momentum $\mathbf{p}$ be

$$\mathscr{H} = \frac{p^2}{2m} + V \qquad (1.2\text{-}7)$$

where V is the potential energy. The Schrödinger equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad (1.2\text{-}8)$$

may be transformed into spherical coordinates as

$$r^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi + \frac{2mr^2}{\hbar^2}(E - V)\psi = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi. \qquad (1.2\text{-}9)$$

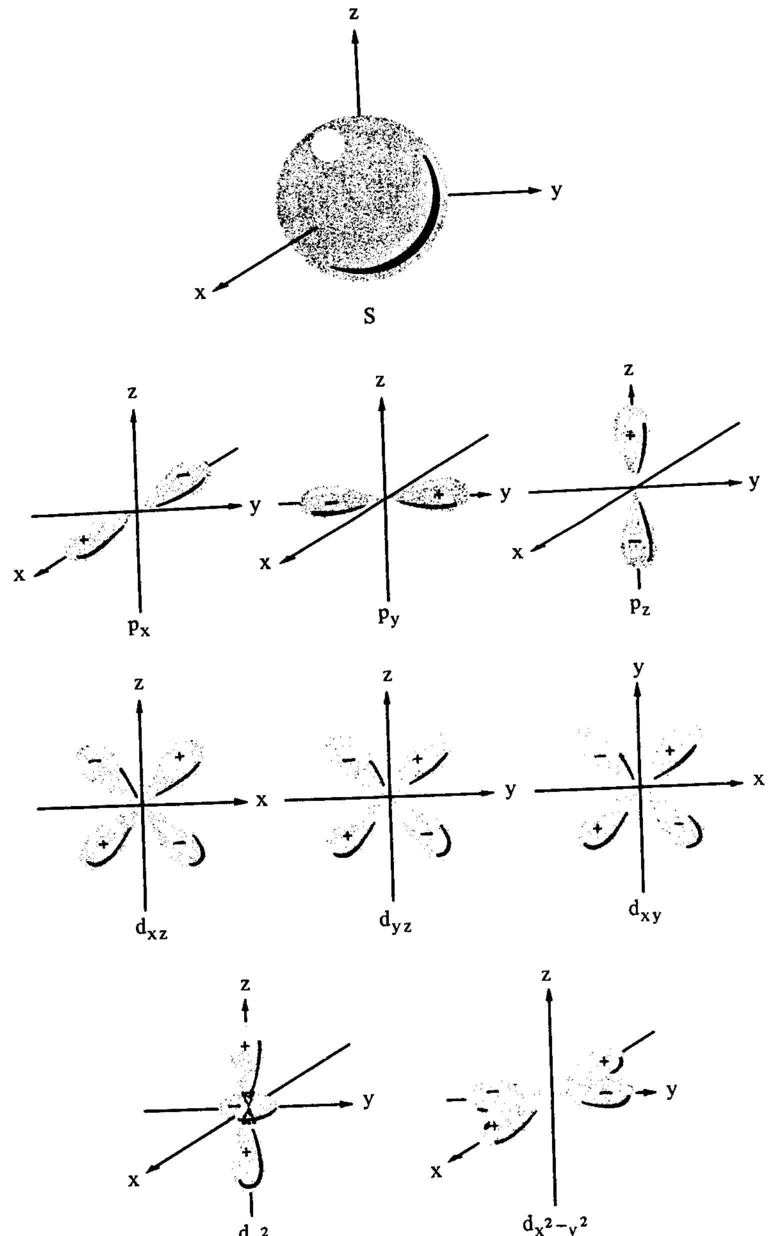


FIG. 1.1 Polar diagrams of s, p, and d functions. (From C. J. Ballhausen and H. B. Gray, "Molecular Orbital Theory," copyright © 1964 by W. A. Benjamin, Inc., Menlo Park, California.)

In a central field for which $V = V(r)$, (1.2-9) is separable into two equations one of which depends on r only and the other on θ and φ. Thus let

$$\psi(r,\theta,\varphi) = R(r)\Theta(\theta,\varphi), \quad (1.2\text{-}10)$$

$$R(r) = \frac{1}{r} P(r). \quad (1.2\text{-}11)$$

The Schrödinger equation (1.2-9) now separates into

$$\frac{d^2P(r)}{dr^2} + \frac{2m}{\hbar^2}[E - V(r)]P(r) = \frac{\lambda}{r^2} P(r), \quad (1.2\text{-}12)$$

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Theta(\theta,\varphi) = \lambda\Theta(\theta,\varphi), \quad (1.2\text{-}13)$$

in which λ is a separation constant. From (1.1-14) it is seen that the operator on the left-hand side of (1.2-13) is just L^2; thus

$$L^2\Theta(\theta,\varphi) = \lambda\Theta(\theta,\varphi). \quad (1.2\text{-}14)$$

Quantum-mechanical wave functions and their first derivatives must be everywhere continuous, single-valued, and finite. When these conditions are imposed on $\psi(r,\theta,\varphi)$, it is found that

$$\Theta(\theta,\varphi) = Y_{lm}(\theta,\varphi), \quad (1.2\text{-}15)$$

$$\lambda = l(l+1). \quad (1.2\text{-}16)$$

In other words, the solutions to the quantum-mechanical central force problem are products of radial functions and angular functions and the latter are the spherical harmonics $Y_{lm}(\theta,\varphi)$ which satisfy

$$L^2 Y_{lm}(\theta,\varphi) = l(l+1)Y_{lm}(\theta,\varphi). \quad (1.2\text{-}17)$$

The relation expressed by (1.2-17) lends itself to the interpretation that $Y_{lm}(\theta,\varphi)$ is an eigenfunction of the operator L^2 and the corresponding eigenvalue is $l(l+1)$. Alternatively, (1.2-17) is derivable from the basic definition for L^2 (1.1-14) and $Y_{lm}(\theta,\varphi)$ (1.2-1). The restrictions on l and m are contained in (1.2-2a) and (1.2-2b); in particular, it should be noted that l and m, known as *quantum numbers* in physical terminology, are integers. In older quantum mechanical formulations $\sqrt{l(l+1)}$ was regarded as the magnitude of the vector **L** and m was the projection of **L** on the z axis. Although this description is somewhat lacking in rigor, it does provide a useful pictorial representation (Fig. 1.2) which serves as the origin for the designation of m as a *projection* quantum number. Also, because m degeneracies are removed by a magnetic field (see Section 17.1), m is also known as a *magnetic* quantum number.

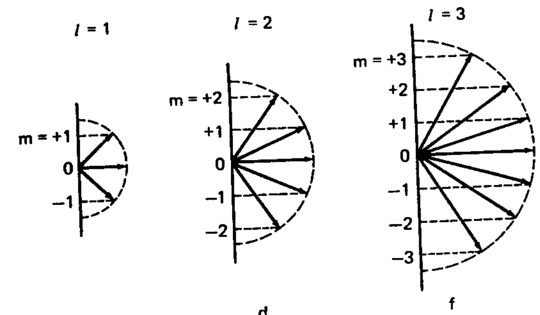


FIG. 1.2 Geometrical relation between the quantum numbers l and m. In these diagrams $\sqrt{l(l+1)}$ is regarded as the magnitude of **L**.

According to (1.1-16), L^2 commutes with all components of **L** and in particular

$$[L^2, L_z] = 0. \quad (1.2\text{-}18)$$

We therefore expect an eigenfunction of L^2 to be simultaneously an eigenfunction of L_z. Since the φ-dependence of $Y_{lm}(\theta,\varphi)$ is entirely confined to $e^{im\varphi}$ and L_z is given by (1.1-3c), we have

$$L_z Y_{lm}(\theta,\varphi) = mY_{lm}(\theta,\varphi). \quad (1.2\text{-}19)$$

Equations (1.2-17) and (1.2-19) exhibit the basic connections between orbital angular momentum operators and spherical harmonics. It is important to note that because of the noncommutativity of the components of **L**, simultaneous eigenfunctions of L^2 and L_z, in general, will not be eigenfunctions of any other component of **L**.

We now list several useful formulas involving spherical harmonics. The reciprocal distance between two points whose position vectors are $\mathbf{r}_1$ and $\mathbf{r}_2$ (Fig. 1.3) is given by

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\omega), \quad (1.2\text{-}20)$$

in which $r_<$ stands for the smaller of the two distances $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$, $r_>$ is the greater of the two distances, and $P_l(\cos\omega)$ is a Legendre polynomial. If $\mathbf{r}_1$ is in the direction (θ_1,φ_1) and $\mathbf{r}_2$ is in the direction (θ_2,φ_2), then the angle ω is the angle between the two directions. The *addition theorem*

$$P_l(\cos\omega) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^*(\theta_1,\varphi_1)Y_{lm}(\theta_2,\varphi_2) \quad (1.2\text{-}21)$$

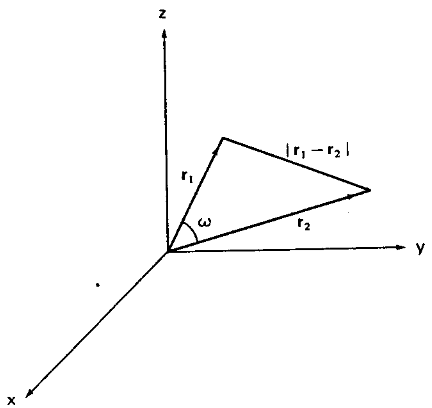


FIG. 1.3 Notation and coordinate system for Eq. (1.2-20).

permits us to replace (1.2-20) by

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\theta_1, \varphi_1) Y_{lm}(\theta_2, \varphi_2). \qquad (1.2\text{-}22)$$

Another variation of (1.2-22) is obtained by writing

$$\begin{aligned} \mathbf{Y}_1^{(l)} \cdot \mathbf{Y}_2^{(l)} &\equiv \mathbf{Y}^{(l)}(\theta_1, \varphi_1) \cdot \mathbf{Y}^{(l)}(\theta_2, \varphi_2) \\ &= \sum_{m=-l}^{l} (-1)^m Y_{l\,-m}(\theta_1, \varphi_1) Y_{lm}(\theta_2, \varphi_2) \\ &= \sum_{m=-l}^{l} Y_{lm}^*(\theta_1, \varphi_1) Y_{lm}(\theta_2, \varphi_2). \qquad (1.2\text{-}23) \end{aligned}$$

Substitution in (1.2-22) yields

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} \mathbf{Y}_1^{(l)} \cdot \mathbf{Y}_2^{(l)}. \qquad (1.2\text{-}24)$$

When $l = 1$ in (1.2-21),

$$P_1(\cos\omega) = \cos\omega = \frac{4\pi}{3} \sum_{m=-l}^{l} Y_{1m}^*(\theta_1, \varphi_1) Y_{1m}(\theta_2, \varphi_2), \qquad (1.2\text{-}25)$$

which then provides an expression for the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$ (Fig. 1.3). Alternatively, if ω is set equal to zero in (1.2-21),

$$P_l(1) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} |Y_{lm}(\theta, \varphi)|^2.$$

Since $P_l(1) = 1$,

$$\sum_{m=-l}^{l} |Y_{lm}(\theta, \varphi)|^2 = \frac{2l+1}{4\pi}. \qquad (1.2\text{-}26)$$

Also, setting $Y_{l'm'}(\theta, \varphi) = Y_{00} = 1/\sqrt{4\pi}$ in (1.2-5) yields

$$\int Y_{lm}(\theta, \varphi)\, d\Omega = \sqrt{4\pi}\, \delta(l, 0)\, \delta(m, 0). \qquad (1.2\text{-}27)$$

A plane wave may be expanded in terms of spherical harmonics as

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y_{lm}(\theta_r, \varphi_r) Y_{lm}^*(\theta_k, \varphi_k), \qquad (1.2\text{-}28)$$

in which $j_l(kr)$ is a spherical Bessel function (Appendix 5), (r, θ_r, φ_r) the coordinates of the point of observation, and (θ_k, φ_k) the direction of the wave vector (Fig. 1.4).

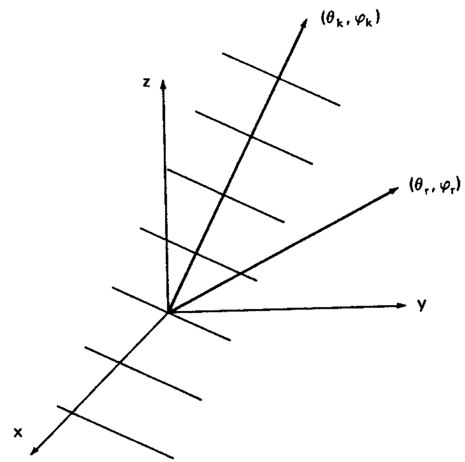


FIG. 1.4 Notation and coordinate system for Eq. (1.2-28).

The integral of the product of three spherical harmonics is given by

$$\begin{aligned} &\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi\, Y_{l'm'}^*(\theta, \varphi) Y_{LM}(\theta, \varphi) Y_{lm}(\theta, \varphi) \\ &= \int Y_{l'm'}^*(\theta, \varphi) Y_{LM}(\theta, \varphi) Y_{lm}(\theta, \varphi)\, d\Omega \\ &\equiv \langle l'm' | Y_{LM} | lm \rangle \\ &= (-1)^{m'} \sqrt{\frac{(2l'+1)(2L+1)(2l+1)}{4\pi}} \begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix} \begin{pmatrix} l' & L & l \\ 0 & 0 & 0 \end{pmatrix}. \qquad (1.2\text{-}29) \end{aligned}$$

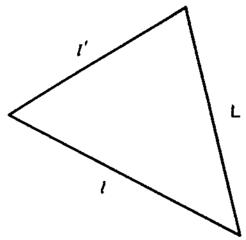


FIG. 1.5 The triangle relation for angular momenta.

