

# A Vector Addition Coefficients of Angular Momenta

In the following, we will give an overview of the vector addition coefficients and their properties together with a variety of contraction and orthogonality relations most frequently used in angular momentum coupling theory. Concerning a more complete description and introduction to the theory of angular momentum coupling we refer to the books by Brink and Satchler (1962); Edmonds (1974) or Zare (1988). For a more extensive compendium of angular momentum coupling equations and relations we refer to the book by Varshalovich *et al.* (1988).

The vector addition coefficients have been numerically calculated and a variety of tables for the Clebsch–Gordan and the  $nj$ -symbols exist. We only mention the extended tables by Rotenberg *et al.* (1959) and Varshalovich *et al.* (1988).

## A.1 Clebsch–Gordan Coefficients and $3j$ -Symbols

The Clebsch–Gordan coefficients, or vector addition coefficients, are defined by the unitary transformation of the coupling of two angular momenta

$$|(ab)c\gamma\rangle = \sum_{\alpha\beta} |a\alpha, b\beta\rangle (a\alpha, b\beta|c\gamma), \quad (\text{A.1})$$

and vanish unless the selection rule

$$\alpha + \beta = \gamma, \quad (\text{A.2})$$

and the triangular condition

$$|a - b| \leq c \leq a + b \quad (\text{A.3})$$

are fulfilled.

The Clebsch–Gordan coefficients are real quantities

$$(a\alpha, b\beta|c\gamma)^* = (a\alpha, b\beta|c\gamma), \quad (\text{A.4})$$

which yields the inverse transformation

$$|a\alpha, b\beta\rangle = \sum_{c\gamma} |(ab)c\gamma\rangle (a\alpha, b\beta|c\gamma). \quad (\text{A.5})$$

Symmetry properties:

$$(a\alpha, b\beta|c\gamma) = (-1)^{a+b-c} (a - \alpha, b - \beta|c - \gamma), \quad (\text{A.6a})$$

$$= (-1)^{a+b-c} (b\beta, a\alpha|c\gamma), \quad (\text{A.6b})$$

$$= \sqrt{\frac{2c+1}{2b+1}} (-1)^{a-\alpha} (a\alpha, c - \gamma|b - \beta), \quad (\text{A.6c})$$

$$= \sqrt{\frac{2c+1}{2a+1}} (-1)^{b+\beta} (c - \gamma, b\beta|a - \alpha). \quad (\text{A.6d})$$

Special cases:

$$(a\alpha, b\beta|00) = \frac{(-1)^{a-\alpha}}{\sqrt{2a+1}} \delta_{ab} \delta_{\alpha-\beta}, \quad (\text{A.7a})$$

$$(a\alpha, 00|c\gamma) = \delta_{ac} \delta_{\alpha\gamma}. \quad (\text{A.7b})$$

If  $c$  and  $\gamma$  take their maximum values, we have:

$$(aa, bb|a + b \ a + b) = 1 \quad (\text{A.7c})$$

The orthonormality of  $|a\alpha, b\beta\rangle$  and  $|(ab)c\gamma\rangle$  yields the orthogonality relations:

$$\sum_{c\gamma} (a\alpha', b\beta'|c\gamma) (a\alpha, b\beta|c\gamma) = \delta_{\alpha'\alpha} \delta_{\beta'\beta}, \quad (\text{A.8a})$$

$$\sum_{\alpha\beta} (a\alpha, b\beta|c'\gamma') (a\alpha, b\beta|c\gamma) = \delta_{c'c} \delta_{\gamma'\gamma}. \quad (\text{A.8b})$$

The Wigner  $3j$ -symbols are defined as

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = \frac{(-1)^{a-b-\gamma}}{\sqrt{2c+1}} (a\alpha, b\beta|c - \gamma). \quad (\text{A.9})$$

Note the appearance of  $-\gamma$  on the right, so that now the selection rule

$$\alpha + \beta + \gamma = 0, \quad (\text{A.10})$$

must be fulfilled.

The  $3j$ -symbol is invariant under cyclic permutations of its columns and is multiplied by  $(-1)^{a+b+c}$  by non-cyclic ones, and by changing the signs of its magnetic components  $\alpha, \beta, \gamma$ . In particular:

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = \begin{pmatrix} b & c & a \\ \beta & \gamma & \alpha \end{pmatrix} = \begin{pmatrix} c & a & b \\ \gamma & \alpha & \beta \end{pmatrix}, \quad (\text{A.11a})$$

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{a+b+c} \begin{pmatrix} b & a & c \\ \beta & \alpha & \gamma \end{pmatrix}, \quad (\text{A.11b})$$

$$= (-1)^{a+b+c} \begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix}. \quad (\text{A.11c})$$

Special cases:

$$\begin{pmatrix} a & b & 0 \\ \alpha & \beta & 0 \end{pmatrix} = \frac{(-1)^{a-\alpha}}{\sqrt{2a+1}} \delta_{ab} \delta_{\alpha-\beta}. \quad (\text{A.12a})$$

If  $\alpha = \beta = \gamma = 0$ , and  $a + b + c$  is odd, we have

$$\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} = 0, \quad (\text{A.12b})$$

and if  $2p \equiv a + b + c$  is even, we have

$$\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} = (-1)^p \sqrt{\Delta(abc)} \frac{p!}{(p-a)!(p-b)!(p-c)!}, \quad (\text{A.12c})$$

where

$$\Delta(abc) \equiv \frac{(a+b-c)!(b+c-a)!(c+a-b)!}{(a+b+c+1)!}. \quad (\text{A.12d})$$

If the arguments of  $\beta$  and  $\gamma$  change by 1 an important relation is

$$\begin{pmatrix} a & b & c \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} = \frac{-1}{2} \begin{pmatrix} a & b & c \\ \frac{1}{2} & \frac{-1}{2} & 0 \end{pmatrix} \frac{(2b+1) + (-1)^{a+b-c}(2a+1)}{\sqrt{c(c+1)}}. \quad (\text{A.13})$$

Orthogonality relations:

$$\sum_{\alpha\beta} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} a & b & c' \\ \alpha & \beta & \gamma' \end{pmatrix} = \frac{1}{2c+1} \delta_{cc'} \delta_{\gamma\gamma'}, \quad (\text{A.14a})$$

$$\sum_{c\gamma} (2c+1) \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} = \delta_{\alpha\alpha'} \delta_{\beta\beta'}. \quad (\text{A.14b})$$

## A.2 Racah Coefficients and 6j-Symbols

The coupling of three angular momenta,  $|m m' m''\rangle \equiv |jm\rangle |j'm'\rangle |j''m''\rangle$ , allows for the generation of two usually different basis sets in the related Hilbert sub-space

$$|(j' j) g', j''; J' M'\rangle = \sum_{\substack{m m' \\ m'' \mu'}} |m m' m''\rangle (j' m', j m | g' \mu') (g' \mu', j'' m'' | J M), \quad (\text{A.15a})$$

or

$$|j', (j j'') g''; J M\rangle = \sum_{\substack{m m' \\ m'' \mu''}} |m m' m''\rangle (j m, j'' m'' | g'' \mu'') (j' m', g'' \mu'' | J M). \quad (\text{A.15b})$$

The  $6j$ -symbols are defined by the unitary transformation between the two basis sets

$$\begin{aligned} \langle j', (jj'')g''; JM | (j'j)g', j''; J'M' \rangle &= \delta_{JJ'} \delta_{MM'} (-1)^{j+j'+j''+J} \\ &\times \sqrt{(2g'+1)(2g''+1)} \left\{ \begin{matrix} j' & j & g' \\ j'' & J & g'' \end{matrix} \right\}, \end{aligned} \quad (\text{A.16})$$

that is, we have

$$\begin{aligned} |(j'j)g', j''; JM \rangle &= \sum_{g''} |j', (jj'')g''; JM \rangle \sqrt{(2g'+1)(2g''+1)} \\ &\times (-1)^{j+j'+j''+J} \left\{ \begin{matrix} j' & j & g' \\ j'' & J & g'' \end{matrix} \right\}. \end{aligned} \quad (\text{A.17})$$

The  $6j$ -symbols are related to the Racah, or  $W$ -coefficients via

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} = (-1)^{a+b+d+e} W(abed; cf). \quad (\text{A.18})$$

Triangular conditions: the  $6j$ -symbol is non-zero only, if the four triangular conditions are fulfilled by the six angular momenta which may be illustrated in the following way

$$\left\{ \begin{matrix} \circ & & \\ & \backslash & / \\ & \circ - \circ & \end{matrix} \right\}, \left\{ \begin{matrix} \circ - \circ - \circ & & \\ & & \end{matrix} \right\}, \left\{ \begin{matrix} & & \circ \\ \circ - \circ & / & \\ & & \end{matrix} \right\}, \left\{ \begin{matrix} & \circ & \\ / & & \backslash \\ \circ & & \circ \end{matrix} \right\}. \quad (\text{A.19})$$

Particularly, the sum of its arguments must be integer

$$a + b + c + d + e + f = n, \quad \text{where } n \in \mathbb{N}. \quad (\text{A.20})$$

Symmetries: the  $6j$ -symbol is invariant under any permutation of its columns, and also for interchanging of the upper and lower arguments in each of any two columns, resulting in symmetry relations between 24 different  $6j$ -symbols, i.e.

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} = \left\{ \begin{matrix} a & c & b \\ d & f & e \end{matrix} \right\} = \left\{ \begin{matrix} b & a & c \\ e & d & f \end{matrix} \right\} = \left\{ \begin{matrix} a & e & f \\ d & b & c \end{matrix} \right\} = \left\{ \begin{matrix} d & c & e \\ a & f & b \end{matrix} \right\}, \quad \text{etc.} \quad (\text{A.21})$$

Special value:

$$\left\{ \begin{matrix} a & b & 0 \\ c & d & f \end{matrix} \right\} = (-1)^{a+c+f} \frac{\delta_{ab} \delta_{cd}}{\sqrt{(2a+1)(2c+1)}}. \quad (\text{A.22})$$

Contraction of  $3j$ -symbols: according to the definition (A.16) the  $6j$ -symbols may be expressed in terms of four  $3j$ -symbols

$$\begin{aligned} \sum_{\substack{\alpha\beta\gamma \\ \alpha'\beta'\gamma'}} (-1)^{A+B+C+\alpha+\beta+\gamma} \begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix} \begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix} \begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma' \end{pmatrix} \\ = \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\}. \end{aligned} \quad (\text{A.23})$$

Note, that the sum runs in fact over two indices, only, as the primed and unprimed magnetic components of the  $3j$ -symbols are not independent; see (A.10). Omitting one index, e.g.  $\gamma'$  from the summation, the left-hand side of (A.23) must be multiplied by  $(2c + 1)$  which yields

$$\sum_{\substack{\alpha\beta\gamma \\ \alpha'\beta'}} (-1)^{A+B+C+\alpha+\beta+\gamma} \begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix} \begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix} \begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix} \begin{pmatrix} a & b & c_1 \\ \alpha' & \beta' & \gamma'_1 \end{pmatrix} \\ = \delta_{cc_1} \delta_{\gamma'\gamma'_1} \frac{1}{2c+1} \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\}. \quad (\text{A.24})$$

Again, the sum is over two indices, only. Further relations can be obtained applying the orthogonality properties (A.14) of the  $3j$ -symbols. Multiplying both sides of (A.23) with the last  $3j$ -symbol yields

$$\sum_{\alpha\beta\gamma} (-1)^{A+B+C+\alpha+\beta+\gamma} \begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix} \begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix} \begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix} \\ = \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma' \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\}. \quad (\text{A.25})$$

Due to the same argument, the sum is over one index, only. Continuing in the same manner, we get

$$\sum_{C\gamma} (-1)^{C+\gamma} (2C+1) \begin{pmatrix} a & B & C \\ \alpha' & \beta & -\gamma \end{pmatrix} \begin{pmatrix} b & A & C \\ \beta' & \alpha & \gamma \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\} \\ = (-1)^{b+B+c+C} \sum_{\gamma'} (-1)^{c+\gamma'} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & -\gamma' \end{pmatrix} \begin{pmatrix} B & A & c \\ \beta & \alpha & \gamma' \end{pmatrix}. \quad (\text{A.26a})$$

Note, that due to (A.10), the formal sum over  $\gamma$  and  $\gamma'$  is over one term, only. Thus, (A.26) may be re-expressed as

$$\sum_C (-1)^{a+b-c+A+B+C-\alpha'-\alpha} (2C+1) \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\} \begin{pmatrix} B & a & C \\ \beta & \alpha' & -\gamma \end{pmatrix} \begin{pmatrix} b & A & C \\ \beta' & \alpha & \gamma \end{pmatrix} \\ = \begin{pmatrix} a & b & c \\ \alpha' & \beta' & -\gamma' \end{pmatrix} \begin{pmatrix} A & B & c \\ \alpha & \beta & \gamma' \end{pmatrix}. \quad (\text{A.26b})$$

