34

Angular Momentum Recoupling: Matrix Elements of Coupled Tensor Operators in an Angular Momentum Coupled Basis

In Chapter 33, we evaluated the matrix elements of a vector-coupled spherical tensor of type $[U^{k_1} \times V^{k_2}]^k_q$ in terms of the reduced matrix elements of both U^{k_1} and V^{k_2} in the appropriate angular momentum–coupled basis,

$$\langle [j_1' \times j_2'] J' M' | [U^{k_1} \times V^{k_2}]^k_q | [j_1 \times j_2] J M \rangle,$$

where we managed to simplify the calculation by judicious use of the Wigner–Eckart theorem and convenient choices of magnetic quantum numbers. In some cases, however, the calculation still involved fairly tedious m sums of expressions involving products of Clebsch–Gordan coefficients. It is the purpose of this chapter to show matrix elements of the above type can be expressed in terms of so-called angular momentum recoupling coefficients. Because values of these recoupling coefficients are available through tabulations or computer codes, and in many cases through algebraic expressions, it will be valuable to study these recoupling coefficients.

A The Recoupling of Three Angular Momenta: Racah Coefficients or 6-j Symbols

So far, we have studied transformations of states involving two commuting angular momentum operators from a basis

$$|j_1 m_1 j_2 m_2\rangle \quad \text{simultaneous eigenvectors of } \vec{j}_1^{\,2}, j_{1_z}, \vec{j}_2^{\,2}, j_{2_z},$$

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to a basis with good total angular momentum, $\vec{J} = \vec{j}_1 + \vec{j}_2$,

$$|j_1 j_2 J M\rangle \quad \text{simultaneous eigenvectors of } \vec{j}_1^{\,2}, \vec{j}_2^{\,2}, \vec{J}^{\,2}, J_z.$$

For states involving three commuting angular momentum operators, we require six angular momentum quantum numbers, hence, six commuting operators, e.g.,

$$\vec{j}_1^{\,2}, j_{1_z}, \vec{j}_2^{\,2}, j_{2_z}, \vec{j}_3^{\,2}, j_{3_z},$$

for a complete specification of the basis:

$$|j_1 m_1 j_2 m_2 j_3 m_3\rangle.$$

As for the case of two angular momenta, it will often be advantageous to use a basis with good total angular momentum in which $\vec{J}^{\,2}$ is diagonal. Now, however, the five commuting operators $\vec{j}_1^{\,2}, \vec{j}_2^{\,2}, \vec{j}_3^{\,2}, \vec{J}^{\,2}$, and $J_z = j_{1_z} + j_{2_z} + j_{3_z}$ will be insufficient. A sixth operator is needed. To find this sixth operator, we could couple to total $\vec{J}$ in two ways

$$\begin{aligned} \vec{J} &= (\vec{j}_1 + \vec{j}_2) + \vec{j}_3 = \vec{J}_{12} + \vec{j}_3 \\ &= \vec{j}_1 + (\vec{j}_2 + \vec{j}_3) = \vec{j}_1 + \vec{J}_{23}, \end{aligned} \tag{1}$$

and use the eigenvectors of the six commuting operators

$$\vec{j}_1^{\,2}, \vec{j}_2^{\,2}, \vec{j}_3^{\,2}, \vec{J}_{12}^{\,2}; \vec{J}^{2}, J_z :$$

$$|[[j_1 j_2] J_{12} j_3] J M\rangle,$$

where we first couple the two angular momenta $\vec{j}_1, \vec{j}_2$ to a state with good $\vec{J}_{12}^{\,2}$, or alternatively, we could use the eigenvectors of the six commuting operators

$$\vec{j}_1^{\,2}, \vec{j}_2^{\,2}, \vec{j}_3^{\,2}, \vec{J}_{23}^{\,2}; \vec{J}^{2}, J_z :$$

$$|[j_1 [j_2 j_3] J_{23}] J M\rangle,$$

where we couple the angular momentum $\vec{j}_1$ to a state in which $\vec{j}_2$ and $\vec{j}_3$ have been coupled to a state of good $\vec{J}_{23}^{\,2}$. The transformation from the one basis to the other must be unitary

$$\begin{aligned} &|[[j_1 j_2] J_{12} j_3] J M\rangle \\ &\quad = \sum_{J_{23}} |[j_1 [j_2 j_3] J_{23}] J M\rangle \langle [j_1 [j_2 j_3] J_{23}] J M | [[j_1 j_2] J_{12} j_3] J M\rangle \\ &\quad = \sum_{J_{23}} |[j_1 [j_2 j_3] J_{23}] J M\rangle U(j_1 j_2 J j_3; J_{12} J_{23}), \end{aligned} \tag{2}$$

where we have renamed the unitary transformation coefficient a U coefficient,

$$\langle [j_1 [j_2 j_3] J_{23}] J M | [[j_1 j_2] J_{12} j_3] J M\rangle = U(j_1 j_2 J j_3; J_{12} J_{23}) \equiv U_{J_{12} J_{23}}(j_1 j_2 J j_3), \tag{3}$$

where we have anticipated this unitary transformation is independent of the magnetic quantum number M. It is a matrix element of the unit operator, a spherical tensor of rank 0, in the total angular momentum basis, hence, M-independent by the Wigner–Eckart theorem. The rather strange order of the angular momentum quantum numbers is that first introduced by Racah through his W coefficient, related to the above U coefficient via

$$U(j_1 j_2 J j_3; J_{12} J_{23}) = \sqrt{(2J_{12}+1)(2J_{23}+1)}\,W(j_1 j_2 J j_3; J_{12} J_{23}). \qquad (4)$$

Finally, we have indicated this unitary transformation could be expressed through the elements of a matrix with row index J_{12} and column index J_{23}, where the matrix elements are functions of the quantum numbers j_1, j_2, J, j_3, common to both bases. The unitary character of the transformation gives us

$$U^{-1}_{J_{23}J_{12}} = U^{*}_{J_{12}J_{23}} = U_{J_{12}J_{23}}. \qquad (5)$$

Because the U coefficients can be expressed in terms of Clebsch–Gordan coefficients, which are real, the U coefficients are real, so the * has been omitted in the last step, and the inverse matrix is given by the transposed matrix, $U^{-1} = \tilde{U}$. Therefore,

$$\begin{aligned} |[j_1[j_2j_3]J_{23}]JM\rangle &= \sum_{J_{12}} U^{-1}_{J_{23}J_{12}} |[[j_1j_2]J_{12}j_3]JM\rangle \\ &= \sum_{J_{12}} U_{J_{12}J_{23}} |[[j_1j_2]J_{12}j_3]JM\rangle \\ &= \sum_{J_{12}} U(j_1j_2Jj_3; J_{12}J_{23}) |[[j_1j_2]J_{12}j_3]JM\rangle. \qquad (6) \end{aligned}$$

Because the signs of angular momentum–coupled functions depend on the order of the couplings, it is important to keep the order of the various couplings, as indicated by the order of the angular momentum couplings inside the [ ] brackets. For this purpose a pictorial representation of eqs. (2) and (6) is also useful. See Figs. 34.2(a) and (b), where the arrow also helps to indicate the order of the couplings. See also Figs. 34.1(a) and (b) for a pictorial representation of the coupling of two angular momenta.