This is known as the *Gaunt formula*; the quantities $\left(\begin{smallmatrix} a & b & c \\ d & e & f \end{smallmatrix}\right)$ are numerical coefficients called *3j symbols* whose properties are described in Section 1.5. The integral (1.2-29) vanishes unless the conditions

$$-m' + M + m = 0, \tag{1.2-30}$$

$$l' + L + l \text{ is an even integer}, \tag{1.2-31}$$

$$\left.\begin{matrix} l' + L - l \\ l' - L + l \\ -l' + L + l \end{matrix}\right\} \geqslant 0 \tag{1.2-32}$$

are satisfied. The symbol $\triangle(l'Ll)$ is often used as shorthand for (1.2-32) together with the condition that $l' + L + l$ is an integer (not necessarily even). These are also known as the triangle conditions (Fig. 1.5). Selected numerical values of (1.2-29) are given in Table 11.1. When the triangle conditions are satisfied,

$$Y_{LM}(\theta,\varphi) = (-1)^{l'-l-M}\sqrt{2L+1}\sum_{mm'}\begin{pmatrix} l & l' & L \\ m & m' & -M \end{pmatrix} Y_{lm}(\theta,\varphi)Y_{l'm'}(\theta,\varphi), \tag{1.2-33}$$

$$Y_{lm}(\theta,\varphi)Y_{l'm'}(\theta,\varphi) = \sum_{LM}\sqrt{\frac{(2l+1)(2l'+1)(2L+1)}{4\pi}} \times \begin{pmatrix} l & l' & L \\ m & m' & M \end{pmatrix}\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} Y^*_{LM}(\theta,\varphi), \tag{1.2-34}$$

$$Y^*_{lm}(\theta,\varphi)Y_{l'm'}(\theta,\varphi) = \sum_{LM}(-1)^{m'}\sqrt{\frac{(2l+1)(2l'+1)(2L+1)}{4\pi}} \times \begin{pmatrix} l & l' & L \\ m & -m' & M \end{pmatrix}\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} Y_{LM}(\theta,\varphi). \tag{1.2-35}$$

Equations (1.2-34) and (1.2-35) are equivalent.

1.3 Generalized Angular Momentum

The commutation rules (1.1-10) for the components of orbital angular momentum operators followed from definition (1.1-1) and the commutation rules (1.1-8a) and (1.1-8b). This development led to the conclusion that the orbital angular momentum quantum numbers, l and m, were integers. However, other kinds of angular momenta are encountered in physical problems and the quantum numbers associated with such angular momenta are not necessarily integers. It is therefore necessary to extend the formalism in such a way as to permit the appearance of nonintegral quantum numbers but without invalidating any of the previous results pertaining to orbital angular momentum.

For this purpose we take the commutation rules (1.1-10) as the starting point of the development. The generalized angular momentum operator **J** is then defined as a vector operator with Hermitian components J_x, J_y, and J_z which satisfy

$$\mathbf{J} \times \mathbf{J} = i\mathbf{J}. \tag{1.3-1}$$

By analogy with (1.1-5), the spherical components are defined as

$$J_{+1} = -\frac{1}{\sqrt{2}}(J_x + iJ_y), \qquad J_0 = J_z, \qquad J_{-1} = \frac{1}{\sqrt{2}}(J_x - iJ_y), \tag{1.3-2}$$

with the inverse relations

$$J_x = -\frac{1}{\sqrt{2}}(J_{+1} - J_{-1}), \qquad J_y = \frac{i}{\sqrt{2}}(J_{+1} + J_{-1}), \qquad J_z = J_0. \tag{1.3-3}$$

It should be remarked that the structural resemblance between (1.3-2) and the spherical harmonics $Y_{1m}(\theta,\varphi)$ (Table 1.1) is not accidental. This aspect will be further explored in the discussion on irreducible tensors in Section 6.1. We also have

$$J^\dagger_{\pm 1} = -J_{\mp 1}, \tag{1.3-4}$$

and, as a direct consequence of (1.3-1),

$$[J_0, J_{\pm 1}] = \pm J_{\pm 1}, \qquad [J_{+1}, J_{-1}] = -J_0. \tag{1.3-5}$$

Since J_x, J_y, and J_z are Hermitian, the total angular momentum operator

$$J^2 = J_x^2 + J_y^2 + J_z^2 \tag{1.3-6a}$$

must also be Hermitian. It may be written in various forms as

$$J^2 = -J_{+1}J_{-1} + J_0^2 - J_{-1}J_{+1} \tag{1.3-6b}$$

$$= \sum_q (-1)^q J_q J_{-q} \qquad (q = 1, 0, -1) \tag{1.3-6c}$$

$$= -2J_{+1}J_{-1} + J_0(J_0 - 1) \tag{1.3-6d}$$

$$= -2J_{-1}J_{+1} + J_0(J_0 + 1) \tag{1.3-6e}$$

in which the last two expressions are based on (1.3-5). J^2 commutes with all rectangular and spherical components of **J**, i.e.,

$$[J^2, J_\mu] = 0. \tag{1.3-7}$$

So far, all the relations that have been written in terms of **J** are duplicates of corresponding relations in terms of **L** given in the previous section. However, at this stage the development proceeds in a new direction. Since J^2 commutes with all components of **J** and, in particular, with J_0, there exist simultaneous eigenfunctions of the two operators. Using the Dirac notation (Appendix 1), let such eigenfunctions, represented symbolically be $|\lambda m\rangle$, satisfy

$$J^2|\lambda m\rangle = \lambda|\lambda m\rangle, \qquad J_0|\lambda m\rangle = m|\lambda m\rangle. \tag{1.3-8}$$

It is seen that in this notation, the eigenfunctions (eigenkets) are labeled by the eigenvalues. Since J^2 and J_0 are both Hermitian, λ and m must be real and

$$\langle\lambda' m'|\lambda m\rangle = \delta_{\lambda'\lambda}\delta_{m'm}. \tag{1.3-9}$$

To proceed further, we invoke a basic postulate of quantum mechanics, namely, that the scalar product of any state vector f with itself is positive definite, i.e.,

$$\langle f|f\rangle \geqslant 0, \qquad \langle f|f\rangle = 0 \quad \text{only if} \quad f = 0. \tag{1.3-10}$$

Using the "turn-over" rule ((A2-4) Appendix 2), the Hermitian property of J_x, and (1.3-10), it is seen that

$$\langle\lambda m|J_x^2|\lambda m\rangle = \langle J_x^\dagger\lambda m|J_x\lambda m\rangle = \langle J_x\lambda m|J_x\lambda m\rangle \geqslant 0. \tag{1.3-11}$$

Similarly,

$$\langle\lambda m|J_y^2|\lambda m\rangle \geqslant 0 \qquad \text{and} \qquad \langle\lambda m|J_z^2|\lambda m\rangle \geqslant 0. \tag{1.3-12}$$

It follows that

$$\langle\lambda m|J^2|\lambda m\rangle \geqslant 0. \tag{1.3-13}$$

But, from (1.3-8) and (1.3-9),

$$\langle\lambda m|J^2|\lambda m\rangle = \lambda;$$

therefore, in view of (1.3-13),

$$\lambda \geqslant 0. \tag{1.3-14}$$

Thus λ is not only real but is positive or zero.

It will now be shown that m has an upper and a lower bound. From (1.3-6e),

$$J_{-1}J_{+1} = \tfrac{1}{2}(J_0^2 + J_0 - J^2).$$

Therefore,

$$\langle\lambda m|J_{-1}J_{+1}|\lambda m\rangle = \tfrac{1}{2}(m^2 + m - \lambda);$$

but

$$\langle\lambda m|J_{-1}J_{+1}|\lambda m\rangle = -\langle J_{+1}\lambda m|J_{+1}\lambda m\rangle, \tag{1.3-15}$$

where the right-hand side of (1.3-15) has again been obtained by the "turn-over" rule. As before,

$$\langle J_{+1}\lambda m|J_{+1}\lambda m\rangle \geqslant 0, \tag{1.3-16}$$

so that

$$\tfrac{1}{2}(m^2 + m - \lambda) \leqslant 0 \tag{1.3-17}$$

or

$$\lambda \geqslant m^2 + m \equiv f(m). \tag{1.3-18}$$

A plot of $f(m)$ as a function of m is shown in Fig. 1.6. Since λ is positive, it is

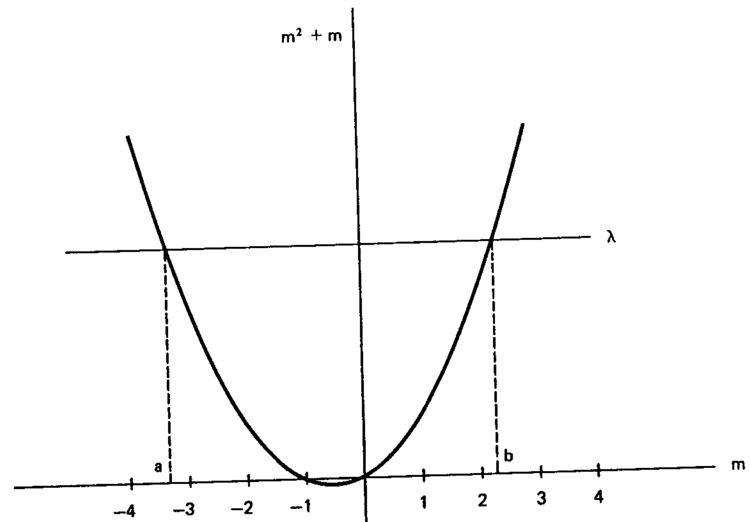


FIG. 1.6 Plot of Eq. (1.3-18).

evident that m possesses an upper bound, say, $b \geqslant 0$ and a lower bound $a \leqslant 0$. Both bounds depend on λ and there are no eigenvalues of J_0 outside of the interval (a, b).

Using the commutator relations (1.3-5),

$$J_0 J_{+1}|\lambda m\rangle = J_{+1}J_0|\lambda m\rangle + J_{+1}|\lambda m\rangle = (m+1)J_{+1}|\lambda m\rangle,$$

from which it is concluded that $J_{+1}|\lambda m\rangle$ is an eigenfunction of J_0 with eigenvalue $(m+1)$. Thus J_{+1}, acting on $|\lambda m\rangle$, has the effect of displacing m upward by one unit. This may be expressed by writing

$$J_{+1}|\lambda m\rangle = c|\lambda\, m+1\rangle, \tag{1.3-19}$$

where c is a constant. Repeating this process, it is found that $J^n_{+1}|\lambda m\rangle$ is an eigenfunction of J_0 with eigenvalue $(m+n)$. Similarly,

$$J_0 J_{-1}|\lambda m\rangle = J_{-1}J_0|\lambda m\rangle - J_{-1}|\lambda m\rangle = (m-1)J_{-1}|\lambda m\rangle,$$

which indicates that

$$J_{-1}|\lambda m\rangle = c'|\lambda\, m-1\rangle, \tag{1.3-20}$$

where c' is another constant. In this case $J^n_{-1}|\lambda m\rangle$ is an eigenfunction of J_0 with eigenvalue $(m-n)$. Because of (1.3-19) and (1.3-20), J_{+1} and J_{-1} are also known as *ladder operators*. We now have the two sequences (or ladders)

$$\begin{aligned} &\vdots \\ J_0 J^2_{+1}|\lambda m\rangle &= (m+2)J^2_{+1}|\lambda m\rangle \\ J_0 J_{+1}|\lambda m\rangle &= (m+1)J_{+1}|\lambda m\rangle \\ J_0|\lambda m\rangle &= m|\lambda m\rangle \\ J_0 J_{-1}|\lambda m\rangle &= (m-1)J_{-1}|\lambda m\rangle \\ J_0 J^2_{-1}|\lambda m\rangle &= (m-2)J^2_{-1}|\lambda m\rangle \\ &\vdots \end{aligned} \tag{1.3-21}$$

However, the sequences do not continue indefinitely in both directions; there is, in fact, an upper and lower bound. To see this, we note that both J_{+1} and J_{-1} commute with J^2 so that

$$J^2 J^n_{\pm 1}|\lambda m\rangle = J^n_{\pm 1}J^2|\lambda m\rangle = \lambda J^n_{\pm 1}|\lambda m\rangle. \tag{1.3-22}$$

This means that $J^n_{\pm 1}|\lambda m\rangle$ is an eigenfunction of J^2 and the corresponding eigenvalue is λ. Thus we have a fixed value of λ and all the eigenvalues of J_0 are confined to an interval such as (a, b) in Fig. 1.6. Let these eigenvalues be

$$m_l, \quad m_l + 1, \quad m_l + 2, \ldots, m_u,$$

where m_l is the lowest eigenvalue in the sequence and does not necessarily

coincide with the endpoint a. Similarly m_u is the highest eigenvalue and does not necessarily coincide with the endpoint b. But to ensure that the eigenvalues $m_l, m_l+1, \ldots, m_u$ remain within the interval (a, b), it is necessary to impose the conditions

$$J_{+1}|\lambda m_u\rangle = 0, \tag{1.3-23a}$$

$$J_{-1}|\lambda m_l\rangle = 0. \tag{1.3-23b}$$

However, from (1.3-6e) and (1.3-8),

$$J_{-1}J_{+1}|\lambda m_u\rangle = \tfrac{1}{2}(J_0^2 + J_0 - J^2)|\lambda m_u\rangle = \tfrac{1}{2}(m_u^2 + m_u - \lambda)|\lambda m_u\rangle. \tag{1.3-24}$$

Condition (1.3-23a) therefore implies that

$$m_u^2 + m_u - \lambda = 0. \tag{1.3-25}$$

In the same fashion,

$$J_{+1}J_{-1}|\lambda m_l\rangle = \tfrac{1}{2}(J_0^2 - J_0 - J^2)|\lambda m_l\rangle = \tfrac{1}{2}(m_l^2 - m_l - \lambda)|\lambda m_l\rangle = 0 \tag{1.3-26}$$

or

$$m_l^2 - m_l - \lambda = 0. \tag{1.3-27}$$

In order to satisfy both (1.3-25) and (1.3-27) we must have

$$m_u = -m_l. \tag{1.3-28}$$

It then follows that it is impossible to have a sequence $m_l, m_l+1, \ldots, m_u$ that satisfies (1.3-28) unless all members of the sequence are either integral or half-integral.