Continuing with this procedure yields

$$\sum_{BC} (-1)^{a+b-c+A+B+C-\alpha'-\alpha} (2B+1)(2C+1) \left\{ \begin{matrix} a & b & c \\ A & B & C \end{matrix} \right\} \\ \times \begin{pmatrix} B & a & C \\ \beta & \alpha' & -\gamma \end{pmatrix} \begin{pmatrix} b & A & C \\ \beta' & \alpha & \gamma \end{pmatrix} \begin{pmatrix} A & B & c \\ \alpha & \beta & \gamma' \end{pmatrix} = \begin{pmatrix} a & b & c \\ \alpha' & \beta' & -\gamma' \end{pmatrix}, \quad (\text{A.27})$$

and

$$\sum_{cBC} (-1)^{a+b-c+A+B+C-\alpha'-\alpha} (2c+1)(2B+1)(2C+1) \begin{Bmatrix} a & b & c \\ A & B & C \end{Bmatrix} \\ \times \begin{pmatrix} B & a & C \\ \beta & \alpha' & -\gamma \end{pmatrix} \begin{pmatrix} b & A & C \\ \beta' & \alpha & \gamma \end{pmatrix} \begin{pmatrix} A & B & c \\ \alpha & \beta & \gamma' \end{pmatrix} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & -\gamma' \end{pmatrix} = 1. \quad (\text{A.28})$$

If  $a + b + e$  is even a special case is

$$(-1)^{a+b+c+d+1} \sqrt{(2a+1)(2b+1)} \begin{pmatrix} a & b & e \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} a & b & e \\ d & c & \frac{1}{2} \end{Bmatrix} = \begin{pmatrix} c & d & e \\ -\frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \quad (\text{A.29})$$

Racah–Elliot relation and orthogonality relations:

$$\sum_x (-1)^{2x} (2x+1) \begin{Bmatrix} a & b & x \\ a & b & f \end{Bmatrix} = 1. \quad (\text{A.30})$$

$$\sum_x (-1)^{a+b+x} (2x+1) \begin{Bmatrix} a & b & x \\ b & a & f \end{Bmatrix} = \delta_{f0} \sqrt{(2a+1)(2b+1)}. \quad (\text{A.31})$$

$$\sum_x (2x+1) \begin{Bmatrix} a & b & x \\ c & d & f \end{Bmatrix} \begin{Bmatrix} c & d & x \\ a & b & g \end{Bmatrix} = \delta_{fg} \frac{1}{(2f+1)}. \quad (\text{A.32})$$

$$\sum_x (-1)^{f+g+x} (2x+1) \begin{Bmatrix} a & b & x \\ c & d & f \end{Bmatrix} \begin{Bmatrix} c & d & x \\ b & a & g \end{Bmatrix} = \begin{Bmatrix} a & d & f \\ b & c & g \end{Bmatrix}. \quad (\text{A.33})$$

$$\sum_x (-1)^{a+b+c+d+e+f+g+h+j+x} (2x+1) \begin{Bmatrix} a & b & x \\ c & d & g \end{Bmatrix} \begin{Bmatrix} c & d & x \\ e & f & h \end{Bmatrix} \begin{Bmatrix} e & f & x \\ b & a & j \end{Bmatrix} \\ = \begin{Bmatrix} g & h & j \\ e & a & d \end{Bmatrix} \begin{Bmatrix} g & h & j \\ f & b & c \end{Bmatrix}. \quad (\text{A.34})$$

### A.3 $9j$ -Symbols

The coupling of four angular momenta **a**, **b**, **d**, and **e** resulting in a total angular momentum **i** with  $z$ -component  $m$  leads to two different basis systems for the Hilbert sub-space of the total angular momentum  $|im\rangle$ :

$$|(ab)c, (de)f; im\rangle \quad \text{and} \quad |(ad)g, (be)h; im\rangle.$$

As in the three vector case, the corresponding eigenfunctions of the basis sets are not independent. They are connected by a linear transformation

$$|(ad)g, (be)h; im\rangle = \sum_{cf} |(ab)c, (de)f; im\rangle \\ \times \langle (ab)c, (de)f; im | (ad)g, (be)h; im \rangle. \quad (\text{A.35})$$

The transformation coefficient in (A.35) that changes the coupling defines the 9j-symbol of Wigner

$$\begin{aligned}
 & \langle (ab)c, (de)f; im | (ad)g, (be)h; im \rangle \\
 &= \sqrt{(2c+1)(2f+1)(2g+1)(2h+1)} \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} \\
 &\equiv X(abc, def, ghi), \tag{A.36}
 \end{aligned}$$

which is identical to the  $X$ -function of Fano.

Triangular conditions: the 9j-symbol vanishes unless the triangular conditions for the triads  $(a, b, c)$ ,  $(d, e, f)$ ,  $(g, h, i)$ ,  $(a, d, g)$ ,  $(b, e, h)$ , and  $(c, f, i)$  are fulfilled.

Symmetry: the 9j-symbol is invariant under interchange of rows and columns (reflection about a diagonal) and is multiplied by  $(-1)^p$ , where  $p = a + b + c + d + e + f + g + h + i$ , upon interchanging of two adjacent rows or columns, resulting in 72 symmetry relations.

Orthogonality:

$$\sum_{cf} (2c+1)(2f+1) \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} \begin{Bmatrix} a & b & c \\ d & e & f \\ j & k & i \end{Bmatrix} = \frac{\delta_{gj}\delta_{hk}}{(2g+1)(2h+1)}. \tag{A.37}$$

Sum rule:

$$\sum_{jk} (2j+1)(2k+1) \begin{Bmatrix} a & b & c \\ d & e & f \\ j & k & i \end{Bmatrix} \begin{Bmatrix} a & e & j \\ d & b & k \\ g & h & i \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}. \tag{A.38}$$

Identical rows or columns: in this case the 9j-symbol vanishes unless the sum of all arguments is even

$$\begin{Bmatrix} a & b & c \\ a & b & c \\ g & h & j \end{Bmatrix} = 0 \quad \text{if } g + h + j = 2k + 1, \tag{A.39a}$$

and

$$\begin{Bmatrix} a & a & c \\ d & d & f \\ g & g & j \end{Bmatrix} = 0 \quad \text{if } c + f + j = 2k + 1, \tag{A.39b}$$

where  $k \in \mathbb{N}$ .

Special values of the arguments: if one argument equals zero the 9j-symbol is reduced to a 6j-symbol

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & 0 \end{Bmatrix} = \delta_{cf}\delta_{gh} \frac{(-1)^{b+c+d+g}}{\sqrt{(2c+1)(2g+1)}} \begin{Bmatrix} a & b & c \\ e & d & g \end{Bmatrix}. \tag{A.40}$$

If two arguments are equal to zero we have

$$\left\{ \begin{array}{ccc} a & b & c \\ d & 0 & f \\ g & h & 0 \end{array} \right\} = \delta_{df} \delta_{bh} \delta_{cf} \delta_{gh} \frac{(-1)^{a-b-c}}{(2b+1)(2c+1)}, \quad (\text{A.41})$$

and for three arguments equal to zero we obtain

$$\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \\ 0 & 0 & 0 \end{array} \right\} = \frac{\delta_{ad} \delta_{be} \delta_{cf}}{\sqrt{(2a+1)(2b+1)(2c+1)}}, \quad (\text{A.42a})$$

and

$$\left\{ \begin{array}{ccc} 0 & b & c \\ d & 0 & f \\ g & h & 0 \end{array} \right\} = \delta_{bc} \delta_{bd} \delta_{bf} \delta_{bg} \delta_{bh} \frac{(-1)^{2b}}{(2b+1)^2}. \quad (\text{A.42b})$$

If one arguments equals unity, the  $9j$ -symbol can be also reduced to a  $6j$ -symbol

$$\left\{ \begin{array}{ccc} a & b & c \\ d & e & c \\ g & g & 1 \end{array} \right\} = (-1)^{b+c+d+g} \frac{a(a+1) - d(d+1) - b(b+1) + e(e+1)}{\sqrt{(g+1)(2g+1)2g(c+1)(2c+1)2c}} \left\{ \begin{array}{ccc} a & b & c \\ e & d & g \end{array} \right\}. \quad (\text{A.43})$$

Important relations to the  $3j$ - and  $6j$ -symbols exist if one of the triads in the  $9j$ -symbol equals  $(1/2, 1/2, 1)$

$$\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} \left\{ \begin{array}{ccc} c & f & 1 \\ \frac{1}{2} & \frac{1}{2} & g \end{array} \right\} = \frac{(-1)^{2g}}{3} \left\{ \begin{array}{ccc} a & b & c \\ \frac{1}{2} & g & e \end{array} \right\} \left\{ \begin{array}{ccc} e & d & f \\ \frac{1}{2} & g & a \end{array} \right\} - \delta_{cf} \frac{(-1)^{b+d-g}}{6(2c+1)} \left\{ \begin{array}{ccc} a & b & c \\ e & d & \frac{1}{2} \end{array} \right\}. \quad (\text{A.44})$$

In addition, if  $c, d, e$  are integer and  $c + d + e$  is even, we get

$$\sqrt{6(2c+1)(2d+1)(2e+1)} \left( \begin{array}{ccc} c & d & e \\ 0 & 0 & 0 \end{array} \right) \left\{ \begin{array}{ccc} a & b & c \\ d & e & c \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} = \left( \begin{array}{ccc} a & b & c \\ \frac{1}{2} & \frac{1}{2} & -1 \end{array} \right). \quad (\text{A.45})$$

If  $c + d + e$  is odd, we have two other relations

$$\left( \begin{array}{ccc} c+1 & d & e \\ 0 & 0 & 0 \end{array} \right) \left\{ \begin{array}{ccc} a & b & c \\ d & e & c+1 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} = (-1)^{b+c+1/2} \left( \begin{array}{ccc} a & b & c \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \times \frac{[(d-a)(2a+1) + (e-b)(2b+1) + c+1]}{\sqrt{6(c+1)(2c+1)(2c+3)(2d+1)(2e+1)}}, \quad (\text{A.46a})$$



and

$$\begin{pmatrix} c-1 & d & e \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ d & e & c-1 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{matrix} \right\} = (-1)^{b+c+1/2} \begin{pmatrix} a & b & c \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \\ \times \frac{[(d-a)(2a+1) + (e-b)(2b+1) - c]}{\sqrt{6c(2c+1)(2c-1)(2d+1)(2e+1)}}. \quad (\text{A.46b})$$

Contraction of 3j-symbols: the following equations are continuously applied as a useful tool in angular momentum coupling theory in order to reduce extended expressions by analytically carrying out the sum over the magnetic quantum numbers.

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = (2a+1) \sum_{\substack{\beta\gamma\delta\epsilon \\ \phi\eta\nu\rho}} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} b & e & h \\ \beta & \epsilon & \eta \end{pmatrix} \begin{pmatrix} c & f & i \\ \gamma & \phi & \nu \end{pmatrix} \\ \times \begin{pmatrix} a & d & g \\ \alpha & \delta & \rho \end{pmatrix} \begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix} \begin{pmatrix} g & h & i \\ \rho & \eta & \nu \end{pmatrix}. \quad (\text{A.47})$$

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix} \right\} = \sum_{\substack{\delta\epsilon\phi \\ \eta\nu\rho}} \begin{pmatrix} b & e & h \\ \beta & \epsilon & \eta \end{pmatrix} \begin{pmatrix} c & f & i \\ \gamma & \phi & \nu \end{pmatrix} \begin{pmatrix} a & d & g \\ \alpha & \delta & \rho \end{pmatrix} \\ \times \begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix} \begin{pmatrix} g & h & i \\ \rho & \eta & \nu \end{pmatrix}. \quad (\text{A.48})$$

$$\sum_{b\beta} (2b+1) \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} b & e & h \\ \beta & \epsilon & \eta \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix} \right\} \\ = \sum_{\delta\phi\nu\rho} \begin{pmatrix} c & f & i \\ \gamma & \phi & \nu \end{pmatrix} \begin{pmatrix} a & d & g \\ \alpha & \delta & \rho \end{pmatrix} \begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix} \begin{pmatrix} g & h & i \\ \rho & \eta & \nu \end{pmatrix}. \quad (\text{A.49})$$

Note, that due to the selection rule (A.10), the sum over  $\beta$  on the left side is over one term, only.

$$\sum_{b\beta c\gamma} (2b+1)(2c+1) \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} b & e & h \\ \beta & \epsilon & \eta \end{pmatrix} \begin{pmatrix} c & f & i \\ \gamma & \phi & \nu \end{pmatrix} \left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix} \right\} \\ = \sum_{\delta\rho} \begin{pmatrix} a & d & g \\ \alpha & \delta & \rho \end{pmatrix} \begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix} \begin{pmatrix} g & h & i \\ \rho & \eta & \nu \end{pmatrix}. \quad (\text{A.50})$$

Due to the same argument, the sums over  $\beta$  and  $\gamma$  on the left, and over  $\delta$  and  $\rho$  on the right side are over one term, only.

