Appendix A
Clebsch–Gordan and Racah Coefficients

In this appendix we summarize the formulae describing the coupling of two or more angular momenta required in our analysis of atomic, molecular and optical collision processes. This leads to the introduction of Clebsch–Gordan coefficients, Racah coefficients, 6-j symbols, 9-j symbols as well as higher order $3n$-j symbols. For a detailed discussion of these topics reference should be made to specialized monographs on angular momentum by Wigner [965, 967], Biedenharn et al. [106], Rose [797], Edmonds [284], Fano and Racah [308] and Brink and Satchler [139] and to the reprint volume by Biedenharn and van Dam [107].

A.1 Clebsch–Gordan Coefficients

Let us consider two independent quantum systems, or parts of a single system, with angular momenta denoted by the angular momentum operators $\mathbf{J_1}$ and $\mathbf{J_2}$. For example, $\mathbf{J_1}$ and $\mathbf{J_2}$ may be the orbital and spin angular momentum operators of a single particle or they may be the orbital angular momentum operators of two different particles. The Cartesian components of these operators satisfy the commutation relations (with $\hbar = 1$)

$$[J_{1x}, J_{1y}] = \mathrm{i}J_{1z}, \quad [J_{1y}, J_{1z}] = \mathrm{i}J_{1x}, \quad [J_{1z}, J_{1x}] = \mathrm{i}J_{1y}, \tag{A.1}$$

$$[\mathbf{J}_1^2, J_{1z}] = 0 \tag{A.2}$$

and

$$[J_{2x}, J_{2y}] = \mathrm{i}J_{2z}, \quad [J_{2y}, J_{2z}] = \mathrm{i}J_{2x}, \quad [J_{2z}, J_{2x}] = \mathrm{i}J_{2y}, \tag{A.3}$$

$$[\mathbf{J}_2^2, J_{2z}] = 0, \tag{A.4}$$

and they commute with each other so that

$$[\mathbf{J}_1, \mathbf{J}_2] = 0. \tag{A.5}$$

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We denote by $\psi_{j_1 m_1}(1)$ and $\psi_{j_2 m_2}(2)$ the simultaneous angular momentum eigenfunctions of these quantum systems which satisfy

$$\mathbf{J}_1^2 \psi_{j_1 m_1}(1) = j_1(j_1+1)\psi_{j_1 m_1}(1), \quad J_{1z}\psi_{j_1 m_1}(1) = m_1 \psi_{j_1 m_1}(1), \tag{A.6}$$

where

$$m_1 = -j_1, -j_1+1, \ldots, j_1, \tag{A.7}$$

and

$$\mathbf{J}_2^2 \psi_{j_2 m_2}(2) = j_2(j_2+1)\psi_{j_2 m_2}(2)\ , \quad J_{2z}\psi_{j_2 m_2}(2) = m_2 \psi_{j_2 m_2}(2), \tag{A.8}$$

where

$$m_2 = -j_2, -j_2+1, \ldots, j_2. \tag{A.9}$$

Simultaneous eigenfunctions of the operators $\mathbf{J}_1^2$, J_{1z}, $\mathbf{J}_2^2$ and J_{2z} are then given by the product $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$. We now define the total angular momentum operator of the two systems by

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2, \tag{A.10}$$

and the z-component of this total angular momentum operator by

$$J_z = J_{1z} + J_{2z}. \tag{A.11}$$

The operators $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$ and J_z form a set of commuting operators. Let us denote by $\psi_{j_1 j_2 j m}(1,2)$ the coupled eigenfunctions which are simultaneous eigenfunctions of the operators $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$ and J_z. These simultaneous eigenfunctions satisfy

$$\begin{aligned} \mathbf{J}^2 \psi_{j_1 j_2 j m}(1,2) &= j(j+1)\psi_{j_1 j_2 j m}(1,2), \\ J_z \psi_{j_1 j_2 j m}(1,2) &= m \psi_{j_1 j_2 j m}(1,2), \end{aligned} \tag{A.12}$$

where

$$j = |j_1 - j_2|,\ |j_1 - j_2| + 1, \ldots, j_1 + j_2, \tag{A.13}$$

and

$$m = -j, -j+1, \ldots, j. \tag{A.14}$$

The $(2j_1+1)(2j_2+1)$ simultaneous eigenfunctions $\psi_{j_1 j_2 j m}(1,2)$ of the operators $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$ and J_z are related to the $(2j_1+1)(2j_2+1)$ product eigenfunctions $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$ of the operators $\mathbf{J}_1^2$, J_{1z}, $\mathbf{J}_2^2$ and J_{2z} by the unitary transformation

$$\psi_{j_1 j_2 jm}(1,2) = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | jm) \psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2). \tag{A.15}$$