It is customary to replace m_u by j; we then have, from (1.3-25),

$$\lambda = j(j+1).$$

Equations (1.3-8) and (1.3-9) may now be written as

$$\begin{aligned} J^2|jm\rangle &= j(j+1)|jm\rangle, \\ J_z|jm\rangle &= J_0|jm\rangle = m|jm\rangle, \\ \langle j'm'|jm\rangle &= \delta_{j'j}\delta_{m'm}. \end{aligned} \tag{1.3-29}$$

Since $m_u\,(=j)$ must be integral or half-integral, the possible values of j are

$$j = 0, \quad \tfrac{1}{2}, \quad 1, \quad \tfrac{3}{2}, \ldots. \tag{1.3-30}$$

Only positive or zero values of j appear because of (1.3-14). Also, since the possible values of m lie between m_l and m_u, we have, in view of (1.3-28),

$$m = j, \quad j-1, \ldots, -j. \tag{1.3-31}$$

As before, m is called the *projection* or *magnetic* quantum number.

The result embodied in (1.3-30) contains the basic distinction between generalized angular momentum and orbital angular momentum. If, in (1.3-30), we were to allow j to assume only integral values, it would merely be necessary to replace $\mathbf{J}$ by $\mathbf{L}$ and j by l to reproduce all the results pertaining to orbital angular momentum operators. However, (1.3-30) also permits j to have half-integral values. This is a new result and suggests the possible existence of angular momentum operators whose properties differ in certain respects from those associated with orbital angular momentum. Indeed, this turns out to be the case and leads to far-reaching physical consequences.

Matrix elements of the various angular momentum operators may now be calculated. From (1.3-29),

$$\langle j'm'|J^2|jm\rangle = j(j+1)\,\delta_{j'j}\,\delta_{m'm}, \tag{1.3-32}$$

$$\langle j'm'|J_0|jm\rangle = m\,\delta_{j'j}\,\delta_{m'm}. \tag{1.3-33}$$

To obtain matrix elements of J_{+1}, we refer to (1.3-24); in the present notation

$$J_{-1}J_{+1}|jm\rangle = \tfrac{1}{2}(J_0{}^2 + J_0 - J^2)|jm\rangle = \tfrac{1}{2}[m(m+1) - j(j+1)]|jm\rangle, \tag{1.3-34}$$

so that

$$\langle jm|J_{-1}J_{+1}|jm\rangle = \tfrac{1}{2}[m(m+1) - j(j+1)]. \tag{1.3-35}$$

From the definition of matrix multiplication (or the closure property) we also have

$$\langle jm|J_{-1}J_{+1}|jm\rangle = \sum_{j'm'} \langle jm|J_{-1}|j'm'\rangle\langle j'm'|J_{+1}|jm\rangle. \tag{1.3-36}$$

The sum in (1.3-36) may be simplified by application of the following theorem: If $[A, B] = 0$, A Hermitian, $A\psi_1 = a_1\psi_1$, $A\psi_2 = a_2\psi_2$, and $a_1 \neq a_2$, then $\langle\psi_1|B|\psi_2\rangle = 0$. In the present case J_{-1} commutes with J^2 and both $|jm\rangle$ and $|j'm'\rangle$ are eigenfunctions of J^2 with eigenvalues $j(j+1)$ and $j'(j'+1)$. Therefore $\langle jm|J_{-1}|j'm'\rangle = 0$ when $j \neq j'$. The same argument applies to J_{+1}; hence

$$\sum_{j'm'} \langle jm|J_{-1}|j'm'\rangle\langle j'm'|J_{+1}|jm\rangle = \sum_{m'} \langle jm|J_{-1}|jm'\rangle\langle jm'|J_{+1}|jm\rangle. \tag{1.3-37}$$

The sum over m' cannot be simplified in the same way because J_{-1} and J_{+1} do not commute with J_0. Nevertheless the sum over m' reduces to one term because J_{-1} acting on $|jm'\rangle$ displaces m' downward by one unit as in (1.3-20), while J_{+1} acting on $|jm'\rangle$ displaces m' upward by one unit as in (1.3-19). The orthogonality condition in (1.3-29) then eliminates all terms from the sum

except $\langle jm|J_{-1}|j\,m+1\rangle\langle j\,m+1|J_{+1}|jm\rangle$. By the "turn-over" rule and (1.3-4)

$$\langle jm|J_{-1}|j\,m+1\rangle\langle j\,m+1|J_{+1}|jm\rangle$$
$$= -\langle J_{+1}jm|j\,m+1\rangle\langle j\,m+1|J_{+1}jm\rangle = -|\langle j\,m+1|J_{+1}|jm\rangle|^2. \tag{1.3-38}$$

Combining (1.3-35), (1.3-36), and (1.3-38), we have

$$\langle j\,m+1|J_{+1}|jm\rangle = -\sqrt{\tfrac{1}{2}[j(j+1) - m(m+1)]} \tag{1.3-39}$$

in which the arbitrary phase factor has been chosen in conformity with the Condon–Shortley convention. All other matrix elements are zero. By a similar development it is found that the nonvanishing matrix elements of J_{-1} are

$$\langle j\,m-1|J_{-1}|jm\rangle = \sqrt{\tfrac{1}{2}[j(j+1) - m(m-1)]}. \tag{1.3-40}$$

Matrix elements of J_x and J_y follow immediately from (1.3-3) in combination with (1.3-39) and (1.3-40). Some numerical values are listed in Table 1.3.

TABLE 1.3

Matrix Elements of $\langle j\,m\pm 1|J_{\pm 1}|jm\rangle = \mp\sqrt{\tfrac{1}{2}[j(j+1) - m(m\pm 1)]}$

j	m	$\langle j\,m+1\|J_{+1}\|jm\rangle$	$\langle j\,m-1\|J_{-1}\|jm\rangle$	j	m	$\langle j\,m+1\|J_{+1}\|jm\rangle$	$\langle j\,m-1\|J_{-1}\|jm\rangle$
$\frac{1}{2}$	$\frac{1}{2}$	0	$\sqrt{\frac{1}{2}}$	2	1	$-\sqrt{2}$	$\sqrt{3}$
$\frac{1}{2}$	$-\frac{1}{2}$	$-\sqrt{\frac{1}{2}}$	0	2	0	$-\sqrt{3}$	$\sqrt{3}$
1	1	0	1	2	-1	$-\sqrt{3}$	$\sqrt{2}$
1	0	-1	1	2	-2	$-\sqrt{2}$	0
1	-1	-1	0	$\frac{5}{2}$	$\frac{5}{2}$	0	$\sqrt{\frac{5}{2}}$
$\frac{3}{2}$	$\frac{3}{2}$	0	$\sqrt{\frac{3}{2}}$	$\frac{5}{2}$	$\frac{3}{2}$	$-\sqrt{\frac{5}{2}}$	2
$\frac{3}{2}$	$\frac{1}{2}$	$-\sqrt{\frac{3}{2}}$	$\sqrt{2}$	$\frac{5}{2}$	$\frac{1}{2}$	-2	$\frac{3}{\sqrt{2}}$
$\frac{3}{2}$	$-\frac{1}{2}$	$-\sqrt{2}$	$\sqrt{\frac{3}{2}}$	$\frac{5}{2}$	$-\frac{1}{2}$	$-\frac{3}{\sqrt{2}}$	2
$\frac{3}{2}$	$-\frac{3}{2}$	$-\sqrt{\frac{3}{2}}$	0	$\frac{5}{2}$	$-\frac{3}{2}$	-2	$\sqrt{\frac{5}{2}}$
2	2	0	$\sqrt{2}$	$\frac{5}{2}$	$-\frac{5}{2}$	$-\sqrt{\frac{5}{2}}$	0

In the interest of avoiding excessively cumbersome language and where misunderstanding is unlikely, it is not uncommon to refer to **J** or its components simply as "angular momenta" rather than "angular momentum operators." Similarly, one may speak of a state as having an angular momentum **J** as a substitute for saying that the wave function of the state is an eigenfunction of J^2 and J_z with eigenvalues $j(j+1)$ and m, respectively. At times the state may simply be labeled by j and m.

1.4 Spin

The eigenfunctions of J^2 and J_0 in (1.3-29) have been symbolized by $|jm\rangle$ with j amd m given by (1.3-30) and (1.3-31). If j is integral, it is known from the properties of orbital angular momentum that the spherical harmonics are eigenfunctions of J^2 $(=L^2)$ and J_0 $(=L_0)$, that is,

$$|jm\rangle = |lm\rangle = Y_{lm}(\theta,\varphi). \tag{1.4-1}$$

When j is half-integral, the eigenfunctions $|jm\rangle$ are not functions of the coordinates—they must be specified in other ways. A case in point is $j=\frac{1}{2}$ which is associated with the spin angular momentum properties of an electron (as well as of other particles, e.g., proton, neutron, etc.)

In discussing the spin properties of a particle it is customary to adopt a notation in which $J = S$ and $j = s$. For a fixed value of s,

$$\begin{aligned} S^2|sm\rangle &= s(s+1)|sm\rangle, \\ S_0|sm\rangle &= m|sm\rangle, \\ \langle sm'|sm\rangle &= \delta_{m'm}, \end{aligned} \tag{1.4-2}$$

from (1.3-29). Also, in conformity with the definition of angular momentum operators

$$\mathbf{S}\times\mathbf{S} = i\mathbf{S}. \tag{1.4-3}$$

We now give the matrices for the various operators when $s=\frac{1}{2}$. Columns will be labeled by the value of m starting with the highest value and progressing to the lowest value; rows will be labeled by m', also in the same sequence. Thus from (1.3-32), the matrix elements of S^2 are

$\langle sm'|S^2|sm\rangle =$ (1.4-4)

m' \ m	$\frac{1}{2}$	$-\frac{1}{2}$
$\frac{1}{2}$	$\frac{3}{4}$	0
$-\frac{1}{2}$	0	$\frac{3}{4}$

or, more compactly,

$$S^2 = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}; \tag{1.4-5}$$

that is, the matrix in (1.4-5) is the matrix representation of the operator S^2 in the basis set

$$|sm\rangle = |\tfrac{1}{2}\tfrac{1}{2}\rangle, |\tfrac{1}{2}-\tfrac{1}{2}\rangle.$$

Similarly, from (1.3-33), (1.3-39), and (1.3-40),

$$S_0 = S_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \tag{1.4-6}$$

$$S_{+1} = \begin{pmatrix} 0 & -\sqrt{\frac{1}{2}} \\ 0 & 0 \end{pmatrix}, \tag{1.4-7}$$

$$S_{-1} = \begin{pmatrix} 0 & 0 \\ \sqrt{\frac{1}{2}} & 0 \end{pmatrix}. \tag{1.4-8}$$

Also, on combining (1.4-7) and (1.4-8) as in (1.3-3),

$$S_x = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}, \tag{1.4-9}$$

$$S_y = i\begin{pmatrix} 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}. \tag{1.4-10}$$

The eigenfunctions $|sm\rangle$ may also be written as

$$|sm\rangle = \begin{cases} |\frac{1}{2}\frac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \alpha, \\ |\frac{1}{2}-\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \beta, \end{cases} \tag{1.4-11}$$

in which $\binom{1}{0}$ and $\binom{0}{1}$ are to be understood as column matrices. These expressions have been designed explicitly to satisfy (1.4-2); thus

$$S^2|\tfrac{1}{2}\tfrac{1}{2}\rangle = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{3}{4}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{2}(\tfrac{1}{2}+1)|\tfrac{1}{2}\tfrac{1}{2}\rangle$$

or

$$S^2\alpha = \tfrac{1}{2}(\tfrac{1}{2}+1)\alpha.$$

Similarly

$$S_0|\tfrac{1}{2}\tfrac{1}{2}\rangle = \begin{pmatrix} \tfrac{1}{2} & 0 \\ 0 & -\tfrac{1}{2} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle$$

or

$$S_0\alpha = \tfrac{1}{2}\alpha.$$

The orthogonality relations in (1.4-2) are also satisfied as, for example, by

$$\begin{aligned} \langle\tfrac{1}{2}\tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle &= \langle\alpha|\alpha\rangle = (1 \quad 0)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1, \\ \langle\tfrac{1}{2}\tfrac{1}{2}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle &= \langle\alpha|\beta\rangle = (1 \quad 0)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0. \end{aligned} \tag{1.4-12}$$

In still another notation, the eigenfunction $|sm\rangle$ is written in the form $\xi(m)$ or ξ_m to suggest that ξ is a function of a "spin coordinate" or "spin variable" m, the latter being the projection quantum number. With $m = \pm\frac{1}{2}$

$$\begin{aligned} \xi(\tfrac{1}{2}) &= \xi_{1/2} = |\tfrac{1}{2}\tfrac{1}{2}\rangle = \alpha, \\ \xi(-\tfrac{1}{2}) &= \xi_{-1/2} = |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle = \beta. \end{aligned} \tag{1.4-13}$$

Evidently, $|sm\rangle$ is not a function of coordinates; mathematically, it is known as a *spinor*.

The *Pauli spin matrices* are defined by

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{1.4-14}$$

Apart from a numerical factor these matrices are the same as those in (1.4-6), (1.4-9), and (1.4-10); in fact

$$\boldsymbol{\sigma} = 2\mathbf{S}. \tag{1.4-15}$$

The difference between $\boldsymbol{\sigma}$ and $\mathbf{S}$ appears to be trivial; nevertheless, it is important to recognize that because $\boldsymbol{\sigma}$ satisfies

$$\boldsymbol{\sigma} \times \boldsymbol{\sigma} = 2i\boldsymbol{\sigma}, \tag{1.4-16}$$

which is *not* of the same form as $\mathbf{S} \times \mathbf{S} = i\mathbf{S}$, the operator $\boldsymbol{\sigma}$ does *not* qualify as an angular momentum operator in contrast to S, which *is* an angular momentum operator.

1.5 Coupling of Two Angular Momenta

In this section we shall explain the sense in which two angular momentum operators, $\mathbf{J}_1$ and $\mathbf{J}_2$, are coupled to form a new angular momentum operator $\mathbf{J}$, and how the respective eigenfunctions and eigenvalues are related.