B Relations between U Coefficients and Clebsch–Gordan Coefficients

By expanding the angular momentum coupled states of eqs. (2) and (6) in terms of uncoupled states via the appropriate Clebsch–Gordan coefficients, we can express the U coefficients in terms of sums of products of Clebsch–Gordan coefficients. Thus,

$$\begin{aligned} &|[[j_1j_2]J_{12}j_3]JM\rangle \\ &\quad = \sum_{m_1m_2m_3} |j_1m_1\rangle|j_2m_2\rangle|j_3m_3\rangle\langle j_1m_1j_2m_2|J_{12}M_{12}\rangle\langle J_{12}M_{12}j_3m_3|JM\rangle \\ &\quad = \sum_{m_1m_2m_3} |j_1m_1\rangle \sum_{J'_{23}} |[j_2j_3]J'_{23}M_{23}\rangle\langle j_2m_2j_3m_3|J'_{23}M_{23}\rangle \\ &\qquad\qquad \times \langle j_1m_1j_2m_2|J_{12}M_{12}\rangle\langle J_{12}M_{12}j_3m_3|JM\rangle \end{aligned}$$

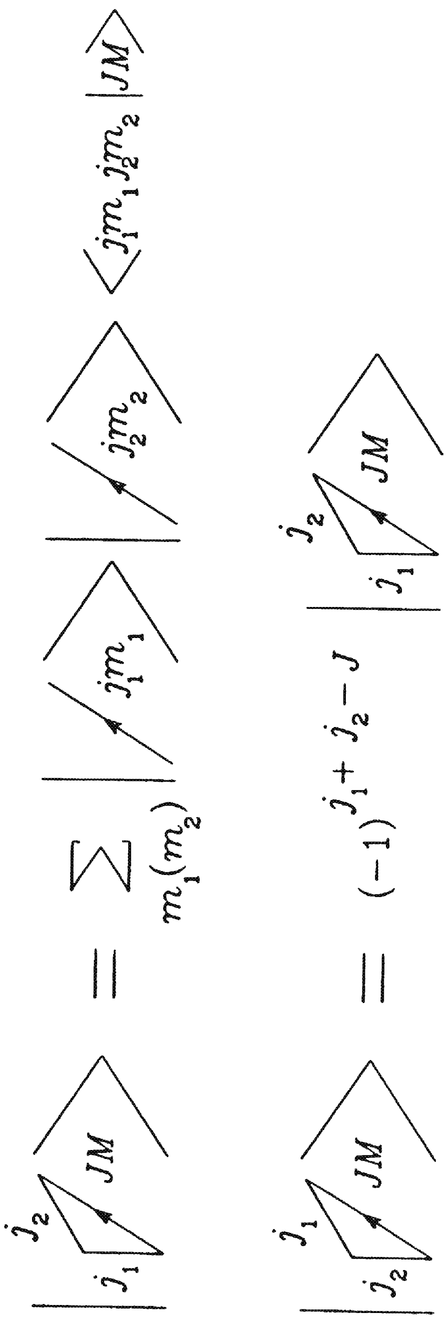

FIGURE 34.1. Coupling of two angular momenta.

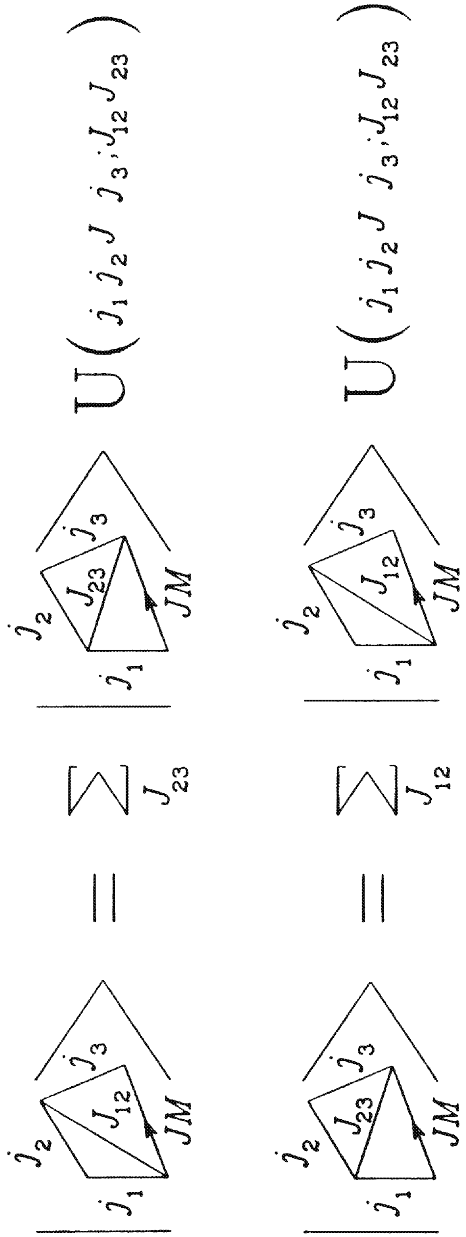

FIGURE 34.2. Recoupling of three angular momenta.

$$= \sum_{m_1 m_2 m_3} \sum_{J'_{23}} \sum_{J'} |[j_1[j_2 j_3]J'_{23}]J'M\rangle \langle j_1 m_1 J'_{23} M_{23}|J'M\rangle$$
$$\times \langle j_2 m_2 j_3 m_3|J'_{23} M_{23}\rangle \langle j_1 m_1 j_2 m_2|J_{12} M_{12}\rangle \langle J_{12} M_{12} j_3 m_3|JM\rangle. \quad (7)$$

Now, left-multiplying this relation by $\langle [j_1[j_2 j_3]J_{23}]JM|$ and using,

$$\langle [j_1[j_2 j_3]J_{23}]JM|[j_1[j_2 j_3]J'_{23}]J'M\rangle = \delta_{J'_{23}J_{23}}\delta_{J'J}, \quad (8)$$

in the last step of the above relation, we are led to

$$U(j_1 j_2 J j_3; J_{12} J_{23}) = \sum_{m_1 m_2 m_3} \langle j_1 m_1 j_2 m_2|J_{12} M_{12}\rangle$$
$$\times \langle J_{12} M_{12} j_3 m_3|JM\rangle \langle j_1 m_1 J_{23} M_{23}|JM\rangle \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle \quad (9)$$

where it is important to remember M is fixed at some specific value, $M = m_1 + m_2 + m_3$, when taking the m_i sums, so that there are essentially only two m_i sums to perform. A second relation can be obtained from

$$|j_1 m_1\rangle |[j_2 j_3]J_{23} M_{23}\rangle = \sum_J |[j_1[j_2 j_3]J_{23}]JM\rangle \langle j_1 m_1 J_{23} M_{23}|JM\rangle$$
$$= \sum_J \sum_{J_{12}} |[[j_1 j_2]J_{12} j_3]JM\rangle U(j_1 j_2 J j_3; J_{12} J_{23}) \langle j_1 m_1 J_{23} M_{23}|JM\rangle$$
$$= \sum_{m_2} |j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle$$
$$= \sum_{m_2} \sum_{J'_{12}} \sum_{J'} |[[j_1 j_2]J'_{12} j_3]J'M\rangle \langle j_1 m_1 j_2 m_2|J'_{12} M_{12}\rangle$$
$$\times \langle J'_{12} M_{12} j_3 m_3|J'M\rangle \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle. \quad (10)$$

Now, using the orthonormality of the states

$$\langle [[j_1 j_2]J_{12} j_3]JM|[[j_1 j_2]J'_{12} j_3]J'M\rangle = \delta_{J_{12}J'_{12}}\delta_{JJ'}, \quad (11)$$

we get

$$U(j_1 j_2 J j_3; J_{12} J_{23}) \langle j_1 m_1 J_{23} M_{23}|JM\rangle =$$
$$\sum_{m_2} \langle j_1 m_1 j_2 m_2|J_{12} M_{12}\rangle \langle J_{12} M_{12} j_3 m_3|JM\rangle \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle. \quad (12)$$

In this relation, m_1, M_{23}, and M, are all fixed. Because the right-hand side, therefore, involves only a single m sum, this relation is particularly useful for the evaluation of U coefficients.

Finally, we get a third relation, by starting with

$$|j_1 m_1 j_2 m_2 j_3 m_3\rangle =$$
$$\sum_{J_{12}} \sum_J |[[j_1 j_2]J_{12} j_3]JM\rangle \langle j_1 m_1 j_2 m_2|J_{12} M_{12}\rangle \langle J_{12} M_{12} j_3 m_3|JM\rangle$$
$$= \sum_{J_{23}} \sum_{J'} |[j_1[j_2 j_3]J_{23}]J'M\rangle \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle \langle j_1 m_1 J_{23} M_{23}|J'M\rangle$$
$$= \sum_{J'_{12} J'} \sum_{J_{23}} |[[j_1 j_2]J'_{12} j_3]J'M\rangle U(j_1 j_2 J' j_3; J'_{12} J_{23})$$
$$\times \langle j_2 m_2 j_3 m_3|J_{23} M_{23}\rangle \langle j_1 m_1 J_{23} M_{23}|J'M\rangle, \quad (13)$$

leading to

$$\langle j_1 m_1 j_2 m_2 | J_{12} M_{12} \rangle \langle J_{12} M_{12} j_3 m_3 | J M \rangle = \sum_{J_{23}} U(j_1 j_2 J j_3; J_{12} J_{23}) \langle j_2 m_2 j_3 m_3 | J_{23} M_{23} \rangle \langle j_1 m_1 J_{23} M_{23} | J M \rangle. \quad (14)$$

In this relation, all the m_i and, hence, the M_{ij} and M are fixed.