The expansion coefficients $(j_1 m_1 j_2 m_2 | jm)$ in this transformation are called vector coupling or Clebsch–Gordan coefficients. These coefficients vanish unless (A.13) and (A.14) are satisfied and

$$m = m_1 + m_2. \tag{A.16}$$

To define these coefficients unambiguously, the relative phases of the eigenfunctions $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$ and $\psi_{j_1 j_2 jm}(1,2)$ must be specified. We adopt here the phase convention of Condon and Shortley [227] where

$$(j_1 j_1 j_2 j_2 | j_1 + j_2 \; j_1 + j_2) = 1. \tag{A.17}$$

With this choice of phase the Clebsch–Gordan coefficients are real and satisfy the orthogonality relations

$$\sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | jm)(j_1 m_1 j_2 m_2 | j' m') = \delta_{jj'} \delta_{mm'}, \tag{A.18}$$

which reduces to a single summation since (A.16) is satisfied, and

$$\sum_{jm} (j_1 m_1 j_2 m_2 | jm)(j_1 m_1' j_2 m_2' | jm) = \delta_{m_1 m_1'} \delta_{m_2 m_2'}. \tag{A.19}$$

Using (A.19) we can invert (A.15) to yield

$$\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2) = \sum_j (j_1 m_1 j_2 m_2 | jm) \psi_{j_1 j_2 jm}(1,2). \tag{A.20}$$

The Clebsch–Gordan coefficients satisfy the following symmetry relations

$$(j_1 m_1 j_2 m_2 | jm) = (-1)^{j_1 + j_2 - j} (j_1 - m_1 j_2 - m_2 | j - m), \tag{A.21}$$

$$= (-1)^{j_1 + j_2 - j} (j_2 m_2 j_1 m_1 | jm), \tag{A.22}$$

$$= (-1)^{j_1 - m_1} \left(\frac{2j+1}{2j_2+1} \right)^{1/2} (j_1 m_1 j - m | j_2 - m_2), \tag{A.23}$$

$$= (-1)^{j_2+m_2}\left(\frac{2j+1}{2j_1+1}\right)^{1/2}(j-mj_2m_2|j_1-m_1), \tag{A.24}$$

$$= (-1)^{j_1-m_1}\left(\frac{2j+1}{2j_2+1}\right)^{1/2}(jmj_1-m_1|j_2m_2), \tag{A.25}$$

$$= (-1)^{j_2+m_2}\left(\frac{2j+1}{2j_1+1}\right)^{1/2}(j_2-m_2jm|j_1m_1). \tag{A.26}$$

The Clebsch–Gordan coefficients also satisfy

$$(j_10j_20|j0) = 0, \quad \text{unless } j_1+j_2+j \text{ is even}, \tag{A.27}$$

and

$$(j_1m_100|jm) = \delta_{j_1j}\delta_{m_1m}. \tag{A.28}$$

Equation (A.27) gives rise to the parity selection rule in applications.

The symmetry relations satisfied by the Clebsch–Gordan coefficients can be simplified by introducing the 3-j symbols defined by Wigner [967]. These are defined by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3}(2j_3+1)^{-1/2}(j_1m_1j_2m_2|j_3-m_3). \tag{A.29}$$

The 3-j symbols are invariant under an even permutation of the columns, while an odd permutation is equivalent to multiplication by $(-1)^{j_1+j_2+j_3}$. Thus

$$(-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix}$$
$$= \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix}. \tag{A.30}$$

Also the analogue of (A.21) is

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \tag{A.31}$$

The orthogonality relations satisfied by the 3-j symbols are

$$\sum_{m_1m_2}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = (2j_3+1)^{-1}\delta_{j_3j_3'}\delta_{m_3m_3'} \tag{A.32}$$

and

$$\sum_{j_3 m_3}(2j_3+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta_{m_1 m_1'}\delta_{m_2 m_2'}. \tag{A.33}$$