It will be assumed that $\mathbf{J}_1$ and $\mathbf{J}_2$ operate in different spaces, by which it is meant that any component of $\mathbf{J}_1$ commutes with any component of $\mathbf{J}_2$, or that

$$[J_{1i}, J_{2j}] = 0, \qquad \text{all} \quad i, j. \tag{1.5-1}$$

Thus $\mathbf{J}_1$ may be a spin angular momentum operator while $\mathbf{J}_2$ is associated with orbital angular momentum, or $\mathbf{J}_1$ and $\mathbf{J}_2$ may be angular momentum operators belonging to two different particles.

According to the general definition of angular momentum operators (1.3-1), $\mathbf{J}_1$ and $\mathbf{J}_2$ satisfy

$$\mathbf{J}_1 \times \mathbf{J}_1 = i\mathbf{J}_1, \qquad \mathbf{J}_2 \times \mathbf{J}_2 = i\mathbf{J}_2, \tag{1.5-2}$$

and there exist sets of orthornormal eigenfunctions such that

$$J_1^2|j_1m_1\rangle = j_1(j_1+1)|j_1m_1\rangle, \qquad J_{1z}|j_1m_1\rangle = m_1|j_1m_1\rangle, \tag{1.5-3}$$

$$J_2^2|j_2m_2\rangle = j_2(j_2+1)|j_2m_2\rangle, \qquad J_{2z}|j_2m_2\rangle = m_2|j_2m_2\rangle, \tag{1.5-4}$$

with

$$\begin{aligned} &j_1, j_2 = 0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2}, \ldots, \\ m_1 = j_1,\ j_1 - 1, \ldots, -j_1, &\qquad m_2 = j_2,\ j_2 - 1, \ldots, -j_2. \end{aligned} \tag{1.5-5}$$

We now define a new operator $\mathbf{J}$ by

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \tag{1.5-6}$$

with the understanding that each component of $\mathbf{J}$ is the sum of the corresponding components of $\mathbf{J}_1$ and $\mathbf{J}_2$, i.e.,

$$J_x = J_{1x} + J_{2x}, \qquad J_{+1} = J_{1\,+1} + J_{2\,+1},$$

with similar relations for other components. Is $\mathbf{J}$ an angular momentum operator? The commutation properties provide the answer; thus

$$\begin{aligned} [J_x, J_y] &= [J_{1x} + J_{2x}, J_{1y} + J_{2y}] \\ &= [J_{1x}, J_{1y}] + [J_{1x}, J_{2y}] + [J_{2x}, J_{1y}] + [J_{2x}, J_{2y}]. \end{aligned} \tag{1.5-7}$$

The second and third commutators vanish because of (1.5-1); Eq. (1.5-7) then becomes

$$[J_x, J_y] = [J_{1x}, J_{1y}] + [J_{2x}, J_{2y}] = i(J_{1z} + J_{2z}) = iJ_z. \tag{1.5-8}$$

Other commutators of the components of J are evaluated in similar fashion; it may therefore be concluded that

$$\mathbf{J} \times \mathbf{J} = i\mathbf{J}, \tag{1.5-9}$$

which is sufficient to identify **J** as an angular momentum operator. We regard (1.5-6) as the defining relation for the coupling of two angular momentum operators, $\mathbf{J}_1$ and $\mathbf{J}_2$, to form a new angular momentum operator **J**. Parenthetically, it may be remarked that arbitrary linear combinations of $\mathbf{J}_1$ and $\mathbf{J}_2$ do not necessarily produce angular momentum operators.

In view of (1.5-9) there exist orthonormal eigenfunctions $|j_1 j_2 jm\rangle$, also abbreviated to $|jm\rangle$, which satisfy

$$J^2|jm\rangle \equiv J^2|j_1 j_2 jm\rangle = j(j+1)|jm\rangle \equiv j(j+1)|j_1 j_2 jm\rangle, \quad J_z|jm\rangle \equiv J_z|j_1 j_2 jm\rangle = m|jm\rangle \equiv m|j_1 j_2 jm\rangle, \tag{1.5-10a}$$

$$j = 0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\dots; \qquad m = j,\ j-1,\dots,-j. \tag{1.5-10b}$$

The mathematical problem is to establish the relationships between the eigenfunctions and eigenvalues of $J_1{}^2, J_{1z}, J_2{}^2, J_{2z}$ on one hand and the eigenfunctions and eigenvalues of J^2, J_z on the other. For this purpose we construct products of $|j_1 m_1\rangle$ and $|j_2 m_2\rangle$ which are written as

$$|j_1 j_2 m_1 m_2\rangle \equiv |j_1 m_1\rangle |j_2 m_2\rangle. \tag{1.5-11}$$

Clearly, such products as well as their linear combinations are still eigenfunctions of $J_1{}^2, J_{1z}, J_2{}^2, J_{2z}$ with the same eigenvalues as in (1.5-3) and (1.5-4) since $\mathbf{J}_1$ and $\mathbf{J}_2$ operate exclusively in their individual spaces. Thus

$$\begin{aligned} J_1{}^2|j_1 j_2 m_1 m_2\rangle &= j_1(j_1+1)|j_1 j_2 m_1 m_2\rangle, \\ J_{1z}|j_1 j_2 m_1 m_2\rangle &= m_1|j_1 j_2 m_1 m_2\rangle, \\ J_2{}^2|j_1 j_2 m_1 m_2\rangle &= j_2(j_2+1)|j_1 j_2 m_1 m_2\rangle, \\ J_{2z}|j_1 j_2 m_1 m_2\rangle &= m_2|j_1 j_2 m_1 m_2\rangle, \end{aligned} \tag{1.5-12}$$

from which it follows that

$$\begin{aligned} J_z|j_1 j_2 m_1 m_2\rangle &= (J_{1z} + J_{2z})|j_1 j_2 m_1 m_2\rangle \\ &= (m_1 + m_2)|j_1 j_2 m_1 m_2\rangle \\ &= m|j_1 j_2 m_1 m_2\rangle \end{aligned} \tag{1.5-13}$$

where

$$m = m_1 + m_2. \tag{1.5-14}$$

Equation (1.5-13) shows that $|j_1 j_2 m_1 m_2\rangle$ is an eigenfunction of J_z. Since J_z commutes with

$$J^2 = (J_{1x} + J_{2x})^2 + (J_{1y} + J_{2y})^2 + (J_{1z} + J_{2z})^2, \tag{1.5-15}$$

we should like an eigenfunction of J_z to be simultaneously an eigenfunction of J^2. Unfortunately, $|j_1 j_2 m_1 m_2\rangle$ is not an eigenfunction of J^2; however, it

is possible to construct linear combinations of the form

$$|j_1 j_2 jm\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle \tag{1.5-16}$$

such that $|j_1 j_2 jm\rangle$ is simultaneously an eigenfunction of J_z and J^2. The quantities $\langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle$ are numerical coefficients which are known as Clebsch–Gordan (CG) coefficients or vector addition coefficients. In a commonly employed terminology one refers to $|j_1 j_2 jm\rangle$ as an eigenfunction in the coupled representation and to $|j_1 j_2 m_1 m_2\rangle$ as an eigenfunction in the uncoupled representation.

The quantum numbers in the coupled representation must be related in some fashion to those in the uncoupled representation. To establish these relations we write

$$\begin{aligned} J_z|j_1 j_2 jm\rangle &= (J_{1z} + J_{2z}) \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle \\ &= \sum_{m_1 m_2} (m_1 + m_2)|j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle. \end{aligned} \tag{1.5-17}$$

If it is stipulated that

$$J_z|j_1 j_2 jm\rangle = m|j_1 j_2 jm\rangle = m \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle, \tag{1.5-18}$$

then

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle = 0 \qquad \text{when} \quad m \neq m_1 + m_2, \tag{1.5-19}$$

and the expression for $|j_1 j_2 jm\rangle$ in (1.5-16) may be rewritten as

$$|j_1 j_2 jm\rangle = \sum_{m_1} |j_1 j_2 m_1\, m-m_1\rangle \langle j_1 j_2 m_1\, m-m_1 | j_1 j_2 jm\rangle, \tag{1.5-20a}$$

or

$$|j_1 j_2 jm\rangle = \sum_{m_2} |j_1 j_2\, m-m_2\, m_2\rangle \langle j_1 j_2\, m-m_2\, m_2 | j_1 j_2 jm\rangle. \tag{1.5-20b}$$

To find the possible values of j it is observed, from (1.5-5), that

$$-j_1 \leqslant m_1 \leqslant j_1, \qquad -j_2 \leqslant m_2 \leqslant j_2 \tag{1.5-21}$$

or, since $m_1 + m_2 = m$,

$$-j_1 \leqslant m - m_2 \leqslant j_1, \qquad -j_2 \leqslant m - m_1 \leqslant j_2. \tag{1.5-22}$$

Now let m assume its maximum value, namely j, and let m_1 and m_2 assume their respective maximum values, j_1 and j_2. For this case, (1.5-22) becomes

$$-j_1 \leqslant j - j_2 \leqslant j_1, \qquad -j_2 \leqslant j - j_1 \leqslant j_2 \tag{1.5-23}$$

or

$$j_2 - j_1 \leqslant j \leqslant j_1 + j_2, \qquad j_1 - j_2 \leqslant j \leqslant j_1 + j_2, \tag{1.5-24}$$

which may be combined into the single expression

$$|j_1 - j_2| \leqslant j \leqslant j_1 + j_2. \tag{1.5-25}$$

Now consider an example: Suppose $j_1 = \frac{1}{2}$ and $j_2 = 1$. From (1.5-10b), the values of j are restricted to integral and half-integral positive values; therefore (1.5-25) will be satisfied by $j = \frac{1}{2}, 1, \frac{3}{2}$. When $j = 1$, the values of m are $1, 0, -1$; but it is also necessary to satisfy $m = m_1 + m_2$ when $m_1 = \pm\frac{1}{2}$ and $m_2 = 1, 0, -1$. This is obviously impossible and the value $j = 1$ must be eliminated. To avoid such inconsistencies it is necessary to supplement (1.5-25) with the condition

$$j_1 + j_2 + j = n \tag{1.5-26}$$

where n is an integer. Since (1.5-25) is equivalent to

$$\left.\begin{matrix} j_1 + j_2 - j \\ j_1 - j_2 + j \\ -j_1 + j_2 + j \end{matrix}\right\} \geqslant 0, \tag{1.5-27}$$

the two conditions (1.5-26) and (1.5-27) taken together are the triangle conditions $\triangle(j_1 j_2 j)$ which we have already encountered in Section 1.2. An equivalent statement for the allowed values of j is

$$j = j_1 + j_2, \quad j_1 + j_2 - 1, \ldots, |j_1 - j_2|. \tag{1.5-28a}$$

The possible values of m must satisfy (1.5-10b) as well as (1.5-14); hence

$$m = m_1 + m_2 = j, \quad j - 1, \ldots, -j. \tag{1.5-28b}$$

We shall now illustrate the derivation of the CG coefficients in a simple case. Let a system with $j_1 = \frac{1}{2}$ be coupled to another system with $j_2 = \frac{1}{2}$. Then $m_1 = \pm\frac{1}{2}$, $m_2 = \pm\frac{1}{2}$. On the basis of (1.5-27) and (1.5-28),

$$j = \begin{cases} 0, & m = 0, \\ 1, & m = 1, 0, -1. \end{cases} \tag{1.5-29}$$

Starting with the maximum value of j $(=1)$ and the maximum value of m $(=1)$,

$$|jm\rangle = |1\ 1\rangle = \overset{j_1 j_2 m_1 m_2}{|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle}. \tag{1.5-30}$$

The right side of (1.5-30) is the only product of $|j_1 m_1\rangle$ and $|j_2 m_2\rangle$ which satisfies $m = m_1 + m_2$ when $m = 1$. Operating on $|1\ 1\rangle$ with J_{-1} we obtain (Table 1.3)

$$J_{-1}|1\ 1\rangle = |1\ 0\rangle. \tag{1.5-31}$$

But

$$\begin{aligned} J_{-1}|1\ 1\rangle &= J_{-1}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle = (J_{1\,-1} + J_{2\,-1})|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle \\ &= \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle; \end{aligned} \tag{1.5-32}$$

therefore

$$|1\ 0\rangle = \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle. \tag{1.5-33}$$

The process is repeated by operating on $|1\ 0\rangle$ with J_{-1}; the result is

$$|1\ {-1}\rangle = |\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\ {-\tfrac{1}{2}}\rangle. \tag{1.5-34}$$

This takes care of the case $j = 1$. For $j = 0$, $m = 0$ there is only one eigenstate $|00\rangle$ which must be orthogonal to $|1\ 1\rangle$, $|1\ 0\rangle$, and $|1\ {-1}\rangle$; this is satisfied by

$$|00\rangle = \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle - \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\ {-\tfrac{1}{2}}\tfrac{1}{2}\rangle. \tag{1.5-35}$$

The CG coefficients may now be organized in tabular form as in the first part of Table 1.4.

All the functions $|jm\rangle$ given by (1.5-30), (1.5-33)–(1.5-35) are eigenfunctions of J_z and J^2. To illustrate, take $|1\ 1\rangle = |\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle$ as in (1.5-30). Quite clearly $|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle$ is an eigenfunction of J_z with an eigenvalue equal to one. To verify that $|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle$ is also an eigenfunction of J^2, write

$$J^2 = (\mathbf{J}_1 + \mathbf{J}_2)\cdot(\mathbf{J}_1 + \mathbf{J}_2) = J_1{}^2 + J_2{}^2 + 2\mathbf{J}_1\cdot\mathbf{J}_2. \tag{1.5-36a}$$

The scalar product $\mathbf{J}_1\cdot\mathbf{J}_2$ can be expressed in terms of the spherical components (1.3-2) (or on the basis of the general form (6.1-18)):

$$\begin{aligned} \mathbf{J}_1\cdot\mathbf{J}_2 &= J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z} \\ &= -J_{1\,+1}J_{2\,-1} + J_{10}J_{20} - J_{1\,-1}J_{2\,+1}. \end{aligned} \tag{1.5-36b}$$

The evaluation of $J^2|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle$ then gives $2|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle = 1(1+1)|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle$ as required by (1.5-10).