All three relations, eqs. (9), (12), and (14) may be useful in the evaluation of U coefficients.

As a very simple example, let us evaluate the U coefficients for the case $j_1 = l, j_2 = \frac{1}{2}, j_3 = \frac{1}{2}$. This recoupling coefficient might be needed in two-electron configurations in which one electron has arbitrary orbital angular momentum, l, whereas the second electron is an s electron with $l = 0$. Here, a U coefficient is needed in the transformation from LS to jj coupling and has the form $U(l\frac{1}{2}J\frac{1}{2}; jS)$, where S is the total two-electron spin and J is the total angular momentum quantum number. Here, J can have the values $l+1, l$, and $l-1$. With $J = l+1$, however, S is fixed uniquely at $S = 1$, and j is fixed uniquely at $j = (l + \frac{1}{2})$. The U transformation matrix is a 1×1 matrix. For any 1×1 transformation, the U coefficient has the value $+1$. Thus,

$$U(l\tfrac{1}{2}(l+1)\tfrac{1}{2}; (l+\tfrac{1}{2})1) = +1. \quad (15)$$

Similarly,

$$U(l\tfrac{1}{2}(l-1)\tfrac{1}{2}; (l-\tfrac{1}{2})1) = +1. \quad (16)$$

When $J = l$, however, S has the two possible values, $S = 0, 1$, and j has the two possible values $j = (l + \frac{1}{2}), (l - \frac{1}{2})$. In this case, the U transformation matrix is a 2×2 matrix. With the simple table of Clebsch–Gordan coefficients of Chapter 28, eqs. (9) or (12) yield

$$U(l\tfrac{1}{2}l\tfrac{1}{2}; jS) = \begin{array}{c} \\ j=(l+\frac{1}{2}) \\ j=(l-\frac{1}{2}) \end{array} \begin{array}{c} \begin{array}{cc} S=0 & S=1 \end{array} \\ \begin{pmatrix} \sqrt{\frac{l+1}{2l+1}} & \sqrt{\frac{l}{2l+1}} \\ -\sqrt{\frac{l}{2l+1}} & \sqrt{\frac{l+1}{2l+1}} \end{pmatrix} \end{array}. \quad (17)$$

C Alternate Forms for the Recoupling Coefficients for Three Angular Momenta

The recoupling coefficients for three commuting angular momentum operators were first introduced by Racah through his W coefficient. The relation between the Racah W coefficient and the unitary U coefficient has been given in eq. (4). Because the Clebsch–Gordan coefficients are subject to $2 \times 3!$ symmetry relations most easily expressed via the 3-j symbol (see Chapter 28) there will of course be similar symmetry relations for the U coefficients. To see the symmetry relations most easily, without factors of $\sqrt{(2J+1)}$ or complicated phase factors, it is useful to introduce the so-called 6-j coefficient or 6-j symbol, conventionally written between curly brackets in two rows,

$$U(j_1 j_2 J j_3; J_{12} J_{23}) = (-1)^{j_1+j_2+j_3+J}\sqrt{(2J_{12}+1)(2J_{23}+1)}\begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{Bmatrix}. \tag{18}$$

The 6-j symbol must satisfy four angular momentum addition triangle relations: The three angular momenta in the first row must satisfy an angular momentum addition triangle relation. Any angular momentum quantum number from the first row satisfies such a triangle relation with two partners from the second row, which must lie in columns different from the column of the symbol in the first row. The 6-j symbol is invariant under the following symmetry transformations:

(1) The 6-j symbol is invariant under any permutation of columns (i.e., six symmetry operations).

(2) The 6-j symbol is invariant under an exchange of the j's in rows 1 and 2 for any two columns:

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = \begin{Bmatrix} d & e & c \\ a & b & f \end{Bmatrix} = \begin{Bmatrix} a & e & f \\ d & b & c \end{Bmatrix} = \begin{Bmatrix} d & b & f \\ a & e & c \end{Bmatrix}. \tag{19}$$

In actual calculations, the unitary form of the recoupling coefficients is often the most useful. In order to make use of its symmetry properties, however, it is clearly advantageous to convert it to 6-j form first. As a simple application of such symmetry properties, let us evaluate the U coefficient in which the quantum number, $J_{23} = 0$, and therefore $J = j_1$, and $j_3 = j_2$. If one of the labels, j_1, j_2, j_3, or J, has the value zero, the U matrix is a 1×1 matrix and the U coefficient has the value $+1$. Therefore,

$$\begin{aligned} U(j_1 j_2 j_1 j_2; J_{12} 0) &= \sqrt{(2J_{12}+1)}(-1)^{2j_1+2j_2}\begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_2 & j_1 & 0 \end{Bmatrix} \\ &= \sqrt{(2J_{12}+1)}(-1)^{2j_1+2j_2}\begin{Bmatrix} J_{12} & j_1 & j_2 \\ 0 & j_2 & j_1 \end{Bmatrix} \\ &= \sqrt{\frac{(2J_{12}+1)}{(2j_1+1)(2j_2+1)}}(-1)^{j_1+j_2-J_{12}}\Big(U(J_{12} j_1 j_2 0; j_2 j_1) = +1\Big). \end{aligned} \tag{20}$$

Therefore,

$$U(j_1 j_2 j_1 j_2; J_{12} 0) = (-1)^{j_1+j_2-J_{12}}\sqrt{\frac{(2J_{12}+1)}{(2j_1+1)(2j_2+1)}}. \tag{21}$$

Similarly,

$$U(j_1 j_1 j_2 j_2; 0 J_{23}) = (-1)^{j_1+j_2-J_{23}}\sqrt{\frac{(2J_{23}+1)}{(2j_1+1)(2j_2+1)}}. \tag{22}$$

D Matrix Element of $(U^k(1) \cdot V^k(2))$ in a Vector-Coupled Basis

To illustrate the usefulness of the recoupling coefficients of Racah type, let us calculate the matrix element of a scalar operator of type

$$(U^k(1) \cdot V^k(2)) = \sum_q (-1)^q U^k_q(1) V^k_{-q}(2) \tag{23}$$

in a $|[j_1 j_2]JM\rangle$ basis, where $U^k_q(1)$ are spherical tensors of rank k built from operators acting in the space of variables of type (1) $\equiv (\vec{r}_1, \vec{\sigma}_1, \ldots)$, similarly for $V^k_{-q}(2)$ and space (2) and where the vectors $|j_1 m_1\rangle$ are angular momentum eigenvectors for the subspace (1), similarly for $|j_2 m_2\rangle$ and space (2). That is, we want to calculate matrix elements of type

$$\langle [j_1' j_2']JM|(U^k(1) \cdot V^k(2))|[j_1 j_2]JM\rangle.$$

These are matrix elements of the type met in Chapter 33. For simplicity, we have left off additional quantum numbers that may be needed for a full specification of the states in question. Expanding the angular momentum coupled states in ket and bra and using the Wigner–Eckart theorem to express the matrix elements of $U^k_q(1)$ and $V^k_{-q}(2)$ in terms of their reduced matrix elements, we have

$$\begin{aligned}&\langle [j_1' j_2']JM|(U^k(1) \cdot V^k(2))|[j_1 j_2]JM\rangle = \\ &\sum_q \sum_{m_1(m_2)} \sum_{m_1'(m_2')} \langle j_1 m_1 j_2 m_2|JM\rangle \langle j_1' m_1' j_2' m_2'|JM\rangle \langle j_1 m_1 kq|j_1' m_1'\rangle \\ &\times \frac{\langle j_1'\|U^k(1)\|j_1\rangle}{\sqrt{(2j_1'+1)}} \langle j_2 m_2 k - q|j_2' m_2'\rangle (-1)^q \frac{\langle j_2'\|V^k(2)\|j_2\rangle}{\sqrt{(2j_2'+1)}}.\end{aligned} \tag{24}$$