We conclude this section by giving the following closed expression for the Clebsch–Gordan coefficients (see Wigner [965])

$$\begin{aligned}
&(j_1 m_1 j_2 m_2|jm) \\
&\quad = \left[\frac{(2j+1)(j+j_1-j_2)!(j-j_1+j_2)!(j_1+j_2-j)!(j+m)!(j-m)!}{(j_1+j_2+j+1)!(j_1-m_1)!(j_1+m_1)!(j_2-m_2)!(j_2+m_2)!}\right] \\
&\quad \times \sum_{\kappa}(-1)^{\kappa+j_2+m_2}\frac{(j_2+j_3+m_1-\kappa)!(j_1-m_1+\kappa)!}{\kappa!(j-j_1+j_2-\kappa)!(j+m-\kappa)!(\kappa+j_1-j_2-m)!} \\
&\quad \times \delta_{m,m_1+m_2},
\end{aligned} \tag{A.34}$$

where the summation is over all integral values of κ such that none of the factorial arguments is negative. The explicit values of the Clebsch–Gordan coefficients when $j_2 = 1/2$ and $j_2 = 1$ are given in Tables A.1 and A.2, respectively.

Table A.1 Clebsch–Gordan coefficients $(j_1\ m-m_2\ \frac{1}{2}\ m_2|j\ m)$

j	$m_2 = 1/2$	$m_2 = -1/2$
$j_1+\frac{1}{2}$	$\left[\frac{j_1+m+\frac{1}{2}}{2j_1+1}\right]^{1/2}$	$\left[\frac{j_1-m+\frac{1}{2}}{2j_1+1}\right]^{1/2}$
$j_1-\frac{1}{2}$	$-\left[\frac{j_1-m+\frac{1}{2}}{2j_1+1}\right]^{1/2}$	$\left[\frac{j_1+m+\frac{1}{2}}{2j_1+1}\right]^{1/2}$

Table A.2 Clebsch–Gordan coefficients $(j_1\ m-m_2\ 1\ m_2|j\ m)$

j	$m_2 = 1$	$m_2 = 0$	$m_2 = -1$
j_1+1	$\left[\frac{(j_1+m)(j_1+m+1)}{(2j_1+1)(2j_1+2)}\right]^{1/2}$	$\left[\frac{(j_1-m+1)(j_1+m+1)}{(2j_1+1)(j_1+1)}\right]^{1/2}$	$\left[\frac{(j_1-m)(j_1-m+1)}{(2j_1+1)(2j_1+2)}\right]^{1/2}$
j_1	$-\left[\frac{(j_1+m)(j_1-m+1)}{2j_1(j_1+1)}\right]^{1/2}$	$\frac{m}{[j_1(j_1+1)]^{1/2}}$	$\left[\frac{(j_1-m)(j_1+m+1)}{2j_1(j_1+1)}\right]^{1/2}$
j_1-1	$\left[\frac{(j_1-m)(j_1-m+1)}{2j_1(2j_1+1)}\right]^{1/2}$	$-\left[\frac{(j_1-m)(j_1+m)}{j_1(2j_1+1)}\right]^{1/2}$	$\left[\frac{(j_1+m+1)(j_1+m)}{2j_1(2j_1+1)}\right]^{1/2}$

A.2 Racah Coefficients

We now consider three independent quantum systems, or parts of a single system, with angular momenta denoted by the operators $\mathbf{J}_1$, $\mathbf{J}_2$ and $\mathbf{J}_3$. We can write the total angular momentum operator $\mathbf{J}$ as

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3. \tag{A.35}$$

However, there is no unique way of carrying out this addition. For example, we can first couple the angular momentum eigenfunctions $\psi_{j_1 m_1}(1)$ and $\psi_{j_2 m_2}(2)$ belonging to $\mathbf{J}_1$ and $\mathbf{J}_2$ to form eigenfunctions of $\mathbf{J_{12}} = \mathbf{J}_1 + \mathbf{J}_2$ according to

$$\psi_{j_1 j_2 j_{12} m_{12}}(1,2) = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | j_{12} m_{12}) \psi_{j_1 m_1}(1) \psi_{j_2 m_2}(2)\ . \tag{A.36}$$

These eigenfunctions can then be coupled with the angular momentum eigenfunctions $\psi_{j_3 m_3}(3)$ belonging to $\mathbf{J}_3$ to form eigenfunctions of $\mathbf{J}$ according to

$$\psi_{jm}(j_{12}) = \sum_{m_{12} m_3} (j_{12} m_{12} j_3 m_3 | jm) \psi_{j_1 j_2 j_{12} m_{12}}(1,2) \psi_{j_3 m_3}(3). \tag{A.37}$$