Contraction of 6j-symbols: analogously, the 9j-symbol may expressed in terms of 6j-symbols

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix} \right\} = \sum_x (-1)^{2x} (2x+1) \left\{ \begin{matrix} a & b & c \\ f & i & x \end{matrix} \right\} \left\{ \begin{matrix} d & e & f \\ b & x & h \end{matrix} \right\} \left\{ \begin{matrix} g & h & i \\ x & a & d \end{matrix} \right\}, \quad (\text{A.51})$$

$$\sum_x (2x+1) \left\{ \begin{matrix} a & f & x \\ d & q & e \\ p & c & b \end{matrix} \right\} \left\{ \begin{matrix} a & f & x \\ e & b & s \end{matrix} \right\} = (-1)^{2s} \left\{ \begin{matrix} a & b & s \\ c & d & p \end{matrix} \right\} \left\{ \begin{matrix} c & d & s \\ e & f & q \end{matrix} \right\}, \quad (\text{A.52})$$

$$\sum_x (-1)^{R+x} (2x+1) \left\{ \begin{matrix} a & f & x \\ d & q & e \\ p & c & b \end{matrix} \right\} \left\{ \begin{matrix} a & f & x \\ b & e & s \end{matrix} \right\} = (-1)^{2s} \left\{ \begin{matrix} p & q & s \\ e & a & d \end{matrix} \right\} \left\{ \begin{matrix} p & q & s \\ f & b & c \end{matrix} \right\}, \quad (\text{A.53})$$

where  $R = a + b + c + d + e + f + p + q$ .

It is sometimes helpful to re-order the coupling of the quantum numbers in the 3nj-symbols. This can be achieved with the recursion relation

$$\begin{aligned} & (-1)^{a+f+b+i} \sum_x (-1)^{2x} (2x+1) \left\{ \begin{matrix} a & b & x \\ d & e & f \\ g & h & i \end{matrix} \right\} \left\{ \begin{matrix} a & b & x \\ c & \lambda & a' \end{matrix} \right\} \left\{ \begin{matrix} i & f & x \\ \lambda & c & f' \end{matrix} \right\} \\ & = (-1)^{a'+f'+g+e} \sum_y (-1)^{2y} (2y+1) \left\{ \begin{matrix} a' & b & y \\ d & e & f' \\ g & h & i \end{matrix} \right\} \left\{ \begin{matrix} f' & e & y \\ d & \lambda & f \end{matrix} \right\} \left\{ \begin{matrix} g & a' & y \\ \lambda & d & a \end{matrix} \right\}. \quad (\text{A.54}) \end{aligned}$$

## B Rotation Matrices and Spherical Harmonics

The behaviour of particles in a scattering system is directly related to its description in the relevant coordinate frame. These relations are dealt with by the theory of rotation matrices. The book of Zare (1988) yields a detailed and broad insight. We are giving a comprehensive overview of the important relations.

### B.1 Transformation Properties of Angular Momentum Under Rotation

Any rotation  $\mathbf{R}_n(\omega)$  can be specified by giving three parameters, two to fit its rotation axis  $\hat{\mathbf{n}}$  and one to fit its rotation angle  $\omega$  about  $\hat{\mathbf{n}}$ . For an arbitrary rotation about  $\hat{\mathbf{n}}$  by an angle  $\omega$ , we obtain

$$\mathbf{R}_n(\omega) = \exp(-i\omega \mathbf{J} \cdot \hat{\mathbf{n}}). \quad (\text{B.1})$$

We note, that an arbitrary rotation cannot change the value of the angular momentum  $J$  since  $\mathbf{J}^2$  commutes with the rotation operator

$$[\mathbf{R}_n(\omega), \mathbf{J}^2] = [\exp(-i\omega \mathbf{J} \cdot \hat{\mathbf{n}}), \mathbf{J}^2] = \sum_{\nu} \frac{1}{\nu!} (-i\omega)^{\nu} [(\mathbf{J} \cdot \hat{\mathbf{n}})^{\nu}, \mathbf{J}^2] = 0. \quad (\text{B.2})$$

Thus, a rotation acting on the angular momentum eigenstates  $|JM\rangle$  of  $\mathbf{J}^2$  and  $J_z$  can only transform  $|JM\rangle$  into a linear combination of other  $M$  values

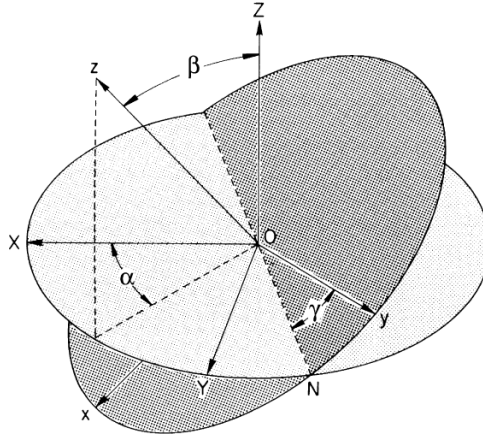
$$|Jm\rangle = \mathbf{R}(\alpha, \beta, \gamma) |JM\rangle = \sum_{M'} \mathcal{D}_{M'M}^{(J)}(\alpha, \beta, \gamma) |JM'\rangle, \quad (\text{B.3})$$

where the expansion coefficients

$$\mathcal{D}_{M'M}^{(J)}(\alpha, \beta, \gamma) = \langle JM' | \mathbf{R}(\alpha, \beta, \gamma) | JM \rangle, \quad (\text{B.4})$$

are the elements of a  $(2J + 1) \times (2J + 1)$  unitary matrix for  $\mathbf{R}$ , called the *rotation matrix*, and form the irreducible representation of the rotation group of dimension  $2J + 1$  corresponding to an angular momentum  $J$  and a rotation around the Euler angles  $(\alpha, \beta, \gamma)$ ; see Fig. B.1.

The Euler angles  $(\alpha, \beta, \gamma)$  are a set of parameters to specify arbitrary rotations by three successive finite rotations; i.e. to make the  $XYZ$  space-fixed coordinate frame coincide with the  $xyz$  body-fixed frame:



**Fig. B.1.** The Euler angles  $\alpha$ ,  $\beta$ , and  $\gamma$  relating the  $XYZ$  space-fixed and the  $xyz$  body-fixed coordinate frames

1. A counterclockwise rotation  $\alpha$  about  $Z$ , the vertical axis. This carries the  $Y$  axis into the line of nodes  $N$ .
2. A counterclockwise rotation  $\beta$  about the line of nodes  $N$ . This carries the  $Z$  axis into the  $z$  axis, i.e. the figure axis of the body.
3. A counterclockwise rotation  $\gamma$  about  $z$ , the figure axis. This carries the line of nodes  $N$  into the  $y$  axis.

Using (B.1), we may express such a rotation as

$$\begin{aligned} \mathbf{R}(\alpha, \beta, \gamma) &= \exp(-i\gamma \mathbf{J} \cdot \hat{\mathbf{n}}_\gamma) \exp(-i\beta \mathbf{J} \cdot \hat{\mathbf{n}}_\beta) \exp(-i\alpha \mathbf{J} \cdot \hat{\mathbf{n}}_\alpha) \\ &= \exp(-i\gamma J_z) \exp(-i\beta J_N) \exp(-i\alpha J_Z), \end{aligned} \quad (\text{B.5})$$

where the form of  $\mathbf{R}$  has been chosen to be an active rotation of the physical system. It can be shown, e.g. Zare (1988), that the three Euler angle rotations may all be carried out in the *same*  $XYZ$  space-fixed coordinate frame if the order of the rotations is reversed. That is, first a rotation  $\gamma$  about the  $Z$  axis, then a rotation  $\beta$  about the  $Y$  axis, and finally a rotation  $\alpha$  about the same  $Z$  axis:

$$\mathbf{R}(\alpha, \beta, \gamma) = \exp(-i\alpha J_Z) \exp(-i\beta J_Y) \exp(-i\gamma J_Z). \quad (\text{B.6})$$

Associated with this is the equivalent rotation of the coordinate frame  $(\gamma, \beta, \alpha)^{-1} = (-\alpha, -\beta, -\gamma)$ , so their usage results in a different sign convention for the angles of rotation.

Substituting (B.6) into (B.4) and using the fact that the basis vectors  $|JM\rangle$  are eigenfunctions of  $J_Z$  the rotation matrices simplify as follows

$$\mathcal{D}_{M'M}^{(J)}(\alpha, \beta, \gamma) = \exp(-i\alpha M') d_{M'M}^{(J)}(\beta) \exp(-i\gamma M), \quad (\text{B.7})$$

where

$$d_{M'M}^{(J)}(\beta) = \langle JM' | \exp(-i\beta J_Y) | JM \rangle, \quad (\text{B.8})$$

are the reduced rotation matrices. They are real quantities and explicit expressions as well as extended tables may be found in the literature (Brink and Satchler 1962; Messiah 1979; Varshalovich *et al.* 1988; Zare 1988).

## B.2 Symmetry Properties of Rotation Matrices

The reduced rotation matrices  $d_{MM'}^{(J)}$  satisfy a number of useful symmetry relations:

$$\begin{aligned} d_{MM'}^{(J)}(\beta) &= (-1)^{M-M'} d_{M'M}^{(J)}(\beta) = d_{-M'-M}^{(J)}(\beta) = d_{M'M}^{(J)}(-\beta) \\ &= (-1)^{J-M} d_{M-M'}^{(J)}(\pi - \beta) = (-1)^{J+M'} d_{M-M'}^{(J)}(\pi + \beta). \end{aligned} \quad (\text{B.9})$$

Note, that rotation by  $-\beta$  is the inverse of rotation by  $\beta$ , that is  $d_{M'M}^{(J)}(-\beta) = [d_{M'M}^{(J)}(\beta)]^{-1}$ . As the  $d_{MM'}^{(J)}$  are real and are elements of a unitary transformation, we get  $[d_{M'M}^{(J)}(\beta)]^{-1} = [d_{M'M}^{(J)}(\beta)]^\dagger = d_{M'M}^{(J)}(\beta)$ .

Using Zare (1988) we obtain special values:

$$d_{M'M}^{(J)}(0) = \delta_{M'M} \quad \text{and} \quad d_{M'M}^{(J)}(\pi) = (-1)^{J+M'} \delta_{M'-M}. \quad (\text{B.10})$$

Combining (B.9) and (B.10) yields the result

$$\begin{aligned} d_{M'M}^{(J)}(2\pi) &= (-1)^{J+M'} d_{-M'-M}^{(J)}(\pi) \\ &= (-1)^{2J} \delta_{M'M} = (-1)^{2J} d_{M'M}^{(J)}(0). \end{aligned} \quad (\text{B.11})$$

The symmetry properties for the rotation matrices  $\mathcal{D}_{MM'}^{(J)}$  are obtained as:

$$\mathcal{D}_{MM'}^{(J)}(\alpha\beta\gamma)^* = (-1)^{M-M'} \mathcal{D}_{-M-M'}^{(J)}(\alpha\beta\gamma) = \mathcal{D}_{M'M}^{(J)}(-\gamma - \beta - \alpha), \quad (\text{B.12})$$

where  $(-\gamma - \beta - \alpha)$  is the rotation inverse to  $(\alpha\beta\gamma)$ . In the following we may use the contraction ( $\omega = \alpha\beta\gamma$ ).

As the rotation matrices are unitary, they satisfy the sum rules:

$$\begin{aligned} \sum_{M'} [\mathcal{D}_{M'M}^{(J)}(\omega)]^\dagger \mathcal{D}_{M'N}^{(J)}(\omega) &= \sum_{M'} d_{M'M}^{(J)}(-\beta) d_{M'N}^{(J)}(\beta) \\ &= \sum_{M'} d_{MM'}^{(J)}(\beta) d_{M'N}^{(J)}(\beta) = \delta_{MN}, \end{aligned} \quad (\text{B.13a})$$

and

$$\begin{aligned} \sum_M [\mathcal{D}_{M'M}^{(J)}(\omega)]^\dagger \mathcal{D}_{N'M}^{(J)}(\omega) &= \sum_M d_{M'M}^{(J)}(-\beta) d_{N'M}^{(J)}(\beta) \\ &= \sum_M d_{MM'}^{(J)}(\beta) d_{N'M}^{(J)}(\beta) = \delta_{M'N'}. \end{aligned} \quad (\text{B.13b})$$

### B.3 The Clebsch–Gordan Series and its Inverse

The connection between the uncoupled  $|J_1 M_1\rangle|J_2 M_2\rangle$  and coupled representations  $|JM\rangle$  under a rotational transformation is given by the so-called *Clebsch–Gordan series*.

$$\begin{aligned} \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega) \\ = \sum_J (J_1 M_1, J_2 M_2 | J M) (J_1 M'_1, J_2 M'_2 | J M') \mathcal{D}_{M' M}^{(J)}(\omega). \end{aligned} \quad (\text{B.14})$$

In principle, the right-hand side must be summed over  $M$  and  $M'$ , too. Applying the selection rule (A.2), the sum can be omitted. The Clebsch–Gordan series can be re-written in terms of  $3j$ -symbols

$$\begin{aligned} \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega) \\ = \sum_J (2J+1) \begin{pmatrix} J_1 & J_1 & J \\ M_1 & M_2 & M \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J \\ M'_1 & M'_2 & M' \end{pmatrix} \mathcal{D}_{M' M}^{(J)}(\omega)^*. \end{aligned} \quad (\text{B.15})$$

Note the complex conjugate rotation matrix on the right hand side which enters by using (A.9) and (B.12).