Now, let us use a symmetry property of the Clebsch–Gordan coefficients to reexpress

$$\langle j_2 m_2 k - q|j_2' m_2'\rangle = (-1)^{k-q} \sqrt{\frac{(2j_2'+1)}{(2j_2+1)}} \langle kq j_2' m_2'|j_2 m_2\rangle. \tag{25}$$

The above matrix element then can be rewritten as

$$\begin{aligned}&\langle [j_1' j_2']JM|(U^k(1) \cdot V^k(2))|[j_1 j_2]JM\rangle = (-1)^k \frac{\langle j_1'\|U^k(1)\|j_1\rangle \langle j_2'\|V^k(2)\|j_2\rangle}{\sqrt{(2j_1'+1)(2j_2+1)}} \\ &\times \sum_q \sum_{m_1(m_2)} \sum_{m_1'(m_2')} \langle j_1 m_1 kq|j_1' m_1'\rangle \langle j_1' m_1' j_2' m_2'|JM\rangle \\ &\quad \times \langle j_1 m_1 j_2 m_2|JM\rangle \langle kq j_2' m_2'|j_2 m_2\rangle.\end{aligned} \tag{26}$$

Comparing the sum over q, m_1, m_1' of the product of the four Clebsch–Gordan coefficients in the last lines with eq. (9), the identification of the six angular momenta in these Clebsch–Gordan coefficients with those of eq. (9) yields

$$\sum_{q,m_1,m_1'} \langle j_1 m_1 kq|j_1' m_1'\rangle \langle j_1' m_1' j_2' m_2'|JM\rangle \langle j_1 m_1 j_2 m_2|JM\rangle \langle kq j_2' m_2'|j_2 m_2\rangle$$

$$= U(j_1 k J j_2'; j_1' j_2), \tag{27}$$

so

$$\begin{aligned}
&\langle [j_1' j_2'] J M | (U^k(1) \cdot V^k(2)) | [j_1 j_2] J M \rangle \\
&= (-1)^k \frac{\langle j_1' \| U^k(1) \| j_1 \rangle \langle j_2' \| V^k(2) \| j_2 \rangle}{\sqrt{(2j_1'+1)(2j_2+1)}} U(j_1 k J j_2'; j_1' j_2) \\
&= (-1)^{j_1 + j_2' + J} \langle j_1' \| U^k(1) \| j_1 \rangle \langle j_2' \| V^k(2) \| j_2 \rangle \begin{Bmatrix} j_1 & k & j_1' \\ j_2' & J & j_2 \end{Bmatrix}.
\end{aligned} \tag{28}$$

E Recoupling of Four Angular Momenta: 9-j Symbols

In a two-electron configuration of an atom, we may be interested in a transformation from an LS-coupled basis to a jj-coupled basis,

$$|\big[[l_1 l_2] L [s_1 s_2] S\big] J M\rangle \longrightarrow |\big[[l_1 s_1] j_1 [l_2 s_2] j_2\big] J M\rangle.$$

This is a special case (with $s_1 = s_2 = \frac{1}{2}$) of a recoupling of four angular momenta; j_1, j_2, j_3, j_4, if we name $j_1 \equiv l_1$, $j_2 \equiv l_2$, and $j_3 \equiv s_1$, $j_4 \equiv s_2$. We need the transformation from a basis in which J_{12} and J_{34} are good quantum numbers to a basis in which J_{13} and J_{24} are good quantum numbers

$$\begin{aligned}
|\big[[j_1 j_2] J_{12} [j_3 j_4] J_{34}\big] J M\rangle &= \sum_{J_{13} J_{24}} |\big[[j_1 j_3] J_{13} [j_2 j_4] J_{24}\big] J M\rangle \\
&\quad \langle \big[[j_1 j_3] J_{13} [j_2 j_4] J_{24}\big] J M | \big[[j_1 j_2] J_{12} [j_3 j_4] J_{34}\big] J M\rangle \\
= \sum_{J_{13} J_{24}} |\big[[j_1 j_3] J_{13} [j_2 j_4] J_{24}\big] J M\rangle \; & U \begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix}.
\end{aligned} \tag{29}$$

See Fig. 34.3 for a pictorial representation of this relation. The $U(\cdots)$ symbol involving the nine j's is again a unitary transformation matrix, again independent of M; now with row and column indices specified by two quantum numbers each,

$$U \begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix} = U_{J_{12} J_{34}, J_{13} J_{24}}. \tag{30}$$

For example, with $j_1 \equiv l_1 = 1$, $j_2 \equiv l_2 = 2$, and $j_3 \equiv s_1 = \frac{1}{2}$, $j_4 \equiv s_2 = \frac{1}{2}$, and resultant total $J = 1$, this would be a 3×3 transformation matrix, where the row labels $J_{12} J_{34} \equiv LS$ have the three possible values 10, 11, 21, and the column labels $J_{13} J_{24} \equiv jj'$ have the three possible values $\frac{1}{2}\frac{3}{2}$, $\frac{3}{2}\frac{3}{2}$, $\frac{3}{2}\frac{5}{2}$. Because the above matrix is again both unitary and real, we have

$$\left(U^{-1}\right)_{J_{13} J_{24}, J_{12} J_{34}} = U_{J_{12} J_{34}, J_{13} J_{24}}. \tag{31}$$

Therefore, the inverse transformation is given by

$$|\big[[j_1 j_3] J_{13} [j_2 j_4] J_{24}\big] J M\rangle$$

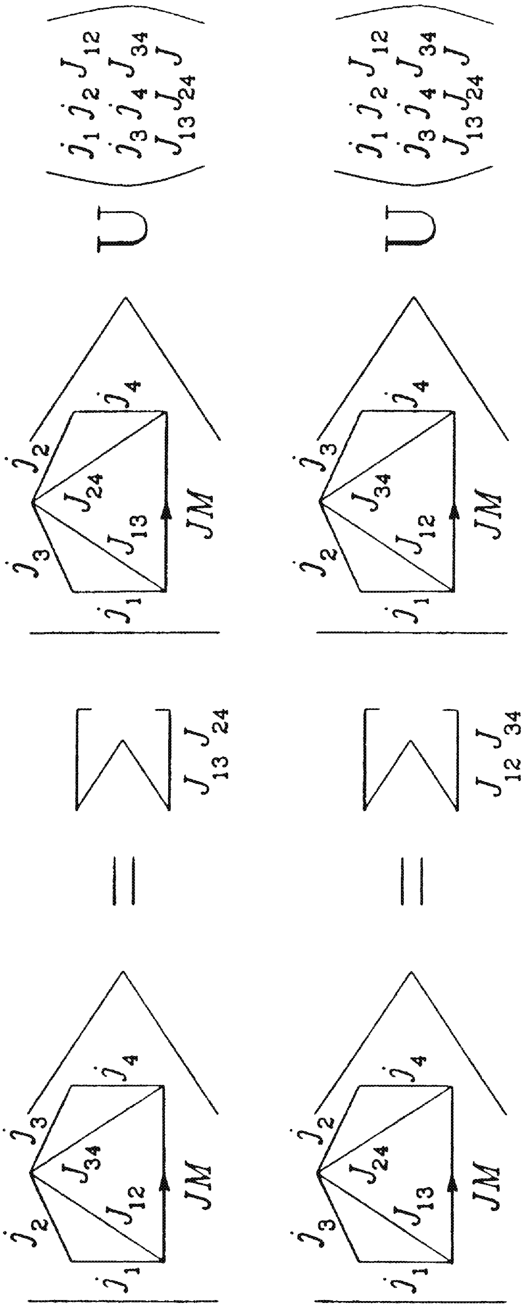

FIGURE 34.3. Recoupling of four angular momenta

$$= \sum_{J_{12}J_{34}} |[[j_1 j_2]J_{12}[j_3 j_4]J_{34}]JM\rangle \; U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix}. \quad (32)$$