This procedure, in which the CG coefficients are generated by the ladder operators (J_{-1} and J_{+1}), becomes quite tedious in more complicated situations. A general formula for these coefficients is (Wigner, 1959):

$$\begin{aligned} \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle &= \delta(m, m_1 + m_2)\sqrt{\frac{(j_1+j_2-j)!(j+j_1-j_2)!(j+j_2-j_1)!(2j+1)}{(j+j_1+j_2+1)!}} \\ &\times \sum_k \frac{(-1)^k\sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!}}{k!(j_1+j_2-j-k)!(j_1-m_1-k)!(j_2+m_2-k)!(j-j_2+m_1+k)!(j-j_1-m_2+k)!} \end{aligned} \tag{1.5-37}$$

TABLE 1.4

Clebsch–Gordan Coefficients $\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$.
$\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle = (-1)^{j_1+j_2-j} \langle j_2 j_1 m_2 m_1 | j_2 j_1 j m \rangle$.

$j_1 = \frac{1}{2}$	$j_2 = \frac{1}{2}$	$j = 1$			$j = 0$
m_1	m_2	$m = 1$	$m = 0$	$m = -1$	$m = 0$
1/2	1/2	1			
1/2	−1/2		$\sqrt{1/2}$		$\sqrt{1/2}$
−1/2	1/2		$\sqrt{1/2}$		$-\sqrt{1/2}$
−1/2	−1/2			1	

$j_1 = 1$	$j_2 = \frac{1}{2}$	$j = \frac{3}{2}$				$j = \frac{1}{2}$	
m_1	m_2	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$
1	1/2	1					
1	−1/2		$\sqrt{1/3}$			$\sqrt{2/3}$	
0	1/2		$\sqrt{2/3}$			$-\sqrt{1/3}$	
0	−1/2			$\sqrt{2/3}$			$\sqrt{1/3}$
−1	1/2			$\sqrt{1/3}$			$-\sqrt{2/3}$
−1	−1/2				1		

$j_1 = \frac{3}{2}$	$j_2 = \frac{1}{2}$	$j = 2$					$j = 1$		
m_1	m_2	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = 1$	$m = 0$	$m = -1$
3/2	1/2	1							
3/2	−1/2		$\sqrt{1/4}$				$\sqrt{3/4}$		
1/2	1/2		$\sqrt{3/4}$				$-\sqrt{1/4}$		
1/2	−1/2			$\sqrt{1/2}$				$\sqrt{1/2}$	
−1/2	1/2			$\sqrt{1/2}$				$-\sqrt{1/2}$	
−1/2	−1/2				$\sqrt{3/4}$				$\sqrt{1/4}$
−3/2	1/2				$\sqrt{1/4}$				$-\sqrt{3/4}$
−3/2	−1/2					1			

TABLE 1.4 (*continued*)

$j_1 = 1$	$j_2 = 1$	$j = 2$					$j = 1$			$j = 0$
m_1	m_2	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = 1$	$m = 0$	$m = -1$	$m = 0$
1	1	1								
1	0		$\sqrt{1/2}$				$\sqrt{1/2}$			
1	−1			$\sqrt{1/6}$				$\sqrt{1/2}$		$\sqrt{1/3}$
0	1		$\sqrt{1/2}$				$-\sqrt{1/2}$			
0	0			$\sqrt{2/3}$				0		$-\sqrt{1/3}$
0	−1				$\sqrt{1/2}$				$\sqrt{1/2}$	
−1	1			$\sqrt{1/6}$				$-\sqrt{1/2}$		$\sqrt{1/3}$
−1	0				$\sqrt{1/2}$				$-\sqrt{1/2}$	
−1	−1					1				

$j_1 = 2$	$j_2 = \frac{1}{2}$	$j = \frac{5}{2}$						$j = \frac{3}{2}$			
m_1	m_2	$m = \frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = -\frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$
2	1/2	1									
2	−1/2		$\sqrt{1/5}$					$\sqrt{4/5}$			
1	1/2		$\sqrt{4/5}$					$-\sqrt{1/5}$			
1	−1/2			$\sqrt{2/5}$					$\sqrt{3/5}$		
0	1/2			$\sqrt{3/5}$					$-\sqrt{2/5}$		
0	−1/2				$\sqrt{3/5}$					$\sqrt{2/5}$	
−1	1/2				$\sqrt{2/5}$					$-\sqrt{3/5}$	
−1	−1/2					$\sqrt{4/5}$					$\sqrt{1/5}$
−2	1/2					$\sqrt{1/5}$					$-\sqrt{4/5}$
−2	−1/2						1				

TABLE 1.4 (continued)

$j_1 = \frac{3}{2}$	$j_2 = 1$	$j = \frac{5}{2}$						$j = \frac{3}{2}$				$j = \frac{1}{2}$	
m_1	m_2	$m = \frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = -\frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$
3/2	1	1											
3/2	0		$\sqrt{2/5}$					$\sqrt{3/5}$					
3/2	−1			$\sqrt{1/10}$					$\sqrt{2/5}$			$\sqrt{1/2}$	
1/2	1		$\sqrt{3/5}$					$-\sqrt{2/5}$					
1/2	0			$\sqrt{3/5}$					$\sqrt{1/15}$			$-\sqrt{1/3}$	
1/2	−1				$\sqrt{3/10}$					$\sqrt{8/15}$			$\sqrt{1/6}$
−1/2	1			$\sqrt{3/10}$					$-\sqrt{8/15}$			$\sqrt{1/6}$	
−1/2	0				$\sqrt{3/5}$					$-\sqrt{1/15}$			$-\sqrt{1/3}$
−1/2	−1					$\sqrt{3/5}$					$\sqrt{2/5}$		
−3/2	1				$\sqrt{1/10}$					$-\sqrt{2/5}$			$\sqrt{1/2}$
−3/2	0					$\sqrt{2/5}$					$-\sqrt{3/5}$		
−3/2	−1						1						

$j_1 = 2$	$j_2 = 1$	$j = 3$							$j = 2$					$j = 1$		
m_1	m_2	$m = 3$	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = -3$	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = 1$	$m = 0$	$m = -1$
2	1	1														
2	0		$\sqrt{1/3}$						$\sqrt{2/3}$							
2	−1			$\sqrt{1/15}$						$\sqrt{1/3}$				$\sqrt{3/5}$		
1	1		$\sqrt{2/3}$						$-\sqrt{1/3}$							
1	0			$\sqrt{8/15}$						$\sqrt{1/6}$				$-\sqrt{3/10}$		
1	−1				$\sqrt{1/5}$						$\sqrt{1/2}$				$\sqrt{3/10}$	
0	1			$\sqrt{6/15}$						$-\sqrt{1/2}$				$\sqrt{1/10}$		
0	0				$\sqrt{3/5}$						0				$-\sqrt{2/5}$	
0	−1					$\sqrt{6/15}$						$\sqrt{1/2}$				$\sqrt{1/10}$
−1	1				$\sqrt{1/5}$						$-\sqrt{1/2}$				$\sqrt{3/10}$	
−1	0					$\sqrt{8/15}$						$-\sqrt{1/6}$				$-\sqrt{3/10}$
−1	−1						$\sqrt{2/3}$						$\sqrt{1/3}$			
−2	1					$\sqrt{1/15}$						$-\sqrt{1/3}$				$\sqrt{3/5}$
−2	0						$\sqrt{1/3}$						$-\sqrt{2/3}$			
−2	−1							1								

with

$$j_1, j_2, j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots, \tag{1.5-38}$$

$$\triangle\,(j_1 j_2 j):\ \begin{cases} j_1 + j_2 + j = n \quad \text{(an integer)}, & (1.5\text{-}39) \\ \left.\begin{matrix} j_1 + j_2 - j \\ j_1 - j_2 + j \\ -j_1 + j_2 + j \end{matrix}\right\} \geqslant 0, & (1.5\text{-}40) \end{cases}$$

$$m_1 = j_1, j_1 - 1, \ldots, -j_1, \quad m_2 = j_2, j_2 - 1, \ldots, -j_2, \quad m = j, j - 1, \ldots, -j. \tag{1.5-41}$$

Numerical values of some of the coupling coefficients are given in Table 1.4 (Heine, 1960); we list a few of their properties:

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle = 0 \quad \text{unless} \quad m = m_1 + m_2, \tag{1.5-42}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle \text{ is real}, \tag{1.5-43}$$

$$\sum_{m_1 m_2} \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j'm'\rangle = \delta_{jj'}\,\delta_{mm'}, \tag{1.5-44a}$$

$$\sum_{jm} \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle \langle j_1 j_2 m_1' m_2' | j_1 j_2 jm\rangle = \delta_{m_1 m_1'}\,\delta_{m_2 m_2'}, \tag{1.5-44b}$$

$$\begin{aligned} &\sqrt{j(j+1) - m(m+1)}\,\langle j_1 j_2 m_1 m_2 | j_1 j_2 j\, m+1\rangle \\ &\quad = \sqrt{j_1(j_1+1) - m_1(m_1-1)}\,\langle j_1 j_2\, m_1 - 1\, m_2 | j_1 j_2 jm\rangle \\ &\quad\quad + \sqrt{j_2(j_2+1) - m_2(m_2-1)}\,\langle j_1 j_2 m_1\, m_2 - 1 | j_1 j_2 jm\rangle, \end{aligned} \tag{1.5-45a}$$

$$\begin{aligned} &\sqrt{j(j+1) - m(m-1)}\,\langle j_1 j_2 m_1 m_2 | j_1 j_2 j\, m-1\rangle \\ &\quad = \sqrt{j_1(j_1+1) - m_1(m_1+1)}\,\langle j_1 j_2\, m_1 + 1\, m_2 | j_1 j_2 jm\rangle \\ &\quad\quad + \sqrt{j_2(j_2+1) - m_2(m_2+1)}\,\langle j_1 j_2 m_1\, m_2 + 1 | j_1 j_2 jm\rangle, \end{aligned} \tag{1.5-45b}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle = (-1)^{j_1 + j_2 - j} \langle j_2 j_1 m_2 m_1 | j_2 j_1 jm\rangle. \tag{1.5-46}$$

The 3j symbols encountered in the Gaunt formula (1.2-29) are closely related to the CG coefficients; they are defined by

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m}}{\sqrt{2j+1}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j\, -m\rangle \tag{1.5-47}$$

in which the left side is a 3j symbol whose general form is written as

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.$$

Among its properties are (Rotenberg *et al.*, 1959)

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}$$

$$= \begin{pmatrix} j_2 & j_3 & j_1 \\ m_3 & m_1 & m_2 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_2 & m_3 & m_1 \end{pmatrix}, \qquad (1.5\text{-}48)$$

$$(-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix}$$

$$= \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}, \qquad (1.5\text{-}49)$$

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta(j_3, j_3')\,\delta(m_3, m_3')}{(2j_3+1)}, \qquad (1.5\text{-}50)$$

$$\sum_{j_3 m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta(m_1, m_1')\,\delta(m_2, m_2'), \qquad (1.5\text{-}51)$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \quad \text{unless} \begin{cases} m_1 + m_2 + m_3 = 0, \\ \triangle(j_1 j_2 j_3). \end{cases} \qquad (1.5\text{-}52)$$

Equation (1.5-16) for the eigenfunction in the coupled representation, written in terms of $3j$ symbols, is

$$|j_1 j_2 jm\rangle = (-1)^{j_2-j_1-m} \sum_{m_1 m_2} \sqrt{2j+1} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} |j_1 j_2 m_1 m_2\rangle. \qquad (1.5\text{-}53)$$

It is also possible to express $|j_1 j_2 m_1 m_2\rangle$ in terms of $|j_1 j_2 jm\rangle$:

$$|j_1 j_2 m_1 m_2\rangle = \sum_{jm} (-1)^{j_2-j_1-m} \sqrt{2j+1} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} |j_1 j_2 jm\rangle. \qquad (1.5\text{-}54)$$

A number of special formulas for $3j$ symbols (Edmonds, 1960) are listed in Table 1.5. Extensive numerical tables are given by Rotenberg *et al.* (1959); a short list of numerical values is given in Table 1.6.

To recapitulate, an eigenfunction $|jm\rangle$ (or $|j_1 j_2 jm\rangle$) in the coupled representation is related to the eigenfunctions $|j_1 j_2 m_1 m_2\rangle$ in the uncoupled representation by

$$|jm\rangle \equiv |j_1 j_2 jm\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle$$

$$= (-1)^{j_2-j_1-m} \sqrt{2j+1} \sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} |j_1 j_2 m_1 m_2\rangle \qquad (1.5\text{-}55)$$

TABLE 1.5

Special Formulas for 3j Symbols

$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = 0 \quad \text{if } j_1 + j_2 + j_3 \text{ is odd}$
$\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2} \\ m & -m-\frac{1}{2} & \frac{1}{2} \end{pmatrix} = (-1)^{j-m-\frac{1}{2}} \sqrt{\frac{j-m+\frac{1}{2}}{(2j+2)(2j+1)}}$
$\begin{pmatrix} j+1 & j & 1 \\ m & -m-1 & 1 \end{pmatrix} = (-1)^{j-m-1} \sqrt{\frac{(j-m)(j-m+1)}{(2j+3)(2j+2)(2j+1)}}$
$\begin{pmatrix} j+1 & j & 1 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m-1} \sqrt{\frac{(j+m+1)(j-m+1)}{(2j+3)(j+1)(2j+1)}}$
$\begin{pmatrix} j & j & 1 \\ m & -m-1 & 1 \end{pmatrix} = (-1)^{j-m} \sqrt{\frac{(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}$
$\begin{pmatrix} j & j & 1 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{m}{\sqrt{(2j+1)(j+1)j}}$
$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{1}{\sqrt{2j+1}}$
$\begin{pmatrix} j & j & 2 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{3m^2 - j(j+1)}{\sqrt{(2j+3)(j+1)(2j+1)2j(2j-1)}}$

with

$$m = m_1 + m_2, \qquad j = j_1 + j_2,\ j_1 + j_2 - 1, \ldots, |j_1 - j_2|.$$

The quantum number j is confined to integral or half-integral values and $m = j, j-1, \ldots, -j$; $|j_1 j_2 m_1 m_2\rangle$ is an eigenfunction of J_1^2, J_2^2, J_{1z}, J_{2z}, and $J_z\,(=J_{1z} + J_{2z})$ with eigenvalues $j_1(j_1+1)$, $j_2(j_2+1)$, m_1, m_2, and $m\,(=m_1+m_2)$, respectively. However, $|j_1 j_2 m_1 m_2\rangle$ is not an eigenfunction of J^2. Note that j_1, j_2, m_1, and m_2 serve to label the eigenfunction as well as to specify the eigenvalues; for this reason, j_1, j_2, m_1, and m_2 are often said to be "good" quantum numbers (in the uncoupled representation). Also, $|j_1 j_2 jm\rangle$ is an eigenfunction of J_1^2, J_2^2, J^2, and J_z with eigenvalues $j_1(j_1+1)$, $j_2(j_2+1)$, $j(j+1)$, and m, respectively, but $|j_1 j_2 jm\rangle$ is not an eigenfunction of J_{1z} and J_{2z}. The "good" quantum numbers in the coupled representation are therefore j_1, j_2, j, and m.