The *inverse Clebsch–Gordan series* yields

$$\begin{aligned} \mathcal{D}_{M' M}^{(J)}(\omega) = \sum_{M_1 M'_1 M_2 M'_2} (J_1 M_1, J_2 M_2 | J M) (J_1 M'_1, J_2 M'_2 | J M') \\ \times \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega). \end{aligned} \quad (\text{B.16})$$

Note, that the summation of the right-hand side is not independent. Applying the selection rule (A.2), either two of the summation indices  $M_1, M'_1$  or  $M_2, M'_2$  can be omitted. Re-writing in terms of  $3j$ -symbols and omitting the sum over  $M_2$  and  $M'_2$  we obtain

$$\begin{aligned} \mathcal{D}_{M' M}^{(J)}(\omega)^* = \sum_{M_1 M'_1} (2J+1) \begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & M \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J \\ M'_1 & M'_2 & M' \end{pmatrix} \\ \times \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega). \end{aligned} \quad (\text{B.17})$$

Analogously, we obtain the relations

$$\begin{aligned} \mathcal{D}_{M' M}^{(J)}(\omega)^* \begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & M \end{pmatrix} \\ = \sum_{M'_1 M'_2} \begin{pmatrix} J_1 & J_2 & J \\ M'_1 & M'_2 & M' \end{pmatrix} \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega), \end{aligned} \quad (\text{B.18a})$$

and

$$\begin{aligned} \mathcal{D}_{M M'}^{(J)}(\omega)^* \begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & M \end{pmatrix} \\ = \sum_{M'_1 M'_2} \begin{pmatrix} J_1 & J_2 & J \\ M'_1 & M'_2 & M' \end{pmatrix} \mathcal{D}_{M_1 M'_1}^{(J_1)}(\omega) \mathcal{D}_{M_2 M'_2}^{(J_2)}(\omega). \end{aligned} \quad (\text{B.18b})$$

Eventually, the contraction of three rotation matrices results in a  $3j$ -symbol

$$\begin{aligned} \sum_{M M_1 M_2} \mathcal{D}_{M M'}^{(J)}(\omega) \mathcal{D}_{M_1 M'_1}^{(J_1)}(\omega) \mathcal{D}_{M_2 M'_2}^{(J_2)}(\omega) \begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & M \end{pmatrix} \\ = \begin{pmatrix} J_1 & J_2 & J \\ M'_1 & M'_2 & M' \end{pmatrix}. \end{aligned} \quad (\text{B.19})$$

The closure relation for two consecutive rotations gives

$$\sum_{M''} \mathcal{D}_{M M''}^{(J)}(\omega_2) \mathcal{D}_{M'' M'}^{(J)}(\omega_1) = \mathcal{D}_{M M'}^{(J)}(\omega), \quad (\text{B.20})$$

where  $\omega = (\alpha\beta\gamma)$  is the resultant of first  $\omega_1 = (\alpha_1\beta_1\gamma_1)$  and second  $\omega_2 = (\alpha_2\beta_2\gamma_2)$ . Analogously, the closure relation for the reduced rotation matrices yields

$$\sum_{M''} d_{M M''}^{(J)}(\beta_2) d_{M'' M'}^{(J)}(\beta_1) = d_{M M'}^{(J)}(\beta_1 + \beta_2). \quad (\text{B.21})$$

## B.4 Integrals Over Rotation Matrices

Integrating over the solid angle element  $d\Omega = d\alpha \sin\beta d\beta d\gamma$  and using (B.12) and (B.14) yields the orthogonality relation results in a between two rotation matrices having the same argument

$$\int d\Omega \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega)^* \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega) = \frac{8\pi^2}{2J_1 + 1} \delta_{J_1 J_2} \delta_{M'_1 M'_2} \delta_{M_1 M_2}. \quad (\text{B.22})$$

Applying the Clebsch–Gordan series and (B.22) allows for evaluating the integral over three rotation matrices of the same argument. With (B.14) we obtain

$$\begin{aligned} \int d\Omega \mathcal{D}_{M'_3 M_3}^{(J_3)}(\omega)^* \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega) \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \\ = \frac{8\pi^2}{2J_3 + 1} (J_1 M_1, J_2 M_2 | J_3 M_3) (J_1 M'_1, J_2 M'_2 | J_3 M'_3), \end{aligned} \quad (\text{B.23a})$$

and using (B.15) yields

$$\begin{aligned} \int d\Omega \mathcal{D}_{M'_3 M_3}^{(J_3)}(\omega) \mathcal{D}_{M'_2 M_2}^{(J_2)}(\omega) \mathcal{D}_{M'_1 M_1}^{(J_1)}(\omega) \\ = 8\pi^2 \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ M'_1 & M'_2 & M'_3 \end{pmatrix}. \end{aligned} \quad (\text{B.23b})$$

## B.5 Relation with the Spherical Harmonics

Special cases: if the angular momentum  $L$  is integer and one magnetic quantum number is equal to zero the dependence on the angles  $\gamma$  or  $\alpha$  becomes obsolete, and the rotation matrices can be expressed in terms of spherical harmonics  $Y_{LM}(\beta, \alpha)$ . For the spherical harmonics the notation  $Y_{LM}(\theta, \phi)$  is more common. In the following, we therefore change the notation of the Euler angles accordingly; i.e.  $\alpha \leftrightarrow \phi$ ,  $\beta \leftrightarrow \theta$ , and  $\gamma \leftrightarrow \chi$ . This yields the relation

$$\mathcal{D}_{M0}^{(L)}(\omega) = d_{M0}^{(L)}(\theta) e^{-iM\phi} = C_{LM}^*(\theta, \phi) = \sqrt{\frac{4\pi}{2L+1}} Y_{LM}^*(\theta, \phi), \quad (\text{B.24})$$

where  $C_{LM}(\theta, \phi)$  are the *renormalized* spherical harmonics introduced by Condon and Shortley (1935). With the first magnetic quantum number equal to zero we obtain

$$\begin{aligned} \mathcal{D}_{0M}^{(L)}(\omega) &= d_{0M}^{(L)}(\theta) e^{-iM\chi} = (-1)^M d_{M0}^{(L)}(\theta) e^{-iM\chi} = (-1)^M C_{LM}^*(\theta, \chi) \\ &= C_{L-M}(\theta, \chi) = \sqrt{\frac{4\pi}{2L+1}} Y_{L-M}(\theta, \chi), \end{aligned} \quad (\text{B.25})$$

where we have used the relation  $Y_{LM}^* = (-1)^M Y_{L-M}$ . Particularly, for  $\chi = \phi = 0$ , the reduced rotation matrices may be also expressed in terms of associated Legendre polynomials  $P_L^M(\cos \theta)$  as

$$d_{M0}^{(L)}(\theta) = C_{LM}^*(\theta, 0) = \sqrt{\frac{(L-M)!}{(L+M)!}} P_L^M(\cos \theta), \quad (\text{B.26})$$

if  $M \geq 0$ , and

$$d_{0M}^{(L)}(\theta) = (-1)^M C_{LM}^*(\theta, 0) = (-1)^M \sqrt{\frac{(L-M)!}{(L+M)!}} P_L^M(\cos \theta). \quad (\text{B.27})$$

Having both magnetic quantum numbers equal to zero we simply get the Legendre polynomials

$$\mathcal{D}_{00}^{(L)}(\omega) = d_{00}^{(L)}(\theta) = P_L(\cos \theta). \quad (\text{B.28})$$

Some of the relations derived above are often applied using spherical harmonics. Using (B.24), the orthogonality relation (B.22) may be expressed as

$$\int \sin \theta d\theta d\phi C_{kq}^*(\theta, \phi) C_{KQ}(\theta, \phi) = \frac{4\pi}{2K+1} \delta_{kK} \delta_{qQ}. \quad (\text{B.29})$$

From the sum rules (B.13a) and (B.13b) we get

$$\sum_q |C_{kq}(\theta, \phi)|^2 = 1, \quad (\text{B.30})$$



and for  $q = 0$  we obtain

$$\sum_k (2k+1) C_{k0}(\theta, \phi) = 2\delta(\cos \theta - 1). \quad (\text{B.31})$$

From the closure relation (B.20) we obtain the addition theorem for the renormalized spherical harmonics

$$\sum_q C_{kq}(\theta, \phi) C_{kq}^*(\theta', \phi') = P_k(\cos \omega), \quad (\text{B.32})$$

where  $\omega$  is the angle between the two directions  $(\theta, \phi)$  and  $(\theta', \phi')$ .

From the Clebsch–Gordan series and its inverse, see (B.15) and (B.17), we obtain similar contractions between two renormalized spherical harmonics of the same argument

$$C_{a\alpha}(\theta, \phi) C_{b\beta}(\theta, \phi) = \sum_c C_{c\gamma}(\theta, \phi) (2c+1) (-1)^\gamma \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix} \begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{B.33})$$

where the sum over  $\gamma$  on the right-hand side is fixed to one argument due to the selection rule (A.10). Summing over the magnetic components on the left-hand side yields

$$\sum_{\alpha\beta} C_{a\alpha}(\theta, \phi) C_{b\beta}(\theta, \phi) \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix} = C_{c\gamma}(\theta, \phi) (-1)^\gamma \begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{B.34})$$

Combining (B.22) and (B.33) yields the integral over three renormalized spherical harmonics

$$\int \sin \theta d\theta d\phi C_{a\alpha}(\theta, \phi) C_{b\beta}(\theta, \phi) C_{c\gamma}(\theta, \phi) = 4\pi \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix} \begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{B.35})$$

For all three magnetic quantum numbers equal to zero, we obtain a similar integral in terms of Legendre polynomials

$$\int \sin \theta d\theta P_a(\cos \theta) P_b(\cos \theta) P_c(\cos \theta) = 2 \left( \begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} \right)^2. \quad (\text{B.36})$$

## B.6 Left–Right Asymmetry of Rotation Matrices

For evaluating asymmetry parameters it is useful to investigate the symmetries of the reduced rotation matrices under the operation  $\theta \rightarrow -\theta$ .

Considering the case of electron impact excitation/ionization we need to consider only a few of the reduced rotation matrices  $d_{Q'Q}^{(K)}(\theta)$  since the quantum numbers  $Q$  and  $Q'$  are restricted by the selection rule

$$|Q| \leq 1, \quad (\text{B.37})$$

and only particular combinations of the reduced rotation matrices can occur (see Sect. 2.5.3).

Due to the definition of the asymmetry parameters we need to consider the sum and the difference of the occurring combinations of reduced rotation matrices with the argument being  $\theta$  and  $-\theta$ , respectively. I.e., we need to consider expressions of the type  $d_{Q'Q}^{(K)}(\theta) \pm d_{Q'Q}^{(K)}(-\theta)$ .

In order to obtain the relevant results the symmetry relations (B.9) of the reduced rotation matrices must be applied. For the simple most case we obtain

$$d_{00}^{(K)}(\theta) - d_{00}^{(K)}(-\theta) = 0, \quad (\text{B.38})$$

and by using (B.28)

$$d_{00}^{(K)}(\theta) + d_{00}^{(K)}(-\theta) = 2d_{00}^{(K)}(\theta) = 2P_K(\cos \theta). \quad (\text{B.39})$$

Analogously, applying (B.26) and (B.27), we obtain for the difference

$$\begin{aligned} d_{10}^{(K)}(\theta) - d_{10}^{(K)}(-\theta) &= d_{10}^{(K)}(\theta) - d_{01}^{(K)}(\theta) = 2C_{K1}^*(\theta, 0) \\ &= \frac{2}{\sqrt{K(K+1)}} P_K^1(\cos \theta). \end{aligned} \quad (\text{B.40})$$

The sum yields

$$\begin{aligned} d_{10}^{(K)}(\theta) + d_{10}^{(K)}(-\theta) &= d_{10}^{(K)}(\theta) + d_{01}^{(K)}(\theta) \\ &= C_{K1}^*(\theta, 0) - C_{K1}^*(\theta, 0) = 0. \end{aligned} \quad (\text{B.41})$$

For the other occurring differences we simply obtain

$$\begin{aligned} \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] - \left[ d_{11}^{(K)}(-\theta) \pm d_{-11}^{(K)}(-\theta) \right] \\ = \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] - \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] = 0, \end{aligned} \quad (\text{B.42})$$

and for the summations we eventually get

$$\begin{aligned} \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] + \left[ d_{11}^{(K)}(-\theta) \pm d_{-11}^{(K)}(-\theta) \right] \\ = \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] + \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right] \\ = 2 \left[ d_{11}^{(K)}(\theta) \pm d_{-11}^{(K)}(\theta) \right]. \end{aligned} \quad (\text{B.43})$$

Note, that the derived relations are valid for any integer rank  $K \geq 0$  of the reduced rotation matrices.