See Fig. 34.3(b). In the arrangement of the positions of the nine j's in the $U(\cdots)$ symbol, each row and each column corresponds to a coupling of two angular momenta to a resultant. The 9-j U coefficient can thus be expressed in terms of sums over products of six Clebsch–Gordan coefficients

$$U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix} =$$

$$\sum_{m_i} \langle j_1 m_1 j_2 m_2 | J_{12} M_{12}\rangle \langle j_3 m_3 j_4 m_4 | J_{34} M_{34}\rangle \langle J_{12} M_{12} J_{34} M_{34} | JM\rangle$$
$$\times \langle j_1 m_1 j_3 m_3 | J_{13} M_{13}\rangle \langle j_2 m_2 j_4 m_4 | J_{24} M_{24}\rangle \langle J_{13} M_{13} J_{24} M_{24} | JM\rangle, \quad (33)$$

where the sum is over all m_i, but with $M = m_1 + m_2 + m_3 + m_4$ fixed at a specific value. Clearly, the symmetry properties of the Clebsch–Gordan coefficients will again lead to many symmetry properties of the unitary 9-j transformation coefficients. These will again have their simplest form not in terms of the unitary 9-j transformation coefficients, but in terms of the so-called 9-j symbol, always written in curly brackets, which is defined by

$$U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix}$$
$$= \sqrt{(2J_{12}+1)(2J_{34}+1)(2J_{13}+1)(2J_{24}+1)} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{Bmatrix}. \quad (34)$$

This $\{\cdots\}$ 9-j symbol has the following symmetry properties:

(1) The 9-j symbol is invariant under any even permutation of rows or columns.

(2) The 9-j symbol is invariant under reflection in either diagonal.

(3) The 9-j symbol changes sign by the factor, $(-1)^{j_1+j_2+j_3+j_4+J_{12}+J_{34}+J_{13}+J_{24}+J}$, involving all nine j's, under any odd permutation of rows or columns.

The 9-j transformation coefficients can be expressed in terms of products of 6-j U coefficients. For example,

$$|[[j_1 j_2]J_{12}[j_3 j_4]J_{34}]JM\rangle$$
$$= \sum_{J_{234}} |[j_1[j_2[j_3 j_4]J_{34}]J_{234}]JM\rangle U(j_1 j_2 J J_{34}; J_{12} J_{234})$$
$$= \sum_{J_{234}} (-1)^{j_3+j_4-J_{34}} |[j_1[j_2[j_4 j_3]J_{34}]J_{234}]JM\rangle U(j_1 j_2 J J_{34}; J_{12} J_{234})$$
$$= \sum_{J_{234}} \sum_{J_{24}} (-1)^{j_3+j_4-J_{34}} |[j_1[[j_2 j_4]J_{24} j_3]J_{234}]JM\rangle$$
$$\times U(j_2 j_4 J_{234} j_3; J_{24} J_{34}) U(j_1 j_2 J J_{34}; J_{12} J_{234})$$
$$= \sum_{J_{234}} \sum_{J_{24}} (-1)^{j_3+j_4-J_{34}} (-1)^{j_3+J_{24}-J_{234}} |[j_1[j_3[j_2 j_4]J_{24}]J_{234}]JM\rangle$$
$$\times U(j_2 j_4 J_{234} j_3 : J_{24} J_{34}) U(j_1 j_2 J J_{34}; J_{12} J_{234})$$

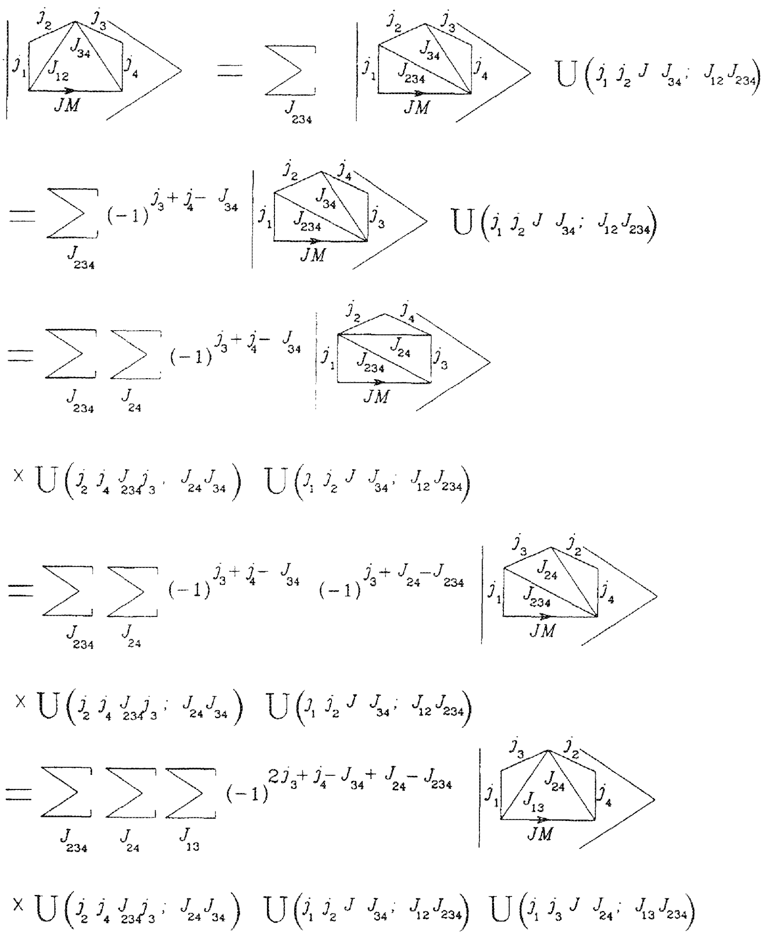

FIGURE 34.4. Pictorial version of eq. (35).

$$
\begin{aligned}
&= \sum_{J_{234}}\sum_{J_{24}}\sum_{J_{13}} (-1)^{2j_3+j_4-J_{34}-J_{234}+J_{24}} |[[j_1 j_3]J_{13}[j_2 j_4]J_{24}]JM\rangle \\
&\quad \times U(j_2 j_4 J_{234} j_3; J_{24} J_{34}) U(j_1 j_2 J J_{34}; J_{12} J_{234}) U(j_1 j_3 J J_{24}; J_{13} J_{234}) \\
&= \sum_{J_{13}, J_{24}} |[[j_1 j_3]J_{13}[j_2 j_4]J_{24}]JM\rangle \; U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix}. \qquad (35)
\end{aligned}
$$

The various steps in this relation are easier to follow in a pictorial representation. See Fig. 34.4. Comparing the last two lines of this relation, we get

$$
U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix} =
$$

$$\sum_{J_{234}}(-1)^{2j_3+j_4-J_{34}-J_{234}+J_{24}}U(j_2j_4J_{234}j_3:J_{24}J_{34})$$
$$\times U(j_1j_2JJ_{34};J_{12}J_{234})U(j_1j_3JJ_{24};J_{13}J_{234})$$
$$=\sum_{J_{234}}(-1)^{2J_{234}}(2J_{234}+1)\sqrt{(2J_{12}+1)(2J_{34}+1)(2J_{13}+1)(2J_{24}+1)}$$
$$\times\begin{Bmatrix} j_2 & j_4 & J_{24} \\ j_3 & J_{234} & J_{34}\end{Bmatrix}\begin{Bmatrix} j_1 & j_2 & J_{12} \\ J_{34} & J & J_{234}\end{Bmatrix}\begin{Bmatrix} j_1 & j_3 & J_{13} \\ J_{24} & J & J_{234}\end{Bmatrix}. \quad (36)$$

This relation is particularly useful if one of the angular momenta has the value zero. For example, if $j_2 = 0$. Then, with $J_{24} = j_4$ and $J_{234} = J_{34}$, we have $U(0j_4J_{34}j_3; j_4J_{34}) = +1$ and with $J_{12} = j_1$ and again $J_{234} = J_{34}$, we have $U(j_10JJ_{34}; j_1J_{34}) = +1$. The above relation collapses to

$$U\begin{pmatrix} j_1 & 0 & j_1 \\ j_3 & j_4 & J_{34} \\ J_{13} & j_4 & J\end{pmatrix} = U(j_1j_3Jj_4; J_{13}J_{34}). \quad (37)$$

This relation can also be seen directly from the pictorial representation of Fig. 34.5, from which we see the triangle, coupling j_1 with 0 to resultant j_1, rides along on the back of a single Racah type of recoupling transformation involving the recoupling of j_1, j_3, and j_4. Similarly, we have

$$U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & 0 & j_3 \\ J_{13} & j_2 & J\end{pmatrix} = (-1)^{j_1+J-J_{12}-J_{13}}U(j_2j_1Jj_3; J_{12}J_{13}). \quad (38)$$

See also Fig. 34.6.