Alternatively, we can first couple $\psi_{j_2 m_2}(2)$ and $\psi_{j_3 m_3}(3)$ to form eigenfunctions of $\mathbf{J_{23}} = \mathbf{J}_2 + \mathbf{J}_3$ according to

$$\psi_{j_2 j_3 j_{23} m_{23}}(2,3) = \sum_{m_2 m_3} (j_2 m_2 j_3 m_3 | j_{23} m_{23}) \psi_{j_2 m_2}(2) \psi_{j_3 m_3}(3) \tag{A.38}$$

and then couple these eigenfunctions with $\psi_{j_1 m_1}(1)$ to form eigenfunctions of $\mathbf{J}$ according to

$$\psi_{jm}(j_{23}) = \sum_{m_1 m_{23}} (j_1 m_1 j_{23} m_{23} | jm) \psi_{j_1 m_1}(1) \psi_{j_2 m_2}(2) \psi_{j_2 j_3 j_{23} m_{23}}(2,3). \tag{A.39}$$

Finally, we can first couple $\psi_{j_1 m_1}(1)$ and $\psi_{j_3 m_3}(3)$ to form eigenfunctions of $\mathbf{J_{13}} = \mathbf{J}_1 + \mathbf{J}_3$ and then couple the resultant eigenfunctions with $\psi_{j_2 m_2}(2)$ to form eigenfunctions of $\mathbf{J}$.

These three representations of the eigenfunctions of $\mathbf{J}$ are related by unitary transformations. For example, we can write

$$\psi_{jm}(j_{12}) = \sum_{j_{23}} R(j_{23}, j_{12}) \psi_{jm}(j_{23}). \tag{A.40}$$

The Racah coefficients W are then defined by the equation (Racah [764–767])

$$R(j_{23}, j_{12}) = [(2j_{23}+1)(2j_{12}+1)]^{1/2} W(j_1 j_2 j j_3; j_{12} j_{23}). \tag{A.41}$$

We can derive a relation between the Racah coefficients and the Clebsch – Gordan coefficients by expressing $\psi_{jm}(j_{12})$ and $\psi_{jm}(j_{23})$ in terms of $\psi_{j_1m_1}(1)$, $\psi_{j_2m_2}(2)$ and $\psi_{j_3m_3}(3)$. Equations (A.36) and (A.37) yield

$$\psi_{jm}(j_{12}) = \sum_{m_1m_{12}} (j_1m_1 j_2m_{12} - m_1|j_{12}m_{12})(j_{12}m_{12} j_3m - m_{12}|jm) \times \psi_{j_1m_1}(1)\psi_{j_2m_{12}-m_1}(2)\psi_{j_3m-m_{12}}(3) \tag{A.42}$$

and (A.38) and (A.39) yield

$$\psi_{jm}(j_{23}) = \sum_{m_2m_{23}} (j_2m_2 j_3m_{23} - m_2|j_{23}m_{23})(j_1m - m_{23} j_{23}m_{23}|jm) \times \psi_{j_1m-m_{23}}(1)\psi_{j_2m_2}(2)\psi_{j_3m_{23}-m_2}(3). \tag{A.43}$$

Substituting (A.42) and (A.43) into (A.40) and using (A.41) gives

$$\sum_f [(2e+1)(2f+1)]^{1/2} W(abcd; ef)(b\beta d\delta|f\beta+\delta)(a\alpha f\beta+\delta|c\alpha+\beta+\delta) = (a\alpha b\beta|e\alpha+\beta)(e\alpha+\beta d\delta|c\alpha+\beta+\delta). \tag{A.44}$$

Using the properties of the Clebsch–Gordan coefficients given by (A.18) and (A.19) and by (A.21), (A.22), (A.23), (A.24), (A.25) and (A.26) we obtain the following additional relations

$$[(2e+1)(2f+1)]^{1/2} W(abcd; ef)(a\alpha f\beta+\delta|c\alpha+\beta+\delta) = \sum_\beta (a\alpha b\beta|e\alpha+\beta)(e\alpha+\beta d\delta|c\alpha+\beta+\delta)(b\beta d\delta|f\beta+\delta), \tag{A.45}$$

where $\beta+\delta$ is a fixed parameter, and

$$[(2e+1)(2f+1)]^{1/2} W(abcd; ef) = \sum_{\alpha\beta} (a\alpha b\beta|e\alpha+\beta)(e\alpha+\beta d\delta|c\alpha+\beta+\delta)(b\beta d\delta|f\beta+\delta) \times (a\alpha f\beta+\delta|c\alpha+\beta+\delta), \tag{A.46}$$

where $\alpha+\beta+\delta$ is a fixed parameter.