Eventually, we give explicit expressions of (B.43) for some cases of interest. For  $K = 1$  we obtain

$$d_{11}^{(1)}(\theta) + d_{-11}^{(1)}(\theta) = 1, \quad (\text{B.44})$$

and

$$d_{11}^{(1)}(\theta) - d_{-11}^{(1)}(\theta) = \cos \theta, \quad (\text{B.45})$$

and for  $K = 2$  we get

$$d_{11}^{(2)}(\theta) + d_{-11}^{(2)}(\theta) = \cos \theta, \quad (\text{B.46})$$

and

$$d_{11}^{(2)}(\theta) - d_{-11}^{(2)}(\theta) = \cos(2\theta). \quad (\text{B.47})$$

The identity of (B.45) and (B.46) is by chance. For  $K = 3$  we obtain

$$d_{11}^{(3)}(\theta) + d_{-11}^{(3)}(\theta) = \frac{1}{4}(5 \cos^2 \theta - 1), \quad (\text{B.48})$$

which is unequal to the result of (B.47).

Eventually, we give expressions for the angular functions for the *magic angle*  $\theta_M = 54.7^\circ$ ,

$$\sin \theta_M = \sqrt{\frac{2}{3}} \quad \text{and} \quad \cos \theta_M = \frac{1}{\sqrt{3}}. \quad (\text{B.49})$$

## C Irreducible Tensorial Sets

Dealing with tensorial sets is essential in interpreting multi-particle scattering processes. Therefore, its application is an important means for the understanding of Auger emission. Important relations are given below. A good introduction into the field may be found in Brink and Satchler (1962) or Zare (1988).

### C.1 Definition and Basic Properties

*Definition:* Tensor operator  $\equiv$  The manifold of operators which, under rotation, linearly transform into each other.

Irreducible tensor operator: The  $(2k + 1)$  operators  $T_{KQ}$ ,  $Q = -K, \dots, +K$ , are called the *standard components of an irreducible tensor operator  $\mathbf{T}_K$  of rank  $K$*  if they transform under rotation as

$$\mathcal{D}T_{KQ}\mathcal{D}^{-1} = \sum_q T_{Kq}\mathcal{D}_{qQ}^{(K)}. \quad (\text{C.1})$$

Scalar operator  $\equiv$  Irreducible tensor operator of rank zero; i.e.,

$$\mathcal{D}T_{00}\mathcal{D}^{-1} = T_{00}\mathcal{D}_{00}^{(0)} = T_{00}. \quad (\text{C.2})$$

Vector operator  $\equiv$  Irreducible tensor operator of first rank; let  $V_x, V_y, V_z$  be its components in the Cartesian  $x, y, z$ -coordinate frame, then its standard components are

$$V_+ = \frac{1}{\sqrt{2}} (V_x + iV_y), \quad (\text{C.3a})$$

$$V_0 = V_z, \quad (\text{C.3b})$$

$$V_- = \frac{1}{\sqrt{2}} (V_x - iV_y). \quad (\text{C.3c})$$

Commutation relations with the angular momentum:

$$[J_{\pm}, T_{kq}] = \sqrt{k(k+1) - q(q \pm 1)} T_{kq \pm 1}, \quad (\text{C.4a})$$

$$[J_z, T_{kq}] = q T_{kq}. \quad (\text{C.4b})$$

Hermitian conjugate:

$$\mathbf{S}_K = \mathbf{T}_K^\dagger \quad \text{if} \quad S_{KQ} = (-1)^Q T_{KQ}^\dagger. \quad (\text{C.5})$$

One of the basic properties of irreducible tensor operators is the *Wigner–Eckart* theorem (see also Sect. 2.2):

$$\begin{aligned} \langle JM | T_{KQ} | J' M' \rangle &= \frac{(-1)^{2K}}{\sqrt{2J+1}} \langle J \| T_K \| J' \rangle (J' M', K Q | JM) \\ &= (-1)^{J-M} \langle J \| T_K \| J' \rangle \begin{pmatrix} J & K & J' \\ -M & Q & M' \end{pmatrix}, \end{aligned} \quad (\text{C.6})$$

where  $\langle J \| T_K \| J' \rangle$  is the so-called reduced matrix element. Its complex conjugate is given (for  $K$  integer) as:

$$\langle J \| T_K \| J' \rangle^* = (-1)^{J'-J} \langle J \| T_K^\dagger \| J' \rangle. \quad (\text{C.7})$$

Note, that the notation of the Wigner–Eckart theorem is not unique in the literature. Our form coincides with the convention used by Blum (1996); Edmonds (1974); Fano and Racah (1959); Messiah (1979); Racah (1942); Varshalovich *et al.* (1988) and Zare (1988). Some authors, including Brink and Satchler (1962); Rose (1957) and Wigner (1959), define the reduced matrix element to be a factor of  $\sqrt{2J+1}$  smaller.

Special values of tensor operators are the *identity operator*

$$\langle J \| \mathbf{1} \| J' \rangle = \delta_{JJ'} \sqrt{2J+1}, \quad (\text{C.8})$$

and the total angular momentum

$$\langle J \| \mathbf{J} \| J' \rangle = \delta_{JJ'} \sqrt{J(J+1)(2J+1)}. \quad (\text{C.9})$$

In the following, some of the multipole expansions useful in physics are given:

$$\exp(i\mathbf{k}\mathbf{r}) = \sum_{\ell} i^{\ell} (2\ell+1) j_{\ell}(kr) \mathbf{C}_{\ell}(\theta_k \phi_k) \mathbf{C}_{\ell}(\theta_r \phi_r), \quad (\text{C.10})$$

$$\delta(\mathbf{a} - \mathbf{b}) = \frac{1}{4\pi a^2} \delta(a-b) \sum_{\ell} (2\ell+1) \mathbf{C}_{\ell}(\theta_a \phi_a) \mathbf{C}_{\ell}(\theta_b \phi_b), \quad (\text{C.11})$$

$$\begin{aligned} \exp(-\gamma[\mathbf{a} - \mathbf{b}]^2) &= \sum_{\ell} i^{-\ell} (2\ell+1) e^{-\gamma(a^2+b^2)} j_{\ell}(2i\gamma ab) \\ &\quad \times \mathbf{C}_{\ell}(\theta_a \phi_a) \mathbf{C}_{\ell}(\theta_b \phi_b), \end{aligned} \quad (\text{C.12})$$

where  $j_{\ell}(kr)$  denote the spherical Bessel functions; and if  $\boldsymbol{\rho} = \mathbf{b} - \mathbf{a}$ , with  $b \geq a$ ,

$$\frac{1}{\rho} = \sum_{\ell} \frac{a^{\ell}}{b^{\ell+1}} \mathbf{C}_{\ell}(\theta_a \phi_a) \mathbf{C}_{\ell}(\theta_b \phi_b), \quad (\text{C.13})$$

$$\frac{e^{ik\rho}}{\rho} = ik h_0^{(1)}(k\rho) = ik \sum_{\ell} (2\ell + 1) j_{\ell}(ka) h_{\ell}^{(1)}(kb) \times \mathbf{C}_{\ell}(\theta_a \phi_a) \mathbf{C}_{\ell}(\theta_b \phi_b), \quad (\text{C.14})$$

$$\frac{e^{-\alpha\rho}}{\alpha\rho} = - \sum_{\ell} (2\ell + 1) j_{\ell}(i\alpha a) h_{\ell}^{(1)}(i\alpha b) \mathbf{C}_{\ell}(\theta_a \phi_a) \mathbf{C}_{\ell}(\theta_b \phi_b), \quad (\text{C.15})$$

where  $h_{\ell}^{(1)}(kr)$  denote the spherical Hankel functions of the first type; and if  $\mathbf{r} = \mathbf{a} + \mathbf{b}$ , we get the expansion

$$r^{\ell} C_{\ell m}(\theta_r, \phi_r) = \sum_{\lambda\mu} \sqrt{\frac{2\ell!}{2\lambda!2(\ell-\lambda)!}} (\ell - \lambda \ m - \mu, \lambda\mu | \ell m) \times a^{\ell-\lambda} b^{\lambda} C_{\ell-\lambda \ m-\mu}(\theta_a \phi_a) C_{\lambda\mu}(\theta_b \phi_b). \quad (\text{C.16})$$

## C.2 Tensorial Products of Irreducible Tensor Operators

*Definition:* Let  $\mathbf{T}_{k_1}$ ,  $\mathbf{U}_{k_2}$  be two irreducible tensor operators of rank  $k_1$  and  $k_2$ , respectively. Then  $\mathbf{T}_{k_1} \otimes \mathbf{U}_{k_2} \equiv$  the manifold of the  $(2k_1 + 1)(2k_2 + 1)$ , not necessarily linear independent, operators  $T_{k_1 q_1} U_{k_2 q_2}$ . It is a (reducible) tensor operator.

$\mathbf{V}_K \equiv [\mathbf{T}_{k_1} \otimes \mathbf{U}_{k_2}]_K$  is the tensorial product of rank  $K$ , which is the irreducible tensor operator of rank  $K$  with its components

$$V_{KQ}(k_1, k_2) = \sum_{q_1 q_2} (k_1 q_1, k_2 q_2 | K Q) T_{k_1 q_1} U_{k_2 q_2}, \quad (\text{C.17})$$

where,  $|k_1 - k_2| \leq K \leq k_1 + k_2$  is a necessary condition. Re-writing (C.17) in terms of  $3j$ -symbols yields

$$V_{KQ}(k_1, k_2) = \sum_{q_1 q_2} (-1)^{k_1 - k_2 + Q} \sqrt{2K + 1} \begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix} T_{k_1 q_1} U_{k_2 q_2}. \quad (\text{C.18})$$

In case that  $k_1 = k_2 = k$ , the scalar product is defined as

$$S \equiv (\mathbf{T}_k \cdot \mathbf{U}_k) = \sum_q (-1)^q T_{kq} U_{k-q}. \quad (\text{C.19})$$

Note, that  $S$  is not irreducible. It is related to the irreducible tensor of rank zero via

$$S = (-1)^k \sqrt{2k + 1} V_{00}(k, k). \quad (\text{C.20})$$

*Reduced matrix elements:* Suppose a composite quantum system to be generated from its joint sub-systems 1 and 2. Let  $\mathbf{J}_1$  and  $\mathbf{J}_2$  be the total angular momenta of the related sub-systems, and  $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$ .

Let  $|\tau_1 J_1 M_1\rangle$  and  $|\tau_2 J_2 M_2\rangle$  be the basis sets of system 1 and 2, respectively.

$\mathbf{T}_{k_1}$  and  $\mathbf{U}_{k_2}$  are irreducible tensor operators which solely interact with the variables in the Hilbert sub-space of system 1 and 2, respectively.

Let  $\mathbf{V}_K$  be the tensorial product of rank  $K$  according to its definition (C.17). Then, in the standard basis  $\{\tau_1 \tau_2 \mathbf{J}_1^2 \mathbf{J}_2^2 J_z\}$  the matrix elements of  $\mathbf{V}_K(k_1, k_2)$  are given as

$$\begin{aligned} \langle \tau_1 \tau_2 J_1 J_2 J \| \mathbf{V}_K \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle &= \sqrt{(2J+1)(2K+1)(2J'+1)} \\ &\times \begin{Bmatrix} J'_1 & J'_2 & J' \\ k_1 & k_2 & K \\ J_1 & J_2 & J \end{Bmatrix} \langle \tau_1 J_1 \| \mathbf{T}_{k_1} \| \tau'_1 J'_1 \rangle \langle \tau_2 J_2 \| \mathbf{U}_{k_2} \| \tau'_2 J'_2 \rangle. \end{aligned} \quad (\text{C.21})$$

*Special cases* occur if the tensor operator acts in one of the sub-systems, only.