F Matrix Element of a Coupled Tensor Operator, $[U^{k_1}(1) \times V^{k_2}(2)]^k_q$ in a Vector-Coupled Basis

To appreciate how the 9-j transformation coefficient can facilitate calculations in an angular momentum coupled basis, let us calculate the matrix element of a vector-coupled tensor operator,

$$[U^{k_1}(1) \times V^{k_2}(2)]^k_q = \sum_{q_1(q_2)}\langle k_1q_1k_2q_2|kq\rangle U^{k_1}_{q_1}(1)V^{k_2}_{q_2}(2), \quad (39)$$

in a $|[j_1j_2]JM\rangle$ basis, where again, the $U^{k_1}_{q_1}(1)$ are spherical tensors of rank k_1 acting on variables of type (1) and where the $|j_1m_1\rangle$ are angular momentum eigenvectors of the space (1), similarly for $V^{k_2}_{q_2}(2)$ and the $|j_2m_2\rangle$ and space (2). The needed matrix element can be expressed in terms of a reduced matrix element via the Wigner–Eckart theorem and can be expanded in terms of Clebsch–Gordan coefficients via

$$\langle[j'_1j'_2]J'M'|[U^{k_1}(1) \times V^{k_2}(2)]^k_q|[j_1j_2]JM\rangle$$
$$= \langle JMkq|J'M'\rangle\frac{\langle[j'_1j'_2]J'\|[U^{k_1}(1) \times V^{k_2}(2)]^k\|[j_1j_2]J\rangle}{\sqrt{(2J'+1)}}$$

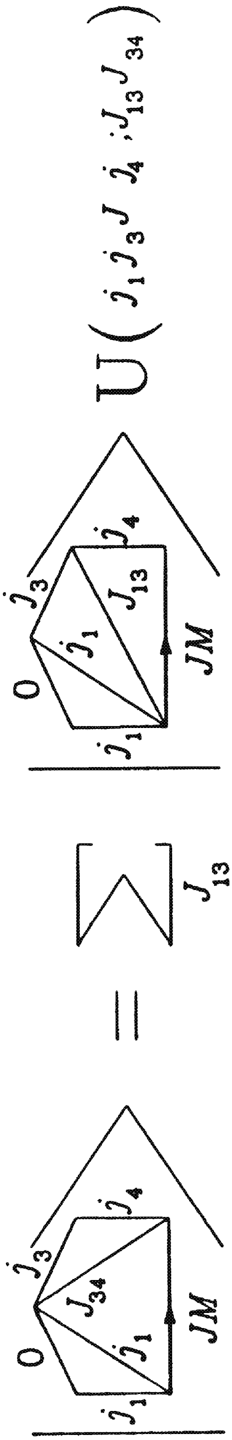

FIGURE 34.5. Pictorial version of Eq. (37).

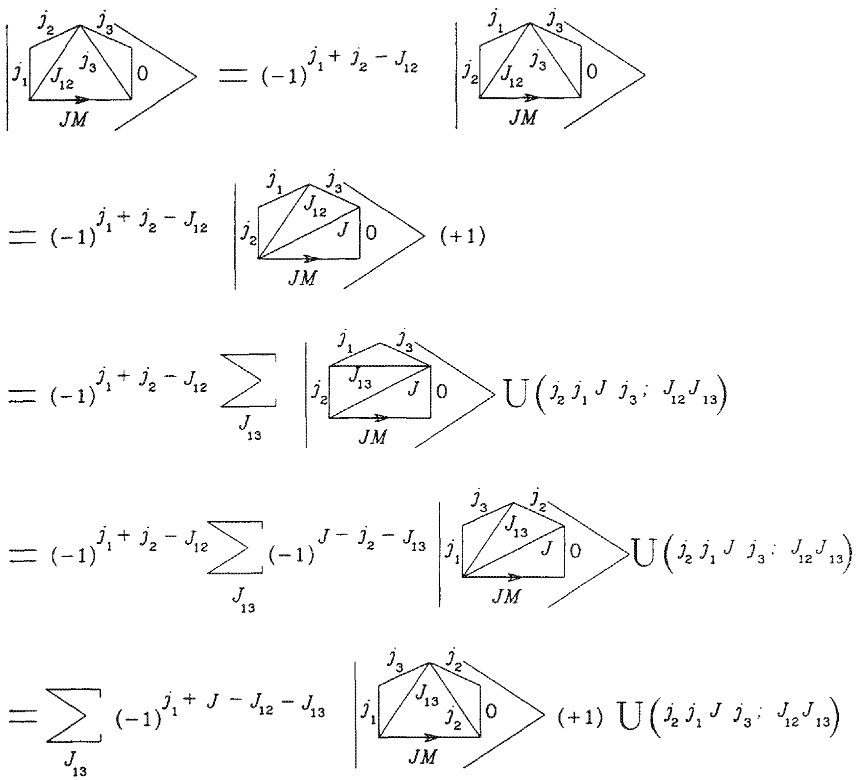

FIGURE 34.6. Pictorial version of eq. (38).

$$= \sum_{m_1 m_1' q_1} \langle j_1 m_1 j_2 m_2 | JM \rangle \langle j_1' m_1' j_2' m_2' | J'M' \rangle \langle k_1 q_1 k_2 q_2 | kq \rangle$$

$$\times \langle j_1 m_1 k_1 q_1 | j_1' m_1' \rangle \frac{\langle j_1' \| U^{k_1} \| j_1 \rangle}{\sqrt{(2j_1'+1)}} \langle j_2 m_2 k_2 q_2 | j_2' m_2' \rangle \frac{\langle j_2' \| V^{k_2} \| j_2 \rangle}{\sqrt{(2j_2'+1)}}, \quad (40)$$

where the magnetic quantum numbers, M, q, and M' are fixed at specific values. If we multiply this equation by $\langle JMkq | J'M' \rangle$, and, keeping M' fixed, sum over all possible values of M and $q = (M' - M)$, the orthogonality relation,

$$\sum_{M,(q)} \langle JMkq | J'M' \rangle^2 = 1,$$

will pick out the reduced matrix element for our coupled tensor operator

$$\frac{\langle [j_1' j_2'] J' \| [U^{k_1}(1) \times V^{k_2}(2)]^k \| [j_1 j_2] J \rangle}{\sqrt{(2J'+1)}}$$
$$= \frac{\langle j_1' \| U^{k_1} \| j_1 \rangle}{\sqrt{(2j_1'+1)}} \frac{\langle j_2' \| V^{k_2} \| j_2 \rangle}{\sqrt{(2j_2'+1)}}$$

$$\times \sum_{m_1,m'_1 q_1 \cdot q_2} \sum \langle j_1 m_1 j_2 m_2 | JM \rangle \langle j'_1 m'_1 j'_2 m'_2 | J'M' \rangle \langle k_1 q_1 k_2 q_2 | kq \rangle$$
$$\times \langle j_1 m_1 k_1 q_1 | j'_1 m'_1 \rangle \langle j_2 m_2 k_2 q_2 | j'_2 m'_2 \rangle \langle JMkq | J'M' \rangle. \qquad (41)$$