Henceforth, *coupling coefficients* will be understood to be either $3j$ symbols or Clebsch–Gordan (CG) coefficients.

TABLE 1.6

Numerical Values of 3j Symbols.[a,b]

j_1	j_2	j_3	m_1	m_2	m_3	
1	1	0	0	0	0	*0$\underline{1}$
2	1	1	0	0	0	1$\underline{11}$
2	2	0	0	0	0	00$\underline{1}$
2	2	2	0	0	0	*10$\underline{11}$,
3	2	1	0	0	0	*01$\underline{11}$,
3	3	0	0	0	0	*000$\underline{1}$,
3	3	2	0	0	0	2$\underline{111}$,
4	2	2	0	0	0	10$\underline{11}$,
4	3	1	0	0	0	2$\underline{2}$0$\underline{1}$,
4	3	3	0	0	0	*100$\underline{1}$,$\underline{1}$
4	4	0	0	0	0	0$\underline{2}$
4	4	2	0	0	0	*2$\underline{2}$1$\underline{1}$,$\underline{1}$
4	4	4	0	0	0	120$\underline{1}$,$\underline{11}$
1/2	1/2	0	1/2	-1/2	0	$\underline{1}$
1	1/2	1/2	0	-1/2	1/2	$\underline{11}$
1	1/2	1/2	1	-1/2	-1/2	*0$\underline{1}$
1	1	0	0	0	0	*0$\underline{1}$
1	1	0	1	-1	0	0$\underline{1}$
1	1	1	-1	0	1	$\underline{11}$
1	1	1	0	-1	1	*$\underline{11}$
1	1	1	0	0	0	0
1	1	1	1	-1	0	$\underline{11}$
1	1	1	1	0	-1	*$\underline{11}$
3/2	1	1/2	-1/2	0	1/2	*$\underline{11}$
3/2	1	1/2	1/2	-1	1/2	$\underline{2}$1
3/2	1	1/2	1/2	0	-1/2	$\underline{11}$
3/2	1	1/2	3/2	-1	-1/2	*$\underline{2}$
3/2	3/2	0	1/2	-1/2	0	*$\underline{2}$
3/2	3/2	0	3/2	-3/2	0	$\underline{2}$
3/2	3/2	1	-1/2	-1/2	1	1$\underline{11}$

j_1	j_2	j_3	m_1	m_2	m_3	
3/2	3/2	1	1/2	-3/2	1	*$\underline{1}$0$\underline{1}$
3/2	3/2	1	1/2	-1/2	0	*$\underline{211}$
3/2	3/2	1	3/2	-3/2	0	$\underline{2}$1$\underline{1}$
3/2	3/2	1	3/2	-1/2	-1	*$\underline{1}$0$\underline{1}$
2	1	1	-1	0	1	*$\underline{1}$0$\underline{1}$
2	1	1	0	-1	1	$\underline{111}$
2	1	1	0	0	0	1$\underline{11}$
2	1	1	1	-1	0	*$\underline{1}$0$\underline{1}$
2	1	1	1	0	-1	*$\underline{1}$0$\underline{1}$
2	1	1	2	-1	-1	00$\underline{1}$
2	3/2	1/2	0	-1/2	1/2	*$\underline{1}$0$\underline{1}$
2	3/2	1/2	1	-3/2	1/2	$\underline{2}$0$\underline{1}$
2	3/2	1/2	1	-1/2	-1/2	$\underline{2}$1$\underline{1}$
2	3/2	1/2	2	-3/2	-1/2	*00$\underline{1}$
2	3/2	3/2	-1	-1/2	3/2	$\underline{1}$0$\underline{1}$
2	3/2	3/2	0	-3/2	3/2	*$\underline{2}$0$\underline{1}$
2	3/2	3/2	0	-1/2	1/2	*$\underline{2}$0$\underline{1}$
2	3/2	3/2	1	-3/2	1/2	$\underline{1}$0$\underline{1}$
2	3/2	3/2	1	-1/2	-1/2	0
2	3/2	3/2	2	-3/2	-1/2	*$\underline{1}$0$\underline{1}$
2	3/2	3/2	2	-1/2	-3/2	$\underline{1}$0$\underline{1}$
2	2	0	0	0	0	00$\underline{1}$
2	2	0	1	-1	0	*00$\underline{1}$
2	2	0	2	-2	0	00$\underline{1}$
2	2	1	-1	0	1	*$\underline{1}$0$\underline{1}$
2	2	1	0	-1	1	$\underline{1}$0$\underline{1}$
2	2	1	0	0	0	0
2	2	1	1	-2	1	*0$\underline{11}$
2	2	1	1	-1	0	*$\underline{111}$
2	2	1	1	0	-1	$\underline{1}$0$\underline{1}$

[a] The table gives values of $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2$ in prime notation which lists only the exponents of the prime numbers in the order 2, 3, 5, 7, 11, ... Negative exponents are underscored. For example,

$$2102\underline{\ } = \frac{2^2 \times 3^1 \times 5^0}{7^2} = \frac{12}{49}.$$

[illegible] use the symmetry properties

TABLE 1.6 (continued)

j_1	j_2	j_3	m_1	m_2	m_3	
2	2	1	2	-2	0	1$\underline{11}$
2	2	1	2	-1	-1	*0$\underline{11}$
2	2	2	-2	0	2	10$\underline{11}$,
2	2	2	-1	-1	2	*01$\underline{11}$,
2	2	2	-1	0	1	$\underline{1}$0$\underline{11}$,
2	2	2	0	-2	2	10$\underline{11}$,
2	2	2	0	-1	1	$\underline{1}$0$\underline{11}$,
2	2	2	0	0	0	*10$\underline{11}$,
2	2	2	1	-2	1	*01$\underline{11}$,
2	2	2	1	-1	0	$\underline{1}$0$\underline{11}$,
2	2	2	1	0	-1	$\underline{1}$0$\underline{11}$,
2	2	2	2	-2	0	10$\underline{11}$
2	2	2	2	-1	-1	*01$\underline{11}$
2	2	2	2	0	-2	10$\underline{11}$
5/2	3/2	1	-1/2	-1/2	1	*$\underline{2}$0$\underline{1}$
5/2	3/2	1	1/2	-3/2	1	$\underline{211}$
5/2	3/2	1	1/2	-1/2	0	$\underline{1}$0$\underline{1}$
5/2	3/2	1	3/2	-3/2	0	*0$\underline{11}$
5/2	3/2	1	3/2	-1/2	-1	*$\underline{1}$0$\underline{1}$
5/2	3/2	1	5/2	-3/2	-1	$\underline{11}$
5/2	2	1/2	-1/2	0	1/2	$\underline{1}$0$\underline{1}$
5/2	2	1/2	1/2	-1	1/2	*0$\underline{11}$
5/2	2	1/2	1/2	0	-1/2	*$\underline{1}$0$\underline{1}$
5/2	2	1/2	3/2	-2	1/2	$\underline{111}$
5/2	2	1/2	3/2	-1	-1/2	1$\underline{11}$
5/2	2	1/2	5/2	-2	-1/2	*$\underline{11}$
5/2	2	3/2	-3/2	0	3/2	*01$\underline{11}$,
5/2	2	3/2	-1/2	-1	3/2	$\underline{2}$2$\underline{11}$,
5/2	2	3/2	-1/2	0	1/2	$\underline{1}$0$\underline{11}$,
5/2	2	3/2	1/2	-2	3/2	*00$\underline{11}$,

j_1	j_2	j_3	m_1	m_2	m_3	
5/2	2	3/2	1/2	-1	1/2	*$\underline{211}$,
5/2	2	3/2	1/2	0	-1/2	$\underline{1}$0$\underline{11}$,
5/2	2	3/2	3/2	-2	1/2	3$\underline{111}$,
5/2	2	3/2	3/2	-1	-1/2	$\underline{1111}$,
5/2	2	3/2	3/2	0	-3/2	*01$\underline{11}$,
5/2	2	3/2	5/2	-2	-1/2	*1$\underline{1}$0$\underline{1}$,
5/2	2	3/2	5/2	-1	-3/2	$\underline{1}$00$\underline{1}$,
5/2	5/2	0	1/2	-1/2	0	$\underline{11}$
5/2	5/2	0	3/2	-3/2	0	*$\underline{11}$
5/2	5/2	0	5/2	-5/2	0	$\underline{11}$
5/2	5/2	1	-1/2	-1/2	1	*01$\underline{11}$,
5/2	5/2	1	1/2	-3/2	1	3$\underline{111}$,
5/2	5/2	1	1/2	-1/2	0	$\underline{1111}$,
5/2	5/2	1	3/2	-5/2	1	*0$\underline{1}$0$\underline{1}$,
5/2	5/2	1	3/2	-3/2	0	*$\underline{1}$1$\underline{11}$,
5/2	5/2	1	3/2	-1/2	-1	3$\underline{111}$,
5/2	5/2	1	5/2	-5/2	0	$\underline{1111}$,
5/2	5/2	1	5/2	-3/2	-1	*0$\underline{1}$0$\underline{1}$,
5/2	5/2	2	-3/2	-1/2	2	$\underline{2}$2$\underline{11}$,
5/2	5/2	2	-1/2	-3/2	2	*$\underline{2}$2$\underline{11}$,
5/2	5/2	2	-1/2	-1/2	1	0
5/2	5/2	2	1/2	-5/2	2	$\underline{2}$00$\underline{1}$,
5/2	5/2	2	1/2	-3/2	1	00$\underline{11}$,
5/2	5/2	2	1/2	-1/2	0	*2$\underline{111}$,
5/2	5/2	2	3/2	-5/2	1	*$\underline{1}$00$\underline{1}$,
5/2	5/2	2	3/2	-3/2	0	$\underline{2111}$,
5/2	5/2	2	3/2	-1/2	-1	00$\underline{11}$,
5/2	5/2	2	5/2	-5/2	0	$\underline{2}$11$\underline{1}$,
5/2	5/2	2	5/2	-3/2	-1	*$\underline{1}$00$\underline{1}$,
5/2	5/2	2	5/2	-1/2	-2	$\underline{2}$00$\underline{1}$,

(1.5-48) and (1.5-49) to (a) interchange the columns so that $j_1 \geqslant j_2 \geqslant j_3$ and (b) change the signs (if necess of m_1, m_2, and m_3 so that $m_2 \leqslant 0$.

[b] Reprinted from "The 3-*j* and 6-*j* Symbols," by Rotenberg, Bivins, Metropolis, and Wooten by mission of the M.I.T. Press, Cambridge, Massachusetts. Copyright ©, 1959 by The Massachusetts Insti of Technology.

1.6 Coupling of Three Angular Momenta

The methods developed for the coupling of two angular momentum operators may, in principle, be extended to any number of operators—but not without additional complications. The coupling of three angular momenta

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 \tag{1.6-1}$$

serves as a useful illustration.