It follows from the above definitions that the six angular momenta in $W(abcd; ef)$ satisfy the following four triangular relations

$$\Delta(abe), \quad \Delta(cde), \quad \Delta(acf), \quad \Delta(bdf), \tag{A.47}$$

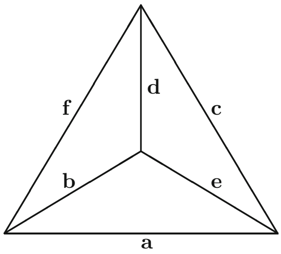

Fig. A.1 Tetrahedron illustrating the triangular relations satisfied by the arguments of the Racah coefficient $W(abcd; ef)$

where, for example, the notation $\Delta(abe)$ means that the three angular momenta a, b and e form the sides of a triangle. These four triangular relations can be combined by representing the six angular momenta by the sides of a tetrahedron as illustrated in Fig. A.1.

The Racah coefficients satisfy certain symmetry relations under the 24 possible permutations of the 6 arguments which preserve the 4 triangular relations. These symmetry relations, which result in at most a change of phase, are given by

$$W(abcd; ef) = W(badc; ef) = W(cdab; ef) = W(acbd; fe) \tag{A.48}$$

and

$$W(abcd; ef) = (-1)^{e+f-a-d} W(ebcf; ad) = (-1)^{e+f-b-c} W(aefd; bc) \tag{A.49}$$

together with the symmetry relations which can be obtained by applying the above symmetry relations more than once.

The Racah coefficients also satisfy the orthogonality relation

$$\sum_e (2e+1)(2f+1) W(abcd; ef) W(abcd; eg) = \delta_{fg} \tag{A.50}$$

and the sum rules

$$\sum_e (-1)^{a+b-e} (2e+1) W(abcd; ef) W(bacd; eg) = W(agfb; dc) \tag{A.51}$$

and

$$\begin{aligned} &\sum_g (2g+1) W(a'gdc; ac') W(bgec'; b'c) W(a'gfb; ab') \\ &\quad = W(adbe; cf) W(a'db'e; c'f). \end{aligned} \tag{A.52}$$

Hence when there is a sum over a product of several Racah coefficients it is often possible to reduce the number of terms in the product. Finally, if one of the arguments of the Racah coefficient is zero we can use the symmetry relations and the following result

$$W(abcd;0f) = \frac{(-1)^{f-b-d}\delta_{ab}\delta_{cd}}{[(2b+1)(2d+1)]^{1/2}} \tag{A.53}$$

to simplify the expression.

A.3 6-j Symbols

The symmetry relations satisfied by the Racah coefficients can be simplified using the 6-j symbols introduced by Wigner [967] which are defined by

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = (-1)^{j_1+j_2+j_4+j_5} W(j_1 j_2 j_5 j_4; j_3 j_6). \tag{A.54}$$

The 6-j symbols are invariant under any permutation of the three columns, i.e.

$$\begin{aligned}\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} &= \begin{Bmatrix} j_2 & j_3 & j_1 \\ j_5 & j_6 & j_4 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_1 & j_2 \\ j_6 & j_4 & j_5 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{Bmatrix} \\ &= \begin{Bmatrix} j_1 & j_3 & j_2 \\ j_4 & j_6 & j_5 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_2 & j_1 \\ j_6 & j_5 & j_4 \end{Bmatrix}.\end{aligned} \tag{A.55}$$

They are also invariant under interchange of the upper and lower arguments in each of any two columns, i.e.

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_5 & j_6 \\ j_4 & j_2 & j_3 \end{Bmatrix} = \begin{Bmatrix} j_4 & j_2 & j_6 \\ j_1 & j_5 & j_3 \end{Bmatrix} = \begin{Bmatrix} j_4 & j_5 & j_3 \\ j_1 & j_2 & j_6 \end{Bmatrix}. \tag{A.56}$$