Let  $\mathbf{U} = \mathbf{1}$  be the identity operator acting on sub-system 2. Then, we have  $K = k_1 = k$ , and (C.21) can be reduced to

$$\begin{aligned} \langle \tau_1 \tau_2 J_1 J_2 J \| \mathbf{T}_k \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle &= \delta_{\tau_2 \tau'_2} \delta_{J_2 J'_2} \langle \tau_1 J_1 \| \mathbf{T}_k \| \tau'_1 J'_1 \rangle \\ &\times (-1)^{J'+J_1+J_2+k} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} J_1 & k & J'_1 \\ J' & J_2 & J \end{Bmatrix}. \end{aligned} \quad (\text{C.22})$$

In the opposite case we have  $\mathbf{T} = \mathbf{1}$  the identity operator acting in sub-system 1. Then,  $K = k_2 = k$ , and (C.21) is reduced to

$$\begin{aligned} \langle \tau_1 \tau_2 J_1 J_2 J \| \mathbf{U}_k \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle &= \delta_{\tau_1 \tau'_1} \delta_{J_1 J'_1} \langle \tau_2 J_2 \| \mathbf{U}_k \| \tau'_2 J'_2 \rangle \\ &\times (-1)^{J+J_1+J'_2+k} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} J_2 & k & J'_2 \\ J' & J_1 & J \end{Bmatrix}. \end{aligned} \quad (\text{C.23})$$

In case of a compound scalar operator  $\mathbf{V}_0(k, k)$  we have  $K = 0$  and  $k_1 = k_2 = k$ . Applying (C.21) and (A.40) yields

$$\begin{aligned} \langle \tau_1 \tau_2 J_1 J_2 J \| \mathbf{V}_0(k, k) \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle &= \langle \tau_1 \tau_2 J_1 J_2 J \| [\mathbf{T}_k \otimes \mathbf{U}_k]_0^{(0)} \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle \\ &= \delta_{JJ'} (-1)^{k+J+J_2+J'_1} \sqrt{\frac{2J+1}{2k+1}} \begin{Bmatrix} J_1 & k & J'_1 \\ J'_2 & J & J_2 \end{Bmatrix} \\ &\times \langle \tau_1 J_1 \| \mathbf{T}_k \| \tau'_1 J'_1 \rangle \langle \tau_2 J_2 \| \mathbf{U}_k \| \tau'_2 J'_2 \rangle. \end{aligned} \quad (\text{C.24})$$

Often, the scalar product  $\mathbf{T}_k \cdot \mathbf{U}_k$  is used in place of  $[\mathbf{T}_k \otimes \mathbf{U}_k]_0^{(0)}$  as the scalar operator. Applying the Wigner–Eckart theorem (C.6) and using (C.19) and (C.20), we can re-write (C.24) as

$$\begin{aligned} \langle \tau_1 \tau_2 J_1 J_2 J M | (\mathbf{T}_k \cdot \mathbf{U}_k) | \tau'_1 \tau'_2 J'_1 J'_2 J' M' \rangle &= \delta_{JJ'} \delta_{MM'} (-1)^k \\ &\times \sqrt{\frac{2k+1}{2J+1}} \langle \tau_1 \tau_2 J_1 J_2 J \| \mathbf{V}_0(k, k) \| \tau'_1 \tau'_2 J'_1 J'_2 J' \rangle \\ &= \delta_{JJ'} \delta_{MM'} (-1)^{J+J_2+J'_1} \begin{Bmatrix} J_1 & k & J'_1 \\ J'_2 & J & J_2 \end{Bmatrix} \\ &\times \langle \tau_1 J_1 \| \mathbf{T}_k \| \tau'_1 J'_1 \rangle \langle \tau_2 J_2 \| \mathbf{U}_k \| \tau'_2 J'_2 \rangle. \end{aligned} \quad (\text{C.25})$$

Eventually, a more general case is the situation when the system is in a state  $|\tau JM\rangle$  with sharp angular momentum  $J$  that is not decomposable into sub-system states. Then, the matrix elements of the compound tensor  $V_{KQ}(k_1, k_2) = [\mathbf{T}_{k_1} \otimes \mathbf{T}_{k_2}]_Q^{(K)}$ , where  $V_{KQ}(k_1, k_2)$  can act only on the set of variables of the system, are obtained as

$$\begin{aligned} \langle \tau J \| \mathbf{V}_K \| \tau' J' \rangle &= \langle \tau J \| [\mathbf{T}_{k_1} \otimes \mathbf{T}_{k_2}]_K \| \tau' J' \rangle \\ &= (-1)^{K+J+J'} \sqrt{2K+1} \sum_{\tau'' J''} \left\{ \begin{matrix} k_1 & k_2 & K \\ J & J' & J'' \end{matrix} \right\} \\ &\quad \times \langle \tau J \| \mathbf{T}_{k_1} \| \tau'' J'' \rangle \langle \tau'' J'' \| \mathbf{T}_{k_2} \| \tau' J' \rangle. \end{aligned} \quad (\text{C.26})$$

A particular application of (C.22) or (C.23) is the reduction of composite systems described in the  $LSJ$  coupling scheme. Suppose  $\mathbf{L} + \mathbf{S} = \mathbf{J}$  and  $\mathbf{L}' + \mathbf{S}' = \mathbf{J}'$ . If the tensor operator  $T_{KQ}$  acts only on the system with angular momenta  $L, L'$  then

$$\begin{aligned} \langle (LS)J \| \mathbf{T}_K \| (L'S')J' \rangle &= \delta_{SS'} (-1)^{L+S+J'+K} \sqrt{(2J+1)(2J'+1)} \\ &\quad \times \left\{ \begin{matrix} L & L' & K \\ J' & J & S \end{matrix} \right\} \langle L \| \mathbf{T}_K \| L' \rangle. \end{aligned} \quad (\text{C.27})$$

Basic reduced matrix elements for the identity and the total angular momentum operator have been given in (C.8) and (C.9), respectively. Reduced matrix elements for the spherical harmonics yield

$$\langle \ell \| \mathbf{Y}_k \| \ell' \rangle = (-1)^\ell \sqrt{\frac{(2\ell+1)(2k+1)(2\ell'+1)}{4\pi}} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{C.28})$$

Using the renormalized spherical harmonics instead gives a more compact relation

$$\langle \ell \| \mathbf{C}_k \| \ell' \rangle = (-1)^\ell \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{C.29})$$

Considering the composite angular momentum – electron spin system the renormalized spherical harmonics act in the angular momentum Hilbert sub-space, only. Applying (C.22) and (C.29) gives

$$\begin{aligned} \langle (\ell 1/2)j \| \mathbf{C}_k \| (\ell' 1/2)j' \rangle &= \sqrt{(2\ell+1)(2\ell'+1)(2j+1)(2j'+1)} \\ &\quad \times (-1)^{j'+1/2+k} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} \ell & k & \ell' \\ j' & \frac{1}{2} & j \end{matrix} \right\}, \end{aligned} \quad (\text{C.30})$$

and combining with (A.29) eventually yields

$$\langle (\ell 1/2)j \| \mathbf{C}_k \| (\ell' 1/2)j' \rangle = (-1)^{j'-1/2-k} \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} j & j' & k \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \quad (\text{C.31})$$

provided that  $\ell + \ell' + k$  is even, and zero otherwise.



## D Expansion of Dipole Matrix Elements

Following Amusia and Cherepkov (1975, pp. 16) the  $T$  matrix elements may be written as

$$\langle JM\mathbf{p}^{(-)}m_s|T_i|J_0M_0\omega\mathbf{n}\lambda\rangle = \sum_{q=1}^N \langle JM\mathbf{p}^{(-)}m_s|\exp^{i\mathbf{k}\cdot\mathbf{r}}(\mathbf{e}_\lambda \cdot \mathbf{p}_q^*)|J_0M_0\rangle, \quad (\text{D.1})$$

where  $N$  denotes the number of electrons in the atomic shell,  $\mathbf{e}_\lambda$  ( $\lambda = \pm 1$ ) is the photon polarization vector which is chosen that  $\mathbf{e}_\lambda \cdot \mathbf{n} = 0$ , and  $\mathbf{p}_q$  is the momentum of the  $q^{th}$  electron of the atom. For completeness we note, that (D.1) holds for photoionization. In the case of photoemission the operator must be replaced by its complex conjugate, i.e.  $\mathbf{e}_\lambda^* \cdot \mathbf{p}_q$ .

Applying the long-wavelength limit of the dipole approximation, i.e.  $kr_q \ll 1$ , the exponential function can be replaced by unity;  $\exp(i\mathbf{k} \cdot \mathbf{r}) \approx 1$ .

Thus, for an arbitrarily polarized photon beam, the  $T$  matrix elements may be written as

$$\begin{aligned} \langle JM\mathbf{p}^{(-)}m_s|T_i|J_0M_0\omega\mathbf{n}\lambda\rangle &= \sum_{q=1}^N \langle JM\mathbf{p}^{(-)}m_s|(\mathbf{e}_\lambda \cdot \mathbf{p}_q^*)|J_0M_0\rangle \\ &= \sum_{q=1}^N i\omega \langle JM\mathbf{p}^{(-)}m_s|(\mathbf{e}_\lambda \cdot \mathbf{r}_q^*)|J_0M_0\rangle, \end{aligned} \quad (\text{D.2})$$

where the first term denotes the “velocity form” and the latter the “length form” of the dipole transition matrix element. The dipole approximation is valid in a rather broad region of energy (Amusia 1990)

$$Z^2 < \omega \ll Z\alpha^{-1}, \quad (\text{D.3})$$

where  $\alpha^{-1} = 137$  denotes the fine structure constant. Throughout this book the length form of the dipole matrix elements is used.

In our chosen coordinate frame the polarization vector  $\mathbf{e}_\lambda$  can be eliminated by noting that in the helicity system the coordinate system is “spanned” by the three unit vectors  $\mathbf{e}_{+1}$ ,  $\mathbf{e}_{-1}$ ,  $\mathbf{n}$ , and that the dipole operator  $\mathbf{r}$  can be therefore expanded in terms of this basis<sup>1</sup>

$$\mathbf{r} = r_{+1}^*\mathbf{e}_{+1} + r_{-1}^*\mathbf{e}_{-1} + r_0^*\mathbf{n}, \quad (\text{D.4})$$

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<sup>1</sup> Here, and throughout the following the index  $q$  and the summation over  $q$ , referring to the  $q^{th}$  electron, are suppressed if not causing ambiguities.

where  $r_{\pm 1}$  and  $r_0$  are the components of  $\mathbf{r}$  along the directions of  $\mathbf{e}_{\pm 1}$  and  $\mathbf{n}$ , respectively. I.e.,  $r_{\pm 1}$  and  $r_0$  are the spherical components of the vector  $\mathbf{r}$ . In this system the scalar product of  $\mathbf{r}$  and  $\mathbf{e}_\lambda$  is given by

$$\mathbf{e}_\lambda \cdot \mathbf{r}^* = r_\lambda. \quad (\text{D.5})$$

The final state electron wavefunction can be expanded into partial waves. Applying the results of Lohmann (1990) we get

$$\begin{aligned} |\mathbf{p}^{(-)} m_s\rangle = \psi_{\mathbf{p} m_s}^{(-)}(\mathbf{r}) &= \frac{1}{|\mathbf{p}|} \sum_{\substack{\ell m j m_j \\ m' \mu}} i^\ell e^{-i\sigma_\ell^j} Y_{\ell m}^*(\hat{\mathbf{p}}) R_{\varepsilon \ell}^j(r) Y_{\ell m'}(\hat{\mathbf{r}}) \chi_\mu \\ &\times (\ell m, 1/2 m_s | j m_j) (\ell m', 1/2 \mu | j m_j), \end{aligned} \quad (\text{D.6})$$

which yields for the expansion coefficients

$$a_{\ell m}^j = \langle j \ell m | \mathbf{p}^{(-)} \rangle = \frac{1}{|\mathbf{p}|} i^\ell e^{-i\sigma_\ell^j} Y_{\ell m}^*(\hat{\mathbf{p}}). \quad (\text{D.7})$$

Inserting the partial wave expansions into the transition matrix element we get

$$\begin{aligned} \langle J M \mathbf{p}^{(-)} m_s | r_\lambda | J_0 M_0 \rangle &= \sum_{\ell m} a_{\ell m}^{j*} \langle J M \ell m 1/2 m_s | r_\lambda | J_0 M_0 \rangle \\ &= \sum_{\substack{\ell m j m_j \\ J_1 M_1}} a_{\ell m}^{j*} \langle (J j) J_1 M_1 | r_\lambda | J_0 M_0 \rangle \\ &\times (\ell m, 1/2 m_s | j m_j) (J M, j m_j | J_1 M_1). \end{aligned} \quad (\text{D.8})$$

Using the fact that  $\hat{\mathbf{r}}_\lambda$  is a tensor operator of rank one and applying the Wigner-Eckart theorem (C.6) we get

$$\langle J_1 M_1 | r_\lambda | J_0 M_0 \rangle = (-1)^{J_1 - M_1} \begin{pmatrix} J_1 & 1 & J_0 \\ -M_1 & \lambda & M_0 \end{pmatrix} \langle J_1 || r || J_0 \rangle. \quad (\text{D.9})$$

With this, we obtain for the dipole matrix element

$$\begin{aligned} \langle J M \mathbf{p}^{(-)} m_s | T_i | J_0 M_0 \omega \mathbf{n} \lambda \rangle &= \langle J M \mathbf{p}^{(-)} m_s | d_\lambda | J_0 M_0 \rangle \\ &= \sum_{\substack{\ell m j m_j \\ J_1 M_1}} a_{\ell m}^{j*} \langle (J j) J_1 || d || J_0 \rangle \\ &\times (-1)^{-\ell + 1/2 - m_j - J + j - J_1} \\ &\times \sqrt{(2j+1)(2J_1+1)} \begin{pmatrix} \ell & 1/2 & j \\ m & m_s & -m_j \end{pmatrix} \\ &\times \begin{pmatrix} J & j & J_1 \\ M & m_j & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & 1 & J_0 \\ -M_1 & \lambda & M_0 \end{pmatrix}, \end{aligned} \quad (\text{D.10})$$

where we introduced the abbreviation  $d_\lambda = i\omega r_\lambda$ . Inserting the expansion coefficients we finally end up with (2.41).