The m sums over the product of the six Clebsch–Gordan coefficients is over all m's except that $M' = m_1 + m_2 + q_1 + q_2$ is fixed. This is precisely the m sum of eq. (33) which yields a single unitary 9-j transformation coefficient. Thus,

$$\frac{\langle [j'_1 j'_2] J' \| [U^{k_1}(1) \times V^{k_2}(2)]^k \| [j_1 j_2] J \rangle}{\sqrt{(2J'+1)}}$$
$$= \frac{\langle j'_1 \| U^{k_1} \| j_1 \rangle}{\sqrt{(2j'_1+1)}} \frac{\langle j'_2 \| V^{k_2} \| j_2 \rangle}{\sqrt{(2j'_2+1)}} U \begin{pmatrix} j_1 & j_2 & J \\ k_1 & k_2 & k \\ j'_1 & j'_2 & J' \end{pmatrix}. \qquad (42)$$

This "grand result" illustrates the full power of the angular momentum recoupling theory and shows how the 9-j transformation coefficients can be put to good use. In special cases, the 9-j transformation coefficients will collapse to a 6-j U coefficient. For example, if the tensor operator acts only in the subspace of type (1), then $V^{k_2}_{q_2} \to 1$, and we can set $k_2 = 0$. Eq. (38) then tells us

$$\frac{\langle [j'_1 j'_2] J' \| U^{k_1}(1) \| [j_1 j_2] J \rangle}{\sqrt{(2J'+1)}}$$
$$= \frac{\langle j'_1 \| U^{k_1} \| j_1 \rangle}{\sqrt{(2j'_1+1)}} (-1)^{j_1 + J' - J - j'_1} U(j_2 j_1 J' k_1; J j'_1), \qquad (43)$$

where we have also used

$$\langle j'_2 \| 1 \| j_2 \rangle = \delta_{j_2 j'_2} \sqrt{(2j'_2 + 1)}.$$

An example of this would be the matrix element of an electric dipole moment operator, which is independent of spin variables, in an $|[ls]jm_j\rangle$ basis

$$\frac{\langle [l's]j' \| \vec{\mu}^{(\text{el.})} \| [ls]j \rangle}{\sqrt{(2j'+1)}} = \frac{\langle l' \| \vec{\mu}^{(\text{el.})} \| l \rangle}{\sqrt{(2l'+1)}} (-1)^{l-l'+j'-j} U(\tfrac{1}{2} l j' 1; j l'). \qquad (44)$$

Another special case would be the case of a scalar operator, with $k = 0$, hence $k_2 = k_1$, and $J' = J$. We leave it as an exercise in the symmetry properties of the 9-j symbol to show our general result of eq. (42) then collapses to the result already derived in eq. (28). Recall $(U^k \cdot V^k) = (-1)^k [(2k+1)]^{\frac{1}{2}} [U^k \times V^k]^0_0$.

Although tabulations of 9-j symbols are not readily available, computer codes are easy to construct. For tabulations of 6-j symbols, see the references to tabulations at the end of Chapter 28. For algebraic expressions for 6-j symbols with at least one $j \leq 2$, see the references at the end of Chapter 28.

G An Application: The Nuclear Hyperfine Interaction in a One-Electron Atom Revisited

In Chapter 33, we calculated the nuclear hyperfine interaction in a one-electron atom with the use of a few Wigner coefficients by making judicious use of the Wigner–Eckart theorem. In particular, we calculated the nuclear hyperfine splitting of a one-electron $p_{3/2}$ state, where our nucleus had a nuclear spin $I = \frac{1}{2}$ as in hydrogen, and we also quoted the result for the partner $p_{1/2}$ state. We can now repeat this calculation in a much more general way by making full use of the angular momentum recoupling machinery of this addendum.

The nuclear hyperfine interaction for a hydrogenic s-state, with $l = 0$, was given in Chapter 33 as

$$H_{\text{h.f.int}} = \frac{mc^2\alpha^4}{2}\frac{m}{M}g_I\frac{8\pi}{3}(\vec{s}\cdot\vec{I})\delta(\vec{r}). \tag{45}$$

For a hydrogenic state with $l \neq 0$, conversely, it was shown to be

$$H_{\text{h.f.int}} = \frac{mc^2\alpha^4}{2}\frac{m}{M}g_I\left[\frac{1}{r^3}\left((\vec{l}\cdot\vec{I}) - \sqrt{8\pi}([Y^2\times s^1]^1\cdot I^1)\right)\right], \tag{46}$$

[see eqs. (5) and (14) of Chapter 33]. If we define the needed hydrogenic integrals via

$$\begin{aligned}
\beta'_{\text{h.f.s.}}(l=0) &= \frac{mc^2\alpha^4}{2}\frac{m}{M}g_I\int d\vec{r}|\psi(\vec{r})_{n00}|^2\frac{8\pi}{3}\delta(\vec{r}) = \frac{mc^2\alpha^4}{2}\frac{m}{M}g_I\frac{2}{3}|R_{n0}(0)|^2,\\
\beta_{\text{h.f.s.}}(l\neq 0) &= \frac{mc^2\alpha^4}{2}\frac{m}{M}g_I\int_0^\infty drr^2|R_{nl}(r)|^2\frac{1}{r^3},
\end{aligned} \tag{47}$$

then we have an effective hyperfine interaction Hamiltonian that can be written

$$\begin{aligned}
H_{\text{h.f.int}} &= \beta_{\text{h.f.s.}}\left[(\vec{l}\cdot\vec{I}) - \sqrt{8\pi}([Y^2\times s^1]^1\cdot I^1)\right], \qquad \text{for } l\neq 0;\\
H_{\text{h.f.int}} &= \beta'_{\text{h.f.s.}}(\vec{s}\cdot\vec{I}), \qquad \text{for } l = 0.
\end{aligned} \tag{48}$$

All terms in these electron-nuclear spin interactions are of the form $(U^{k=1}(1)\cdot V^{k=1}(2))$, where the space (1) is that of the electron and includes both electron orbital and electron spin variables, whereas the space (2) is that of the nuclear intrinsic variables characterized by the nuclear spin vector, $\vec{I}$. We will of course need the coupling scheme $\vec{l}+\vec{s} = \vec{j}$ for the electron variables, and we will assume the fine structure splitting is much greater than the hyperfine structure splitting, so j is a good quantum number. Finally, we will couple electron $\vec{j}$ with the nuclear spin, $\vec{I}$, to resultant total angular momentum, $\vec{F}$: $\vec{j}+\vec{I} = \vec{F}$. All of the needed matrix elements are then given in terms of electron reduced matrix elements, the nuclear spin reduced matrix element, and a single 6-j symbol by formula (28) of this chapter. For example,

$$\langle[[ls]jI]FM_F|(\vec{l}\cdot\vec{I})|[[ls]jI]FM_F\rangle$$

$$= (-1)^{j+I+F}\langle [ls]j\|\vec{l}\|[ls]j\rangle\langle I\|\vec{I}\|I\rangle \begin{Bmatrix} j & 1 & j \\ I & F & I \end{Bmatrix}, \tag{49}$$

with similar expressions for matrix elements of the operators $(\vec{s}\cdot\vec{I})$ and $([Y^2\times s^1]^1\cdot\vec{I})$. The reduced matrix elements of the electronic operators, $\vec{l}$, $\vec{s}$, and $[Y^2\times s^1]^1_q$ in the $|[ls]jm_j\rangle$ basis of the $\vec{l}+\vec{s}=\vec{j}$-coupled scheme are all given through formula (42) of this chapter. For example,

$$\frac{\langle [ls]j\|\vec{s}\|[ls]j\rangle}{\sqrt{(2j+1)}} = \frac{\langle l\|1\|l\rangle}{\sqrt{(2l+1)}}\frac{\langle s\|\vec{s}\|s\rangle}{\sqrt{(2s+1)}}\, U\begin{pmatrix} l & \frac{1}{2} & j \\ 0 & 1 & 1 \\ l & \frac{1}{2} & j \end{pmatrix}. \tag{50}$$