A.4 9-j Symbols

In many applications we need to transform between two coupling schemes involving four angular momenta. This occurs, for example, in the transformation from jj-coupling to LS-coupling for two particles possessing both orbital and spin angular momenta. In this example the total angular momentum vector of the first particle is given by

$$\mathbf{j_1} = \boldsymbol{\ell}_1 + \mathbf{s_1} \tag{A.57}$$

and of the second particle is given by

$$\mathbf{j_2} = \boldsymbol{\ell}_2 + \mathbf{s_2}. \tag{A.58}$$

The total angular momentum of the two-particle system in jj-coupling is then given by

$$\mathbf{J} = \mathbf{j_1} + \mathbf{j_2}. \tag{A.59}$$

Alternatively, the total orbital angular momentum vector of the two particles is given by

$$\mathbf{L} = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2, \tag{A.60}$$

and the total spin angular momentum vector is given by

$$\mathbf{S} = \mathbf{s_1} + \mathbf{s_2}. \tag{A.61}$$

The total angular momentum of the two-particle system in LS coupling is then given by

$$\mathbf{J} = \mathbf{L} + \mathbf{S}. \tag{A.62}$$

The transformation between these coupling schemes is related to the 9-j symbol introduced by Wigner [967] by the following equation

$$\begin{aligned} &< (\ell_1 s_1)j_1, (\ell_2 s_2)j_2; JM|(\ell_1\ell_2)L, (s_1 s_2)S; JM > \\ &= [(2j_1+1)(2j_2+1)(2L+1)(2S+1)]^{1/2} \left\{ \begin{matrix} \ell_1 & s_1 & j_1 \\ \ell_2 & s_2 & j_2 \\ L & S & J \end{matrix} \right\}, \end{aligned} \tag{A.63}$$

which is independent of the total magnetic quantum number M. The 9-j symbol in the curly bracket in this equation can be written as the sum over products of three 6-j symbols by expressing the bra vector in (A.63) in terms of the ket vector in (A.63) through repeated use of the recoupling transformation defined by (A.40) and (A.41). We obtain in the general case

$$\begin{aligned} \left\{ \begin{matrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{matrix} \right\} &= \sum_\kappa (-1)^{2\kappa}(2\kappa+1) \left\{ \begin{matrix} j_1 & j_3 & j_{13} \\ j_{24} & j & \kappa \end{matrix} \right\} \left\{ \begin{matrix} j_2 & j_4 & j_{24} \\ j_3 & \kappa & j_{34} \end{matrix} \right\} \\ &\times \left\{ \begin{matrix} j_{12} & j_{34} & j \\ \kappa & j_1 & j_2 \end{matrix} \right\}. \end{aligned} \tag{A.64}$$

An even permutation of the rows or columns of the 9-j symbol leaves it unchanged as does the transposition obtained by interchanging rows and columns. An odd permutation of the rows or columns causes the 9-j symbol to be multiplied by the factor

$$f = (-1)^{j_1+j_2+j_{12}+j_3+j_4+j_{34}+j_{13}+j_{24}+j}. \tag{A.65}$$

The 9-j symbols satisfy the orthogonality relation

$$\sum_{j_{12}j_{34}} (2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j'_{13} & j'_{24} & j \end{Bmatrix}$$
$$= \delta_{j_{13}j'_{13}}\delta_{j_{24}j'_{24}} \tag{A.66}$$

and the sum rule

$$\sum_{j_{13}j_{23}} (-1)^{2j_2+j_{24}+j_{23}-j_{34}}(2j_{13}+1)(2j_{24}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} \begin{Bmatrix} j_1 & j_3 & j_{13} \\ j_4 & j_2 & j_{24} \\ j_{14} & j_{23} & j \end{Bmatrix}$$
$$= \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_4 & j_3 & j_{34} \\ j_{14} & j_{23} & j \end{Bmatrix}. \tag{A.67}$$

When one of the arguments of the 9-j symbol is zero we can use the symmetry relations and the following result

$$\begin{Bmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{Bmatrix} = \frac{(-1)^{b+c+e+f}}{[(2e+1)(2f+1)]^{1/2}} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} \tag{A.68}$$

to reduce the 9-j symbol to a 6-j symbol times a factor.

A.5 Higher Order 3n-j Symbols

We conclude this appendix by noting that in the theory of electron and photon interactions with complex atoms and ions with many open shells, it is often necessary to consider the recoupling of more than four angular momenta. For example, in the case of recoupling five angular momenta, 12-j symbols arise whose properties have been discussed by Jahn and Hope [498] and by Ord-Smith [708]. However, we will not discuss these higher order 3n-j symbols further here but remark that in practical calculations they can be evaluated in terms of sums over products of Racah coefficients by repeated use of (A.40) and (A.41), and general computer programs have been written for this purpose by Shapiro [870], Burke [154] and Bar-Shalom and Klapisch [56].