Clearly, (1.6-1) may be written as

$$\mathbf{J}_1 + \mathbf{J}_2 = \mathbf{J}_{12}, \qquad \mathbf{J}_{12} + \mathbf{J}_3 = \mathbf{J}. \tag{1.6-2}$$

Each step then involves two angular momenta and these may be handled by the methods of the last section. Thus suppose

$$j_1 = 1, \qquad j_2 = \tfrac{1}{2}, \qquad j_3 = \tfrac{1}{2}.$$

When $\mathbf{J}_1$ and $\mathbf{J}_2$ are coupled to form $\mathbf{J}_{12}$, the possible values of $\mathbf{J}_{12}$ are $\frac{1}{2}$ and $\frac{3}{2}$. We indicate these by writing

$$j_1 j_2(j_{12}) = \begin{cases} 1\tfrac{1}{2}(\tfrac{1}{2}), \\ 1\tfrac{1}{2}(\tfrac{3}{2}). \end{cases} \tag{1.6-3}$$

On further coupling of $\mathbf{J}_{12}$ with $\mathbf{J}_3$ to form $\mathbf{J}$, the possible values of j may be written in a notation which keeps track of the coupling sequence:

$$j_1 j_2(j_{12}) j_3; j = \begin{cases} 1\tfrac{1}{2}(\tfrac{1}{2})\tfrac{1}{2};\ 0, \\ 1\tfrac{1}{2}(\tfrac{1}{2})\tfrac{1}{2};\ 1, \\ 1\tfrac{1}{2}(\tfrac{3}{2})\tfrac{1}{2};\ 1, \\ 1\tfrac{1}{2}(\tfrac{3}{2})\tfrac{1}{2};\ 2. \end{cases} \tag{1.6-4}$$

We may also construct the eigenfunctions $|jm\rangle$ from $|j_1 m_1\rangle$, $|j_2 m_2\rangle$, and $|j_3 m_3\rangle$. As a first step $|j_{12} m_{12}\rangle$ is written as a linear combinations of products of $|j_1 m_1\rangle$ and $|j_2 m_2\rangle$:

$$\begin{aligned} |j_{12} m_{12}\rangle = |\tfrac{1}{2}\tfrac{1}{2}\rangle_{12} &= \sqrt{\tfrac{2}{3}}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{3}}|1\ 0\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \\ |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle_{12} &= \sqrt{\tfrac{1}{3}}|1\ 0\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \sqrt{\tfrac{2}{3}}|1\ -1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \\ |\tfrac{3}{2}\tfrac{3}{2}\rangle_{12} &= |1\ 1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \\ |\tfrac{3}{2}\tfrac{1}{2}\rangle_{12} &= \sqrt{\tfrac{1}{3}}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}|1\ 0\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \\ |\tfrac{3}{2}\ -\tfrac{1}{2}\rangle_{12} &= \sqrt{\tfrac{2}{3}}|1\ 0\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}|1\ -1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \\ |\tfrac{3}{2}\ -\tfrac{3}{2}\rangle_{12} &= |1\ -1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle. \end{aligned} \tag{1.6-5}$$

Now suppose we wish to calculate $|jm\rangle = |1\ 1\rangle$. Again it is possible to find the required linear combinations of $|j_{12} m_{12}\rangle$ and $|j_3 m_3\rangle$. Indeed, on the

basis of (1.6-4) we expect to find two such expressions; they are

$$\begin{aligned} |j_1 j_2(j_{12}) j_3; jm\rangle &= |1\tfrac{1}{2}(\tfrac{1}{2})\tfrac{1}{2};\ 1\ 1\rangle \\ &= |\tfrac{1}{2}\tfrac{1}{2}\rangle_{12}|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ &= \sqrt{\tfrac{2}{3}}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{3}}|1\ 0\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \end{aligned} \tag{1.6-6a}$$

$$\begin{aligned} |j_1 j_2(j_{12}) j_3; jm\rangle &= |1\tfrac{1}{2}(\tfrac{3}{2})\tfrac{1}{2};\ 1\ 1\rangle \\ &= \sqrt{\tfrac{3}{4}}|\tfrac{3}{2}\tfrac{3}{2}\rangle_{12}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{4}}|\tfrac{3}{2}\tfrac{1}{2}\rangle_{12}|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ &= \sqrt{\tfrac{3}{4}}|1\ 1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \tfrac{1}{2}\sqrt{\tfrac{3}{2}}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ &\quad - \sqrt{\tfrac{1}{6}}|1\ 0\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle. \end{aligned} \tag{1.6-6b}$$

The sequential scheme (1.6-2) has led us in a stepwise fashion to (1.6-6a) and (1.6-6b) which provide two expressions for $|jm\rangle = |1\ 1\rangle$ in terms of the products $|j_1 m_1\rangle|j_2 m_2\rangle|j_3 m_3\rangle$. However, the replacement of (1.6-1) by (1.6-2) is certainly not unique. Another possible coupling scheme is

$$\mathbf{J}_2 + \mathbf{J}_3 = \mathbf{J}_{23}, \qquad \mathbf{J}_1 + \mathbf{J}_{23} = \mathbf{J}. \tag{1.6-7}$$

In place of (1.6-3) and (1.6-4) we now have

$$j_2 j_3(j_{23}) = \begin{cases} \tfrac{1}{2}\tfrac{1}{2}(0), \\ \tfrac{1}{2}\tfrac{1}{2}(1), \end{cases}$$

and

$$j_1, j_2 j_3(j_{23}); j = \begin{cases} 1,\ \tfrac{1}{2}\tfrac{1}{2}(0);\ 1 \\ 1,\ \tfrac{1}{2}\tfrac{1}{2}(1);\ 0 \\ 1,\ \tfrac{1}{2}\tfrac{1}{2}(1);\ 1 \\ 1,\ \tfrac{1}{2}\tfrac{1}{2}(1);\ 2. \end{cases} \tag{1.6-8}$$

The possible values of j are the same as those in (1.6-4) even though the coupling has been carried out in a different sequence. The eigenfunctions $|j_{23} m_{23}\rangle$ are

$$\begin{aligned} |j_{23} m_{23}\rangle = |0\ 0\rangle_{23} &= \sqrt{\tfrac{1}{2}}|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{2}}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ |1\ 1\rangle_{23} &= |\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ |1\ 0\rangle_{23} &= \sqrt{\tfrac{1}{2}}|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{2}}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle \\ |1\ -1\rangle_{23} &= |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle, \end{aligned} \tag{1.6-9}$$

and $|jm\rangle = |1\ 1\rangle$ now assumes the two forms

$$\begin{aligned} |j_1, j_2 j_3(j_{23}); jm\rangle &= |1,\ \tfrac{1}{2}\tfrac{1}{2}(0);\ 1\ 1\rangle \\ &= |1\ 1\rangle|00\rangle_{23} \\ &= \sqrt{\tfrac{1}{2}}|1\ 1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{2}}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle, \end{aligned} \tag{1.6-10a}$$

$$
\begin{aligned}
|j_1, j_2 j_3(j_{23}); jm\rangle &= |1, \tfrac{1}{2}\tfrac{1}{2}(1); 1\ 1\rangle \\
&= \sqrt{\tfrac{1}{2}}|1\ 1\rangle|1\ 0\rangle_{23} - \sqrt{\tfrac{1}{2}}|1\ 0\rangle|1\ 1\rangle_{23} \\
&= \tfrac{1}{2}|1\ 1\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle + \tfrac{1}{2}|1\ 1\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle \\
&\quad -\sqrt{\tfrac{1}{2}}|1\ 0\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle. \qquad (1.6\text{-}10b)
\end{aligned}
$$

We now have four separate expressions for $|jm\rangle = |1\ 1\rangle$, namely (1.6-6a) and (1.6-6b) and (1.6-10a) and (1.6-10b).

This example illustrates the following properties:

1. When three angular momentum operators J_1, J_2, and J_3 are coupled to form $\mathbf{J}$, the possible values of j are the same regardless of the coupling scheme.
2. The eigenfunctions $|jm\rangle$ are not uniquely determined by specifying $|j_1 m_1\rangle$, $|j_2 m_2\rangle$, and $|j_3 m_3\rangle$ but depend on the details of the coupling scheme.

Thus, in general,

$$|j_1 j_2(j_{12}) j_3; j\rangle \neq |j_1, j_2 j_3(j_{23}); j\rangle.$$

However, the two eigenfunctions are related by a unitary transformation (Sobelman, 1972)

$$|j_1, j_2 j_3(j_{23}); j\rangle = \sum_{j_{12}} |j_1 j_2(j_{12}) j_3; j\rangle\langle j_1 j_2(j_{12}) j_3; j | j_1, j_2 j_3(j_{23}); j\rangle \qquad (1.6\text{-}11)$$

in which

$$
\begin{aligned}
&\langle j_1 j_2(j_{12}) j_3; j | j_1, j_2 j_3(j_{23}); j\rangle \\
&\quad = (-1)^{j_1+j_2+j_3+j}\sqrt{(2j_{12}+1)(2j_{23}+1)}\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}. \qquad (1.6\text{-}12)
\end{aligned}
$$

The quantity in the braces is a $6j$ symbol whose general form is

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$$

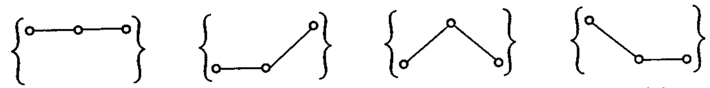
and whose definition is given by (Rotenberg *et al.*, 1959)

$$
\begin{aligned}
\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} &= (-1)^{j_1+j_2+l_1+l_2}\Delta(j_1 j_2 j_3)\Delta(l_1 l_2 j_3)\Delta(l_1 j_2 l_3)\Delta(j_1 l_2 l_3) \\
&\quad \times \sum_k \frac{(-1)^k (j_1+j_2+l_1+l_2+1-k)!}{k!(j_1+j_2-j_3-k)!(l_1+l_2-j_3-k)!(j_1+l_2-l_3-k)!} \\
&\qquad\qquad \overline{(l_1+j_2-l_3-k)!(-j_1-l_1+j_3+l_3+k)!(-j_2-l_2+j_3+l_3+k)!} \qquad (1.6\text{-}13)
\end{aligned}
$$

where

$$\Delta(abc) = \sqrt{\frac{(a+b-c)!(a-b+c)!(b+c-a)!}{(a+b+c+1)!}}.$$

The four triangle relations may be represented symbolically as



$\Delta(j_1 j_2 j_3)$ $\quad$ $\Delta(l_1 l_2 j_3)$ $\quad$ $\Delta(l_1 j_2 l_3)$ $\quad$ $\Delta(j_1 l_2 l_3)$

The $6j$ symbols are invariant under

(a) an interchange of columns,
(b) an interchange of any two numbers in the bottom row with the corresponding two numbers in the top row.

Thus

$$
\begin{aligned}
\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} &= \begin{Bmatrix} j_2 & j_1 & j_3 \\ l_2 & l_1 & l_3 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_3 & j_2 \\ l_1 & l_3 & l_2 \end{Bmatrix} = \cdots \\
&= \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = \begin{Bmatrix} l_1 & l_2 & j_3 \\ j_1 & j_2 & l_3 \end{Bmatrix} = \cdots. \qquad (1.6\text{-}14)
\end{aligned}
$$

Among their properties are

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = (-1)^{j_1+j_2+l_1+l_2} W(j_1 j_2 l_2 l_1; j_3 l_3) \qquad (1.6\text{-}15)$$

in which $W(j_1 j_2 l_2 l_1; j_3 l_3)$ is the Racah W coefficient,

$$\sum_{j_3}(2j_3+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3' \end{Bmatrix} = \frac{\delta(l_3, l_3')}{2l_3+1}, \qquad (1.6\text{-}16)$$

$$\sum_{l_3}(-1)^{j+j_3+l_3}(2l_3+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\begin{Bmatrix} j_1 & l_1 & j \\ j_2 & l_2 & l_3 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_2 & l_1 & j \end{Bmatrix}. \qquad (1.6\text{-}17)$$

A number of special formulas are listed in Table 1.7; numerical values are given in Table 1.8 which is also taken from the tables of Rotenberg *et al.* (1959).

To illustrate the use of (1.6-11) and (1.6-12) it is possible to write

$$|1, \tfrac{1}{2}\tfrac{1}{2}(0); 1\ 1\rangle = -\sqrt{\tfrac{1}{3}}|1\tfrac{1}{2}(\tfrac{1}{2})\tfrac{1}{2}; 1\ 1\rangle + \sqrt{\tfrac{2}{3}}|1\tfrac{1}{2}(\tfrac{3}{2})\tfrac{1}{2}; 1\ 1\rangle \qquad (1.6\text{-}18)$$

TABLE 1.7 (continued)

$$\begin{Bmatrix} a & b & c \\ 2 & c-1 & b \end{Bmatrix} = (-1)^s 2 \times \frac{[(a+b+1)(a-b)-c^2+1]\,[6(s+1)(s-2a)(s-2b)(s-2c+1)]^{1/2}}{[(2b-1)2b(2b+1)(2b+2)(2b+3)(2c-2)(2c-1)2c(2c+1)(2c+2)]^{1/2}},$$

$$\begin{Bmatrix} a & b & c \\ 2 & c-1 & b+1 \end{Bmatrix} = (-1)^s \times \frac{4[(a+b+2)(a-b-1)-(c-1)(b+c+2)]\,[(s-2b-1)(s-2b)(s-2c+1)(s-2c+2)]^{1/2}}{[2b(2b+1)(2b+2)(2b+3)(2b+4)(2c-2)(2c-1)2c(2c+1)(2c+2)]^{1/2}},$$

$$\begin{Bmatrix} a & b & c \\ 2 & c & b \end{Bmatrix} = (-1)^s \frac{2[3X(X+1)-4b(b+1)c(c+1)]}{[(2b-1)2b(2b+1)(2b+2)(2b+3)(2c-1)2c(2c+1)(2c+2)(2c+3)]^{1/2}}.$$

in which numerical values of the $6j$ symbols have been obtained from Table 1.8. Similarly

$$|1,\tfrac{1}{2}\tfrac{1}{2}(1);\,1\,1\rangle = \sqrt{\tfrac{2}{3}}\,|1\tfrac{1}{2}(\tfrac{1}{2})\tfrac{1}{2};\,1\,1\rangle + \sqrt{\tfrac{1}{3}}\,|1\tfrac{1}{2}(\tfrac{3}{2})\tfrac{1}{2};\,1\,1\rangle. \qquad (1.6\text{-}19)$$

On substituting (1.6-6a) and (1.6-6b) into (1.6-18) and (1.6-19) it is readily verified that the results are those given by (1.6-10a) and (1.6-10b).

1.7 Summary and Examples

Definition J_x, J_y, and J_z are components of an angular momentum operator $\mathbf{J}$ if

(a) J_x, J_y, and J_z are Hermitian,
(b) J_x, J_y, and J_z satisfy

$$\mathbf{J}\times\mathbf{J} = i\mathbf{J},$$
$$[J_i, J_j] = i\varepsilon_{ijk}J_k, \qquad (1.7\text{-}1)$$
$$[J_i, J_j] = iJ_k \quad (i, j, k \text{ cyclic}),$$

where ε_{ijk} is the antisymmetric unit tensor of rank 3. The three forms of (1.7-1) are equivalent.