# E Anisotropy Parameters for Electron Impact Ionization

## E.1 Expansion of Matrix Elements

The transition matrix elements of (2.92) can be evaluated applying a triple partial wave expansion (see Appendix D)

$$\begin{aligned}
 \langle JM \mathbf{p}_1^{(-)} m_{s_1} \mathbf{p}_2^{(-)} m_{s_2} | V | J_0 M_0 \mathbf{p}_0^{(+)} m_{s_0} \rangle &= \sum_{\substack{\ell_0 \ell_1 m_1 \\ \ell_2 m_2}} a_{\ell_1 m_1}^{j_1 *} b_{\ell_2 m_2}^{j_2 *} c_{\ell_0}^{j_0} \\
 &\times \langle JM \ell_1 m_1 1/2 m_{s_1} \ell_2 m_2 1/2 m_{s_2} | V | J_0 M_0 \ell_0 0 1/2 m_{s_0} \rangle \\
 &= \sum_{\substack{\ell_0 \ell_1 m_1 \ell_2 m_2 j_0 m_{j_0} \\ j_1 m_{j_1} j_2 m_{j_2} \\ J_1 M_1 J_2 M_2 J_f M_f}} a_{\ell_1 m_1}^{j_1 *} b_{\ell_2 m_2}^{j_2 *} c_{\ell_0}^{j_0} \\
 &\times \langle ([J j_1] J_1 j_2) J_f M_f | V | (J_0 j_0) J_2 M_2 \rangle \\
 &\times (\ell_1 m_1, 1/2 m_{s_1} | j_1 m_{j_1}) (\ell_2 m_2, 1/2 m_{s_2} | j_2 m_{j_2}) \\
 &\times (\ell_0 0, 1/2 m_{s_0} | j_0 m_{j_0}) (JM, j_1 m_{j_1} | J_1 M_1) \\
 &\times (J_1 M_1, j_2 m_{j_2} | J_f M_f) (J_0 M_0, j_0 m_{j_0} | J_2 M_2). \tag{E.1}
 \end{aligned}$$

Using the fact that  $V$  is a zero-order tensor operator and applying the Wigner–Eckart theorem (C.6) we get

$$\begin{aligned}
 \langle J_f M_f | V | J_2 M_2 \rangle &= (-1)^{J_f - M_f} \begin{pmatrix} J_f & 0 & J_2 \\ -M_f & 0 & M_2 \end{pmatrix} \langle J_f \| V \| J_2 \rangle \\
 &= \frac{1}{\sqrt{2J_f + 1}} \langle J_f \| V \| J_2 \rangle \delta_{J_f J_2} \delta_{M_f M_2}. \tag{E.2}
 \end{aligned}$$

With this, we finally obtain for the transition matrix element

$$\begin{aligned}
\langle JM\mathbf{p}_1^{(-)}m_{s1}\mathbf{p}_2^{(-)}m_{s2}|V|J_0M_0\mathbf{p}_0^{(+)}m_{s0}\rangle = & \sum_{\substack{\ell_0\ell_1m_1\ell_2m_2j_0m_{j_0} \\ j_1m_{j_1}j_2m_{j_2} \\ J_1M_1J_fM_f}} a_{\ell_1m_1}^{j_1*} \\
& \times b_{\ell_2m_2}^{j_2*} c_{\ell_0}^{j_0} \langle ([Jj_1]J_1j_2)J_f \| V \| (J_0j_0)J_f \rangle \\
& \times (-1)^{-\ell_1+1/2-m_{j_1}-\ell_2+1/2-m_{j_2}-\ell_0+1/2-m_{j_0}} \\
& \times (-1)^{-J+j_1-M_1-J_1+j_2-M_f-J_0+j_0-M_f} \\
& \times \sqrt{(2j_1+1)(2j_2+1)(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \begin{pmatrix} \ell_1 & 1/2 & j_1 \\ m_1 & m_{s1} & -m_{j_1} \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j_2 \\ m_2 & m_{s2} & -m_{j_2} \end{pmatrix} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s0} & -m_{j_0} \end{pmatrix} \\
& \times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix}. \quad (\text{E.3})
\end{aligned}$$

## E.2 Derivation of Anisotropy Parameters

Inserting the derived expression (E.3) for the transition matrix element twice into (2.92) the anisotropy parameter  $B_e$  can be written as

$$\begin{aligned}
B_e(K'Q',kq) = & \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \int d\mathbf{p}_1 \int d\mathbf{p}_2 \sum_{\substack{MM'm_{s1}m_{s2} \\ m_{s0}m'_{s0}M_0}} \\
& \times \sum_{\substack{\ell_0\ell_1m_1\ell_2m_2 \\ j_0m_{j_0}j_1m_{j_1}j_2m_{j_2} \\ J_1M_1J_fM_f}} \sum_{\substack{\ell'_0\ell'_1m'_1\ell'_2m'_2 \\ j_0m'_{j_0}j'_1m'_{j_1}j'_2m'_{j_2} \\ J'_1M'_1J'_fM'_f}} (-1)^{J-M+1/2-m_{s0}} \\
& \times a_{\ell_1m_1}^{j_1*} b_{\ell_2m_2}^{j_2*} c_{\ell_0}^{j_0} \langle ([Jj_1]J_1j_2)J_f \| V \| (J_0j_0)J_f \rangle \\
& \times a_{\ell'_1m'_1}^{j'_1*} b_{\ell'_2m'_2}^{j'_2*} c_{\ell'_0}^{j'_0} \langle ([Jj'_1]J'_1j'_2)J'_f \| V \| (J_0j'_0)J'_f \rangle \\
& \times (-1)^{-\ell_1+1/2-m_{j_1}-\ell_2+1/2-m_{j_2}-\ell_0+1/2-m_{j_0}} \\
& \times (-1)^{-J+j_1-M_1-J_1+j_2-M_f-J_0+j_0-M_f} \\
& \times (-1)^{-\ell'_1+1/2-m'_{j_1}-\ell'_2+1/2-m'_{j_2}-\ell'_0+1/2-m'_{j_0}} \\
& \times (-1)^{-J+j'_1-M'_1-J'_1+j'_2-M'_f-J_0+j'_0-M'_f} \\
& \times \sqrt{(2j_1+1)(2j_2+1)(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2j'_1+1)(2j'_2+1)(2j'_0+1)(2J'_1+1)(2J'_f+1)}
\end{aligned}$$

$$\begin{aligned}
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} J & J & K' \\ M & -M' & -Q' \end{pmatrix} \\
& \times \begin{pmatrix} \ell_1 & 1/2 & j_1 \\ m_1 & m_{s_1} & -m_{j_1} \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j_2 \\ m_2 & m_{s_2} & -m_{j_2} \end{pmatrix} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \\
& \times \begin{pmatrix} \ell'_1 & 1/2 & j'_1 \\ m'_1 & m_{s_1} & -m'_{j_1} \end{pmatrix} \begin{pmatrix} \ell'_2 & 1/2 & j'_2 \\ m'_2 & m_{s_2} & -m'_{j_2} \end{pmatrix} \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix} \\
& \times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix} \\
& \times \begin{pmatrix} J & j'_1 & J'_1 \\ M' & m'_{j_1} & -M'_1 \end{pmatrix} \begin{pmatrix} J'_1 & j'_2 & J'_f \\ M'_1 & m'_{j_2} & -M'_f \end{pmatrix} \begin{pmatrix} J_0 & j'_0 & J'_f \\ M_0 & m'_{j_0} & -M'_f \end{pmatrix}. \quad (\text{E.4})
\end{aligned}$$

The integration over the solid angles and the energy distribution of the electrons  $e_1^-$  and  $e_2^-$  can be carried out,

$$\int d\mathbf{p}_1 a_{\ell_1 m_1}^{j_1 *} a_{\ell'_1 m'_1}^{j'_1} = e^{i(\sigma_{\ell_1}^{j_1} - \sigma_{\ell'_1}^{j'_1})} \delta_{\ell_1 \ell'_1} \delta_{m_1 m'_1} \Delta E_1, \quad (\text{E.5})$$

and

$$\int d\mathbf{p}_2 b_{\ell_2 m_2}^{j_2 *} b_{\ell'_2 m'_2}^{j'_2} = e^{i(\sigma_{\ell_2}^{j_2} - \sigma_{\ell'_2}^{j'_2})} \delta_{\ell_2 \ell'_2} \delta_{m_2 m'_2} \Delta E_2. \quad (\text{E.6})$$

Note, that the phase difference can still be non-zero because without further assumptions we generally have  $j_1 \neq j'_1$  and  $j_2 \neq j'_2$ .

Applying the above selection rules and defining  $\Delta E_{12} = \Delta E_1 + \Delta E_2$  we obtain

$$\begin{aligned}
B_e(K' Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{MM'm_{s_1}m_{s_2} \\ m_{s_0}m'_{s_0}M_0}} \sum_{\substack{\ell_0 \ell_1 m_1 \ell_2 m_2 \\ j_0 m_{j_0} j_1 m_{j_1} j_2 m_{j_2} \\ J_1 M_1 J_f M_f}} \\
&\times \sum_{\substack{\ell'_0 J'_1 M'_1 J'_f M'_f \\ j'_0 m'_{j_0} j'_1 m'_{j_1} j'_2 m'_{j_2}}} (-1)^{J-M+1/2-m_{s_0}} e^{i(\sigma_{\ell_1}^{j_1} - \sigma_{\ell'_1}^{j'_1})} e^{i(\sigma_{\ell_2}^{j_2} - \sigma_{\ell'_2}^{j'_2})} \\
&\times c_{\ell_0}^{j_0} \langle ([J j_1] J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
&\times c_{\ell'_0}^{j'_0 *} \langle ([J j'_1] J'_1 j'_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
&\times (-1)^{-\ell_1+1/2-m_{j_1}-\ell_2+1/2-m_{j_2}-\ell_0+1/2-m_{j_0}} \\
&\times (-1)^{-J+j_1-M_1-J_1+j_2-M_f-J_0+j_0-M_f} \\
&\times (-1)^{-\ell_1+1/2-m'_{j_1}-\ell_2+1/2-m'_{j_2}-\ell'_0+1/2-m'_{j_0}} \\
&\times (-1)^{-J+j'_1-M'_1-J'_1+j'_2-M'_f-J_0+j'_0-M'_f} \\
&\times \sqrt{(2j_1+1)(2j_2+1)(2j_0+1)(2J_1+1)(2J_f+1)}
\end{aligned}$$

$$\begin{aligned}
& \times \sqrt{(2j'_1 + 1)(2j'_2 + 1)(2j'_0 + 1)(2J'_1 + 1)(2J'_f + 1)} \\
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} J & J & K' \\ M & -M' & -Q' \end{pmatrix} \\
& \times \begin{pmatrix} \ell_1 & 1/2 & j_1 \\ m_1 & m_{s_1} & -m_{j_1} \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j_2 \\ m_2 & m_{s_2} & -m_{j_2} \end{pmatrix} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \\
& \times \begin{pmatrix} \ell_1 & 1/2 & j'_1 \\ m_1 & m_{s_1} & -m'_{j_1} \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j'_2 \\ m_2 & m_{s_2} & -m'_{j_2} \end{pmatrix} \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix} \\
& \times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix} \\
& \times \begin{pmatrix} J & j'_1 & J'_1 \\ M' & m'_{j_1} & -M'_1 \end{pmatrix} \begin{pmatrix} J'_1 & j'_2 & J'_f \\ M'_1 & m'_{j_2} & -M'_f \end{pmatrix} \begin{pmatrix} J_0 & j'_0 & J'_f \\ M_0 & m'_{j_0} & -M'_f \end{pmatrix}. \quad (\text{E.7})
\end{aligned}$$