Because we are interested in the reduced matrix element of $\vec{s}$ mainly for states with orbital angular momentum, $l=0$, the needed unitary 9-j coefficient, with all zeros in the first column, corresponds to a 1×1 unitary transformation and thus has the value, $+1$. The reduced matrix elements for the unit operator and the angular momentum vector operator are given for any angular momentum basis by eqs. (4) and (7) of Chapter 32. Thus,

$$\langle l\|1\|l\rangle = \sqrt{(2l+1)}, \qquad \langle s\|\vec{s}\|s\rangle = \sqrt{(2s+1)s(s+1)} = \sqrt{\tfrac{3}{2}};$$

so, with $[ls]j = [0\frac{1}{2}]\frac{1}{2}$

$$\langle [0\tfrac{1}{2}]\tfrac{1}{2}\|\vec{s}\|[0\tfrac{1}{2}]\tfrac{1}{2}\rangle = \sqrt{\tfrac{3}{2}}.$$

Similarly,

$$\frac{\langle [ls]j\|\vec{l}\|[ls]j\rangle}{\sqrt{(2j+1)}} = \frac{\langle l\|\vec{l}\|l\rangle}{\sqrt{(2l+1)}}\frac{\langle s\|1\|s\rangle}{\sqrt{(2s+1)}}\, U\begin{pmatrix} l & \frac{1}{2} & j \\ 1 & 0 & 1 \\ l & \frac{1}{2} & j \end{pmatrix}$$
$$= \sqrt{l(l+1)}U(\tfrac{1}{2}lj1; jl), \tag{51}$$

where we have used eq. (38) to convert the unitary 9-j coefficient with one zero to a unitary Racah coefficient. This can be read from tables of 6-j symbols. For $l=1$, this U coefficient has the values: $\sqrt{\frac{5}{6}}$ for $j=\frac{3}{2}$, and $\sqrt{\frac{2}{3}}$ for $j=\frac{1}{2}$. Therefore,

$$\langle [1\tfrac{1}{2}]\tfrac{3}{2}\|\vec{l}\|[1\tfrac{1}{2}]\tfrac{3}{2}\rangle = 2\sqrt{\tfrac{5}{3}}; \qquad \langle [1\tfrac{1}{2}]\tfrac{1}{2}\|\vec{l}\|[1\tfrac{1}{2}]\tfrac{1}{2}\rangle = 2\sqrt{\tfrac{2}{3}}.$$

Finally,

$$\langle [ls]j\|[Y^2\times s^1]^1\|[ls]j\rangle = \sqrt{(2j+1)}\frac{\langle l\|Y^2\|l\rangle}{\sqrt{(2l+1)}}\frac{\langle \frac{1}{2}\|\vec{s}\|\frac{1}{2}\rangle}{\sqrt{2}}\, U\begin{pmatrix} l & \frac{1}{2} & j \\ 2 & 1 & 1 \\ l & \frac{1}{2} & j \end{pmatrix}, \tag{52}$$

where the reduced matrix element of Y^2 was given in Chapter 32. It has the value

$$\frac{\langle l\|Y^2\|l\rangle}{\sqrt{(2l+1)}} = \sqrt{\frac{5}{4\pi}}\langle l020|l0\rangle = -\frac{1}{\sqrt{2\pi}} \quad \text{for } l=1.$$

The unitary 9-j coefficients above can be given in terms of 6-j symbols through eq. (36). For $l=1$, and both $j=\frac{3}{2}$ and $j=\frac{1}{2}$, the sum over J_{234} in this relation collapses to a single term: J_{234} has the unique value $\frac{3}{2}$. The above 9-j U coefficients have the values $-1/(3\sqrt{5})$ and $+(2/3)$ for $j=\frac{3}{2}$ and $j=\frac{1}{2}$, respectively. Thus,

$$\langle[1\tfrac{1}{2}]\tfrac{3}{2}\|[Y^2\times s^1]^1\|[1\tfrac{1}{2}]\tfrac{3}{2}\rangle = \frac{1}{\sqrt{30\pi}}, \qquad \langle[1\tfrac{1}{2}]\tfrac{1}{2}\|[Y^2\times s^1]^1\|[1\tfrac{1}{2}]\tfrac{1}{2}\rangle = -\frac{1}{\sqrt{3\pi}}.$$

With these electron reduced matrix elements, together with the nuclear spin reduced matrix element,

$$\langle I\|\vec{I}\|I\rangle = \sqrt{(2I+1)I(I+1)}, \tag{53}$$

the nuclear hyperfine interaction in a one-electron atom is then given by, first for the case $l\neq 0$,

$$\begin{aligned}\langle[[ls]jI]FM_F|H_{\text{h.f.int.}}|[[ls]jI]FM_F\rangle &= \beta_{\text{h.f.s.}}\sqrt{(2I+1)I(I+1)}\\ &\times\Big[\langle[ls]j\|\vec{l}\|[ls]j\rangle-\sqrt{8\pi}\langle[ls]j\|[Y^2\times s^1]^1\|[ls]j\rangle\Big]\\ &\times(-1)^{j+I+F}\begin{Bmatrix} j & 1 & j\\ I & F & I\end{Bmatrix},\end{aligned} \tag{54}$$

and for the case, $l=0$, with $j=\frac{1}{2}$,

$$\begin{aligned}\langle[[ls]jI]FM_F|H_{\text{h.f.int.}}|[[ls]jI]FM_F\rangle &= \beta'_{\text{h.f.s.}}\sqrt{(2I+1)I(I+1)}\\ &\times\langle[ls]j\|\vec{s}\|[ls]j\rangle(-1)^{j+I+F}\begin{Bmatrix} j & 1 & j\\ I & F & I\end{Bmatrix}.\end{aligned} \tag{55}$$

For the cases, $l=1$ and $l=0$, with $I=\frac{1}{2}$, we will need the 6-j symbols

$$\begin{Bmatrix} \frac{3}{2} & 1 & \frac{3}{2}\\ \frac{1}{2} & 2 & \frac{1}{2}\end{Bmatrix} = \frac{1}{2\sqrt{10}}, \qquad \begin{Bmatrix} \frac{3}{2} & 1 & \frac{3}{2}\\ \frac{1}{2} & 1 & \frac{1}{2}\end{Bmatrix} = \frac{\sqrt{5}}{6\sqrt{2}},$$

$$\begin{Bmatrix} \frac{1}{2} & 1 & \frac{1}{2}\\ \frac{1}{2} & 1 & \frac{1}{2}\end{Bmatrix} = \frac{1}{6}, \qquad \begin{Bmatrix} \frac{1}{2} & 1 & \frac{1}{2}\\ \frac{1}{2} & 0 & \frac{1}{2}\end{Bmatrix} = \frac{1}{2},$$

so, with $l=1$, and both $I=\frac{1}{2}$ and $s=\frac{1}{2}$,

$$\begin{aligned}\langle[[1s]jI]FM_F|H_{\text{h.f.int.}}|[[1s]jI]FM_F\rangle &= +\tfrac{2}{5}\beta_{\text{h.f.s.}} \quad \text{for } j=\tfrac{3}{2},\quad F=2,\\ \langle[[1s]jI]FM_F|H_{\text{h.f.int.}}|[[1s]jI]FM_F\rangle &= -\tfrac{2}{3}\beta_{\text{h.f.s.}} \quad \text{for } j=\tfrac{3}{2},\quad F=1,\\ \langle[[1s]jI]FM_F|H_{\text{h.f.int.}}|[[1s]jI]FM_F\rangle &= +\tfrac{2}{3}\beta_{\text{h.f.s.}} \quad \text{for } j=\tfrac{1}{2},\quad F=1,\\ \langle[[1s]jI]FM_F|H_{\text{h.f.int.}}|[[1s]jI]FM_F\rangle &= -2\beta_{\text{h.f.s.}} \quad \text{for } j=\tfrac{1}{2},\quad F=0,\end{aligned} \tag{56}$$

and for $l=0$ states,

$$\begin{aligned}\langle[[0s]sI]FM_F|H_{\text{h.f.int.}}|[[0s]sI]FM_F\rangle &= +\tfrac{1}{4}\beta'_{\text{h.f.s.}}, \qquad \text{for } F=1,\\ \langle[[0s]sI]FM_F|H_{\text{h.f.int.}}|[[0s]sI]FM_F\rangle &= -\tfrac{3}{4}\beta'_{\text{h.f.s.}}, \qquad \text{for } F=0.\end{aligned} \tag{57}$$