TABLE 1.8

Numerical Values of 6j Symbols[a,b]

j_1	j_2	j_3	l_1	l_2	l_3		j_1	j_2	j_3	l_1	l_2	l_3	
1/2	1/2	0	0	0	1/2	*1	2	1	1	1	1	1	22
1/2	1/2	0	1/2	1/2	0	*2	2	1	1	2	1	1	222
1	1/2	1/2	0	1/2	1/2	2	2	3/2	1/2	0	1/2	3/2	3
1	1/2	1/2	1	1/2	1/2	22	2	3/2	1/2	1/2	1	1	21
1	1	0	0	0	1	01	2	3/2	1/2	1	1/2	3/2	301
1	1	0	1/2	1/2	1/2	11	2	3/2	1/2	1	3/2	1/2	4
1	1	0	1	1	0	02	2	3/2	1/2	1	3/2	3/2	*201
1	1	0	1	1	1	*02	2	3/2	1/2	3/2	1	1	311
1	1	1	1/2	1/2	1/2	*02	2	3/2	1/2	2	3/2	1/2	402
1	1	1	1	0	1	*02	2	3/2	1/2	2	3/2	3/2	*202
1	1	1	1	1	0	*02	2	3/2	3/2	0	3/2	3/2	*4
1	1	1	1	1	1	22	2	3/2	3/2	1/2	1	1	*31
3/2	1	1/2	0	1/2	1	*11	2	3/2	3/2	1	1/2	3/2	*201
3/2	1	1/2	1/2	1	1/2	*02	2	3/2	3/2	1	3/2	1/2	*201
3/2	1	1/2	1	1/2	1	*22	2	3/2	3/2	1	3/2	3/2	402
3/2	1	1/2	3/2	1	1/2	*42	2	3/2	3/2	3/2	1	1	*112
3/2	3/2	0	0	0	3/2	*2	2	3/2	3/2	2	1/2	3/2	*202
3/2	3/2	0	1/2	1/2	1	*3	2	3/2	3/2	2	3/2	1/2	*202
3/2	3/2	0	1	1	1/2	*21	2	3/2	3/2	2	3/2	3/2	422
3/2	3/2	0	1	1	3/2	21	2	2	0	0	0	2	001
3/2	3/2	0	3/2	3/2	0	*4	2	2	0	1/2	1/2	3/2	101
3/2	3/2	0	3/2	3/2	1	4	2	2	0	1	1	1	011
3/2	3/2	1	1/2	1/2	1	321	2	2	0	1	1	2	*011
3/2	3/2	1	1	0	3/2	21	2	2	0	3/2	3/2	1/2	201
3/2	3/2	1	1	1	1/2	321	2	2	0	3/2	3/2	3/2	*201
3/2	3/2	1	1	1	3/2	*121	2	2	0	2	2	0	002
3/2	3/2	1	3/2	1/2	1	22	2	2	0	2	2	1	*002
3/2	3/2	1	3/2	3/2	0	4	2	2	0	2	2	2	002
3/2	3/2	1	3/2	3/2	1	*4220,2	2	2	1	1/2	1/2	3/2	*201
2	1	1	0	1	1	02	2	2	1	1	0	2	*011

TABLE 1.8 (continued)

j_1	j_2	j_3	l_1	l_2	l_3		j_1	j_2	j_3	l_1	l_2	l_3	
2	2	1	1	1	1	*201	2	2	2	1	1	1	2121,
2	2	1	1	1	2	221	2	2	2	1	1	2	2121,
2	2	1	3/2	1/2	3/2	*301	2	2	2	3/2	1/2	3/2	3021,
2	2	1	3/2	3/2	1/2	*322	2	2	2	3/2	3/2	1/2	3021,
2	2	1	3/2	3/2	3/2	102	2	2	2	3/2	3/2	3/2	0
2	2	1	2	1	1	*202	2	2	2	2	0	2	002
2	2	1	2	1	2	2121,	2	2	2	2	1	1	2121,
2	2	1	2	2	0	*002	2	2	2	2	1	2	*202
2	2	1	2	2	1	22	2	2	2	2	2	0	002
2	2	1	2	2	2	*202	2	2	2	2	2	1	*202
							2	2	2	2	2	2	*2222,

[a] The table lists $\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}^2$ in prime notation (see Table 1.6). To find the value of a 6*j* symbol use the symmetry properties (1.6-14) to (a) place the largest of the six parameters in the upper left-hand corner (j_1 position), (b) place the largest of the remaining four parameters in the middle of the top row (j_2 position), and (c) make $l_1 > l_2$ if $j_1 = j_2$.

[b] Reprinted from "The 3-*j* and 6-*j* Symbols," by Rotenberg, Bivins, Metropolis, and Wooten by permission of the M.I.T. Press, Cambridge, Massachusetts. Copyright ©, 1959 by the Massachusetts Institute of Technology.

Spherical Components

$$J_{+1} = -\frac{1}{\sqrt{2}}[J_x + iJ_y] = -J^\dagger_{-1}, \qquad J_{-1} = \frac{1}{\sqrt{2}}[J_x - iJ_y] = -J^\dagger_{+1},$$
$$J_x = -\frac{1}{\sqrt{2}}[J_{+1} - J_{-1}], \qquad J_y = \frac{i}{\sqrt{2}}[J_{+1} + J_{-1}], \qquad J_z = J_0 \tag{1.7-2}$$

J^2

$$J^2 = J_x^2 + J_y^2 + J_z^2 = -J_{+1}J_{-1} + J_0 - J_{-1}J_{+1}$$
$$= \sum_q (-1)^q J_q J_{-q} \qquad (q = 1, 0, -1)$$
$$= -2J_{+1}J_{-1} + J_0(J_0 - 1) = -2J_{-1}J_{+1} + J_0(J_0 + 1). \tag{1.7-3}$$

Commutators

$$[J_0, J_{\pm 1}] = \pm J_{\pm 1}, \qquad [J_{+1}, J_{-1}] = -J_0. \tag{1.7-4}$$

In terms of the CG coefficients, (1.7-4) has the form

$$[J_p, J_q] = -\sqrt{2}\langle 1\,1\,pq|1\,1\,1\,p+q\rangle J_{p+q} \qquad (p, q = 1, 0, -1), \tag{1.7-5}$$
$$[J_\mu, J^2] = 0 \qquad (J_\mu = J_x, J_y, J_z, J_{+1}, J_{-1}). \tag{1.7-6}$$

Operators and Eigenstates

$$J^2|jm\rangle = j(j+1)|jm\rangle,$$
$$J_z|jm\rangle = J_0|jm\rangle = m|jm\rangle, \tag{1.7-7}$$
$$J_{\pm 1}|jm\rangle = \mp\sqrt{\tfrac{1}{2}[j(j+1) - (m \pm 1)m]}\,|j\,m \pm 1\rangle$$
$$j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \tfrac{5}{2}, \ldots, \qquad m = j, j-1, \ldots, -j. \tag{1.7-8}$$

Matrix Elements

$$\langle j'm'|J^2|jm\rangle = j(j+1)\,\delta_{j'j}\delta_{m'm}, \tag{1.7-9}$$
$$\langle j'm'|J_0|jm\rangle = m\,\delta_{j'j}\delta_{m'm} = \langle j'm'|J_z|jm\rangle, \tag{1.7-10}$$
$$\langle j'm'|J_{+1}|jm\rangle = -\sqrt{\tfrac{1}{2}[j(j+1) - (m+1)m]}\,\delta_{j'j}\delta_{m'\,m+1}, \tag{1.7-11}$$
$$\langle j'm'|J_{-1}|jm\rangle = \sqrt{\tfrac{1}{2}[j(j+1) - (m-1)m]}\,\delta_{j'j}\delta_{m'\,m-1}. \tag{1.7-12}$$

An alternative expression for the matrix element of J_{+1}, J_0, or J_{-1} is derived in Section 6.3:

$$\langle j'm'|J_q|jm\rangle = (-1)^{j-m'}\begin{pmatrix} j' & 1 & j \\ -m' & q & m \end{pmatrix}\sqrt{(2j'+1)(j'+1)}\,\delta_{j'j} \qquad (q = 1, 0, -1). \tag{1.7-13}$$

For the rectangular components

$$\langle j\,m+1|J_x|jm\rangle = \tfrac{1}{2}\sqrt{j(j+1) - m(m+1)},$$
$$\langle j\,m-1|J_x|jm\rangle = \tfrac{1}{2}\sqrt{j(j+1) - m(m-1)}, \tag{1.7-14}$$
$$\langle j\,m+1|J_y|jm\rangle = -\tfrac{i}{2}\sqrt{j(j+1) - m(m+1)},$$
$$\langle j\,m-1|J_y|jm\rangle = \tfrac{i}{2}\sqrt{j(j+1) - m(m-1)}. \tag{1.7-15}$$

Examples (see (1.4-4) for format)

$j \equiv s = \frac{1}{2}$; $\mathbf{J} \equiv \mathbf{S}$

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = S_0,$$
$$S_{+1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, \qquad S_{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad S^2 = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1.7-16}$$

$$|jm\rangle \equiv |sm\rangle = \begin{cases} |\tfrac{1}{2}\,\tfrac{1}{2}\rangle \equiv \alpha \equiv \xi_{1/2} \equiv \xi(\tfrac{1}{2}) = \begin{pmatrix}1\\0\end{pmatrix}, \\ |\tfrac{1}{2}\,-\tfrac{1}{2}\rangle \equiv \beta \equiv \xi_{-1/2} \equiv \xi(-\tfrac{1}{2}) = \begin{pmatrix}0\\1\end{pmatrix}, \end{cases} \tag{1.7-17}$$

$$\begin{aligned} S_x\alpha &= \beta/2, & S_x\beta &= \alpha/2, \\ S_y\alpha &= i\beta/2, & S_y\beta &= -i\alpha/2, \\ S_z\alpha &= S_0\alpha = \alpha/2, & S_z\beta &= S_0\beta = -\beta/2, \\ S_{+1}\alpha &= 0, & S_{+1}\beta &= -\alpha/\sqrt{2}, \\ S_{-1}\alpha &= \beta/\sqrt{2}, & S_{-1}\beta &= 0, \\ S^2\alpha &= \tfrac{3}{4}\alpha, & S^2\beta &= \tfrac{3}{4}\beta. \end{aligned} \tag{1.7-18}$$

$j = 1$

$$J_x = \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}, \qquad J_y = \frac{i}{\sqrt{2}}\begin{pmatrix}0&-1&0\\1&0&-1\\0&1&0\end{pmatrix},$$

$$J_0 = J_z = \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}, \qquad J^2 = \begin{pmatrix}2&0&0\\0&2&0\\0&0&2\end{pmatrix}, \tag{1.7-19}$$

$$J_{+1} = \begin{pmatrix}0&-1&0\\0&0&-1\\0&0&0\end{pmatrix}, \qquad J_{-1} = \begin{pmatrix}0&0&0\\1&0&0\\0&1&0\end{pmatrix}.$$

Coupling of Angular Momentum Operators The coupling of two angular momentum operators $\mathbf{J}_1$ and $\mathbf{J}_2$ is expressed by the relation

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \tag{1.7-20}$$

where $\mathbf{J}$ is also an angular momentum operator, and

$$\begin{aligned} J_1{}^2|j_1m_1\rangle &= j_1(j_1+1)|j_1m_1\rangle, & J_{1z}|j_2m_2\rangle &= j_2(j_2+1)|j_1m_1\rangle, \\ J_2{}^2|j_2m_2\rangle &= j_2(j_2+1)|j_1m_1\rangle, & J_{2z}|j_2m_2\rangle &= m_2|j_2m_2\rangle, \end{aligned} \tag{1.7-21}$$

with

$$j_1, j_2 = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots, \quad m_1 = j_1, j_1 - 1, \ldots, -j_1, \quad m_2 = j_2, j_2 - 1, \ldots, -j_2. \tag{1.7-22}$$

The coupled and uncoupled representations are related by

$$\begin{aligned} |jm\rangle \equiv |j_1j_2jm\rangle &= \sum_{m_1m_2} |j_1j_2m_1m_2\rangle\langle j_1j_2m_1m_2|j_1j_2jm\rangle \\ &= (-1)^{j_2-j_1-m}\sqrt{2j+1}\sum_{m_1m_2}\begin{pmatrix}j_1 & j_2 & j\\ m_1 & m_2 & -m\end{pmatrix}|j_1j_2m_1m_2\rangle \end{aligned} \tag{1.7-23}$$

where

$$\begin{aligned} j &= j_1 + j_2,\ \ j_1 + j_2 - 1, \ldots, |j_1 - j_2| \\ &= 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots, \\ m &= m_1 + m_2 = j,\ \ j - 1, \ldots, -j, \\ & j_1 + j_2 + j = n \qquad \text{(an integer).} \end{aligned} \tag{1.7-24}$$

Example Coupling of two electronic spins

$$j_1 \equiv s_1 = \tfrac{1}{2}, \qquad m_1 = \pm\tfrac{1}{2}, \qquad |s_1m_1\rangle = \begin{cases} |\tfrac{1}{2}\,\tfrac{1}{2}\rangle_1 = \alpha(1), \\ |\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_1 = \beta(1), \end{cases}$$

$$j_2 = s_2 = \tfrac{1}{2}, \qquad m_2 = \pm\tfrac{1}{2}, \qquad |s_2m_2\rangle = \begin{cases} |\tfrac{1}{2}\,\tfrac{1}{2}\rangle_2 = \alpha(2), \\ |\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_2 = \beta(2), \end{cases}$$

$$j \equiv S = \begin{cases} 1, & m \equiv M = 1, 0, -1, \\ 0, & m \equiv M = 0. \end{cases}$$

$$\begin{aligned} |SM\rangle = |1\ 1\rangle &= \alpha(1)\alpha(2), \\ |1\ 0\rangle &= \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)], \\ |1\ -1\rangle &= \beta(1)\beta(2), \\ |0\ 0\rangle &= \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]. \end{aligned} \tag{1.7-25}$$

Three angular momentum operators $\mathbf{J}_1, \mathbf{J}_2$, and $\mathbf{J}_3$ may be coupled to form a resultant $\mathbf{J}$

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3. \tag{1.7-26}$$

However, the eigenfunctions of $\mathbf{J}$ depend on the coupling sequence and are related through unitary transformations of the form

$$\begin{aligned} |j_1, j_2j_3(j_{23}); j\rangle &= \sum_{j_{12}} (-1)^{j_1+j_2+j_3+j}\sqrt{(2j_{12}+1)(2j_{23}+1)} \\ &\quad \times \begin{Bmatrix}j_1 & j_2 & j_{12}\\ j_3 & j & j_{23}\end{Bmatrix}|j_1j_2(j_{12})j_3; j\rangle. \end{aligned} \tag{1.7-27}$$