Now, applying the orthogonality relations of the 3  $j$ -symbols (A.8a), the summation over  $m_1, m_{s_1}$  and  $m_2, m_{s_2}$  can be carried out which gives the selection rules

$$j_1 = j'_1, \quad m_{j_1} = m'_{j_1}, \quad (\text{E.8})$$

and

$$j_2 = j'_2, \quad m_{j_2} = m'_{j_2}. \quad (\text{E.9})$$

Thus, the phase difference disappears which yields

$$\begin{aligned}
B_e(K'Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{MM'M_0 \\ m_{s_0}m'_{s_0}}} \sum_{\substack{\ell_0\ell_1\ell_2j_0m_{j_0} \\ j_1m_{j_1}j_2m_{j_2} \\ J_1M_1J_fM_f}} \sum_{\substack{\ell'_0j'_0m'_{j_0} \\ J'_1M'_1J'_fM'_f}} \\
& \times c_{\ell_0}^{j_0} \langle ([Jj_1]J_1j_2)J_f \| V \| (J_0j_0)J_f \rangle \\
& \times c_{\ell'_0}^{j'_0} \langle ([Jj_1]J'_1j_2)J'_f \| V \| (J_0j'_0)J'_f \rangle \\
& \times (-1)^{J-M+1/2-m_{s_0}+\ell'_0-\ell_0+j_0-j'_0+m_{j_0}-m'_{j_0}} \\
& \times (-1)^{J'_1-J_1+M_1-M'_1+2M_f-2M'_f} \\
& \times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} J & J & K' \\ M & -M' & -Q' \end{pmatrix} \\
& \times \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
& \times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix} \\
& \times \begin{pmatrix} J & j_1 & J'_1 \\ M' & m_{j_1} & -M'_1 \end{pmatrix} \begin{pmatrix} J'_1 & j_2 & J'_f \\ M'_1 & m_{j_2} & -M'_f \end{pmatrix} \begin{pmatrix} J_0 & j'_0 & J'_f \\ M_0 & m'_{j_0} & -M'_f \end{pmatrix}.
\end{aligned} \tag{E.10}$$

Carrying out the sum over  $M$ ,  $M'$ , and  $m_{j_1}$  by using (A.25) the  $2^{nd}$ ,  $5^{th}$ , and  $8^{th}$   $3j$ -symbols can be contracted

$$\begin{aligned}
B_e(K'Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{\ell_0 \ell_1 \ell_2 M_0 \\ m_{s_0} m'_{s_0}}} \sum_{\substack{j_0 m_{j_0} j_1 j_2 m_{j_2} \\ J_1 M_1 J_f M_f}} \sum_{\substack{\ell'_0 j'_0 m'_{j_0} \\ J'_1 M'_1 J'_f M'_f}} \\
& \times c_{\ell_0}^{j_0} \langle ([Jj_1]J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
& \times c_{\ell'_0}^{j'_0 *} \langle ([Jj_1]J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
& \times (-1)^{1/2-m_{s_0}+\ell'_0-\ell_0+j_0-j'_0+m_{j_0}-m'_{j_0}} \\
& \times (-1)^{J-j_1+J'_1-J_1+M_1-2M'_1+2M_f-2M'_f} \\
& \times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} J_1 & J'_1 & K' \\ -M_1 & M'_1 & -Q' \end{pmatrix} \left\{ \begin{matrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{matrix} \right\} \\
& \times \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix} \\
& \times \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix} \begin{pmatrix} J'_1 & j_2 & J'_f \\ M'_1 & m_{j_2} & -M'_f \end{pmatrix} \begin{pmatrix} J_0 & j'_0 & J'_f \\ M_0 & m'_{j_0} & -M'_f \end{pmatrix}.
\end{aligned} \tag{E.11}$$

Further, summing over  $M_1$ ,  $M'_1$ , and  $m_{j_2}$  and again using (A.25) the  $2^{nd}$ ,  $4^{th}$ , and  $7^{th}$   $3j$ -symbols are contracted to

$$\begin{aligned}
B_e(K'Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{\ell_1 \ell_2 j_1 j_2 \\ M_0 m_{s_0} m'_{s_0}}} \sum_{\substack{\ell_0 j_0 m_{j_0} \\ J_1 J_f M_f}} \sum_{\substack{\ell'_0 j'_0 m'_{j_0} \\ J'_1 J'_f M'_f}} \\
& \times c_{\ell_0}^{j_0} \langle ([Jj_1]J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
& \times c_{\ell'_0}^{j'_0 *} \langle ([Jj_1]J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
& \times (-1)^{1/2-m_{s_0}+\ell'_0-\ell_0+j_0-j'_0+m_{j_0}-m'_{j_0}}
\end{aligned}$$

$$\begin{aligned}
& \times (-1)^{K'+J'_1-J_1+J-j_1-j_2+2M_f-M'_f} \\
& \times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} J_f & J'_f & K' \\ -M_f & M'_f & Q' \end{pmatrix} \\
& \times \left\{ \begin{matrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{matrix} \right\} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix} \\
& \times \left\{ \begin{matrix} J_f & J'_f & K' \\ J'_1 & J_1 & j_2 \end{matrix} \right\} \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix} \begin{pmatrix} J_0 & j'_0 & J'_f \\ M_0 & m'_{j_0} & -M'_f \end{pmatrix} .
\end{aligned} \tag{E.12}$$

Once more, applying (A.25) for carrying out the sum over  $M_f$ ,  $M'_f$ , and  $M_0$  the  $2^{nd}$ ,  $4^{th}$ , and  $6^{th}$   $3j$ -symbols yield

$$\begin{aligned}
B_e(K'Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{\ell_1 \ell_2 j_1 j_2 \\ m_{s_0} m'_{s_0}}} \sum_{\substack{\ell_0 j_0 m_{j_0} \\ J_1 J_f}} \sum_{\substack{\ell'_0 j'_0 m'_{j_0} \\ J'_1 J'_f}} \\
& \times c_{\ell_0}^{j_0} \langle ([Jj_1]J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
& \times c_{\ell'_0}^{j'_0 *} \langle ([Jj_1]J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
& \times (-1)^{J'_1-J_1+J-j_1-j_2-J_f-J'_f-J_0} \\
& \times (-1)^{K'+\ell'_0-\ell_0+j_0-j'_0-1/2+q} \\
& \times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
& \times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m'_{s_0} & -q \end{pmatrix} \begin{pmatrix} j'_0 & j_0 & K' \\ m'_{j_0} & -m_{j_0} & Q' \end{pmatrix} \\
& \times \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} \ell'_0 & 1/2 & j'_0 \\ 0 & m'_{s_0} & -m'_{j_0} \end{pmatrix} \\
& \times \left\{ \begin{matrix} j'_0 & j_0 & K' \\ J_f & J'_f & J_0 \end{matrix} \right\} \left\{ \begin{matrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{matrix} \right\} \left\{ \begin{matrix} J_f & J'_f & K' \\ J'_1 & J_1 & j_2 \end{matrix} \right\} .
\end{aligned} \tag{E.13}$$

Eventually, carrying out the sum over  $m_{s_0}$ ,  $m'_{s_0}$ ,  $m_{j_0}$ , and  $m'_{j_0}$  the remaining four  $3j$ -symbols can be contracted to form a  $9j$ -symbol via (A.49) by introducing the artificial angular momentum  $b$  and its magnetic component  $\beta$ .



$$\begin{aligned}
B_e(K' Q', kq) &= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{\ell_1 \ell_2 j_1 j_2 \\ b\beta}} \sum_{\substack{\ell_0 j_0 \ell'_0 j'_0 \\ J_1 J_f J'_1 J'_f}} (2b+1) \\
&\times c_{\ell_0}^{j_0} \langle ([J j_1] J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
&\times c_{\ell'_0}^{j'_0 *} \langle ([J j_1] J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
&\times (-1)^{J_1 - J'_1 - J + j_1 + j_2 + J_f + J'_f + J_0 + \ell_0 - j'_0 + 1 - q} \\
&\times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
&\times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
&\times \begin{pmatrix} K' & b & k \\ Q' & \beta & -q \end{pmatrix} \begin{pmatrix} b & \ell_0 & \ell'_0 \\ \beta & 0 & 0 \end{pmatrix} \begin{Bmatrix} K' & b & k \\ j_0 & \ell_0 & 1/2 \\ j'_0 & \ell'_0 & 1/2 \end{Bmatrix} \\
&\times \begin{Bmatrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{Bmatrix} \begin{Bmatrix} J_f & J'_f & K' \\ J'_1 & J_1 & j_2 \end{Bmatrix} \begin{Bmatrix} j'_0 & j_0 & K' \\ J_f & J'_f & J_0 \end{Bmatrix}. \quad (E.14)
\end{aligned}$$

The second  $3j$ -symbol immediately gives  $\beta = 0$ . Thus, the first  $3j$ -symbol yields the important selection rule

$$q = Q'. \quad (E.15)$$

With this, the anisotropy parameter can be redefined as

$$\begin{aligned}
B_e(K' kq) &= B_e(K' Q', kq) \delta_{Q'q} \\
&= \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{b\ell_1 j_1 \\ \ell_2 j_2}} \sum_{\substack{\ell_0 j_0 \ell'_0 j'_0 \\ J_1 J_f J'_1 J'_f}} (2b+1) \\
&\times c_{\ell_0}^{j_0} \langle ([J j_1] J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\
&\times c_{\ell'_0}^{j'_0 *} \langle ([J j_1] J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\
&\times (-1)^{J_1 - J'_1 - J + j_1 + j_2 + J_f + J'_f + J_0 + \ell_0 - j'_0 + 1 - q} \\
&\times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)} \\
&\times \sqrt{(2j'_0+1)(2J'_1+1)(2J'_f+1)} \\
&\times \begin{pmatrix} K' & b & k \\ q & 0 & -q \end{pmatrix} \begin{pmatrix} b & \ell_0 & \ell'_0 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} K' & b & k \\ j_0 & \ell_0 & 1/2 \\ j'_0 & \ell'_0 & 1/2 \end{Bmatrix} \\
&\times \begin{Bmatrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{Bmatrix} \begin{Bmatrix} J_f & J'_f & K' \\ J'_1 & J_1 & j_2 \end{Bmatrix} \begin{Bmatrix} j'_0 & j_0 & K' \\ J_f & J'_f & J_0 \end{Bmatrix}. \quad (E.16)
\end{aligned}$$

Eventually, inserting the expansion coefficient

$$c_{\ell_0}^{j_0} = \langle \ell_0 0 | \mathbf{p}_0^{(+)} \rangle = \sqrt{\frac{2\ell_0 + 1}{4\pi |\mathbf{p}_0|^2}} i^{\ell_0} e^{i\sigma_{\ell_0}^{j_0}}, \quad (\text{E.17})$$

which has been obtained in full analogy to the method used in Appendix D, e.g. see (D.7), the anisotropy parameter can be written as

$$\begin{aligned} B_e(K' k q) = & \frac{\Delta E_{12}}{4\pi |\mathbf{p}_0|^2} \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \sum_{\substack{b\ell_1 j_1 \\ \ell_2 j_2}} \sum_{\substack{\ell_0 j_0 \ell'_0 j'_0 \\ J_1 J_f J'_1 J'_f}} (2b+1) \\ & \times i^{\ell_0 - \ell'_0} e^{i(\sigma_{\ell_0}^{j_0} - \sigma_{\ell'_0}^{j'_0})} \\ & \times \langle ([J j_1] J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle \\ & \times \langle ([J j_1] J'_1 j_2) J'_f \| V \| (J_0 j'_0) J'_f \rangle \\ & \times (-1)^{J_1 - J'_1 - J + j_1 + j_2 + J_f + J'_f + J_0 + \ell_0 - j'_0 + 1 - q} \\ & \times \sqrt{(2\ell_0 + 1)(2j_0 + 1)(2J_1 + 1)(2J_f + 1)} \\ & \times \sqrt{(2\ell'_0 + 1)(2j'_0 + 1)(2J'_1 + 1)(2J'_f + 1)} \\ & \times \begin{pmatrix} K' & b & k \\ q & 0 & -q \end{pmatrix} \begin{pmatrix} b & \ell_0 & \ell'_0 \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} K' & b & k \\ j_0 & \ell_0 & 1/2 \\ j'_0 & \ell'_0 & 1/2 \end{matrix} \right\} \\ & \times \left\{ \begin{matrix} J'_1 & J_1 & K' \\ J & J & j_1 \end{matrix} \right\} \left\{ \begin{matrix} J_f & J'_f & K' \\ J'_1 & J_1 & j_2 \end{matrix} \right\} \left\{ \begin{matrix} j'_0 & j_0 & K' \\ J_f & J'_f & J_0 \end{matrix} \right\}. \end{aligned} \quad (\text{E.18})$$

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