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

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

and vanish unless the selection rule

$$\alpha + \beta = \gamma, \tag{A.2}$$

and the triangular condition

$$|a - b| \leq c \leq a + b \tag{A.3}$$

are fulfilled.

The Clebsch–Gordan coefficients are real quantities

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

which yields the inverse transformation

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

Symmetry properties:

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

Special cases:

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

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

If c and γ take their maximum values, we have:

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

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

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

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

The Wigner $3j$-symbols are defined as

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

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

$$\alpha+\beta+\gamma = 0, \tag{A.10}$$

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 α, β, γ. In particular:

$$\begin{pmatrix} a & b & c\\ \alpha & \beta & \gamma\end{pmatrix} = \begin{pmatrix} b & c & a\\ \beta & \gamma & \alpha\end{pmatrix} = \begin{pmatrix} c & a & b\\ \gamma & \alpha & \beta\end{pmatrix}, \tag{A.11a}$$

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

Special cases:

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

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

$$\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} = 0, \tag{A.12b}$$

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

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

where

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

If the arguments of β and γ change by 1 an important relation is

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

Orthogonality relations:

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

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

A.2 Racah Coefficients and 6j-Symbols

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

$$\left|(j'j)g', j''; J'M'\right\rangle = \sum_{\substack{mm' \\ m''\mu'}} \left|m\, m'\, m''\right\rangle \left(j'm', jm|g'\mu'\right) \left(g'\mu', j''m''|JM\right), \tag{A.15a}$$

or

$$\left|j', (jj'')g''; JM\right\rangle = \sum_{\substack{mm' \\ m''\mu''}} \left|m\, m'\, m''\right\rangle \left(jm, j''m''|g''\mu''\right) \left(j'm', g''\mu''|JM\right). \tag{A.15b}$$

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

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

that is, we have

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

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

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = (-1)^{a+b+d+e} W(abed; cf). \tag{A.18}$$

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

$$\left\{\begin{array}{ccccc} \circ & \diagdown & & & \\ & & \circ & - & \circ \end{array}\right\}, \left\{\begin{array}{ccccc} \circ & - & \circ & - & \circ \\ & & & & \end{array}\right\}, \left\{\begin{array}{ccccc} & & & \diagup & \circ \\ \circ & - & \circ & & \end{array}\right\}, \left\{\begin{array}{ccccc} & \diagup & \circ & \diagdown & \\ \circ & & & & \circ \end{array}\right\}. \tag{A.19}$$

Particularly, the sum of its arguments must be integer

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

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.

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = \begin{Bmatrix} a & c & b \\ d & f & e \end{Bmatrix} = \begin{Bmatrix} b & a & c \\ e & d & f \end{Bmatrix} = \begin{Bmatrix} a & e & f \\ d & b & c \end{Bmatrix} = \begin{Bmatrix} d & c & e \\ a & f & b \end{Bmatrix}, \quad \text{etc.} \tag{A.21}$$

Special value:

$$\begin{Bmatrix} a & b & 0 \\ c & d & f \end{Bmatrix} = (-1)^{a+c+f} \frac{\delta_{ab}\delta_{cd}}{\sqrt{(2a+1)(2c+1)}}\,. \tag{A.22}$$

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

$$\begin{aligned}\sum_{\substack{\alpha\beta\gamma \\ \alpha'\beta'\gamma'}} (-1)^{A+B+C+\alpha+\beta+\gamma} \begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix} \begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix} \begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma' \end{pmatrix} \\ = \begin{Bmatrix} a & b & c \\ A & B & C \end{Bmatrix}\,.\end{aligned} \tag{A.23}$$

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. γ' from the summation, the left-hand side of (A.23) must be multiplied by $(2c+1)$ which yields

$$\sum_{\substack{\alpha\beta\gamma \\ \alpha'\beta'}} (-1)^{A+B+C+\alpha+\beta+\gamma} \begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix} \begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix} \begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix} \begin{pmatrix} a & b & c_1 \\ \alpha' & \beta' & \gamma_1' \end{pmatrix}$$
$$= \delta_{cc_1}\delta_{\gamma'\gamma_1'} \frac{1}{2c+1} \begin{Bmatrix} a & b & c \\ A & B & C \end{Bmatrix}. \tag{A.24}$$

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

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

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

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

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

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

Continuing with this procedure yields

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

and

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

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

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

Racah–Elliot relation and orthogonality relations:

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

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

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

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

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

A.3 9*j*-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

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

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

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

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

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

and for three arguments equal to zero we obtain

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ 0 & 0 & 0 \end{Bmatrix} = \frac{\delta_{ad}\delta_{be}\delta_{cf}}{\sqrt{(2a+1)(2b+1)(2c+1)}}, \tag{A.42a}$$

and

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

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

$$\begin{Bmatrix} a & b & c \\ d & e & c \\ g & g & 1 \end{Bmatrix} = (-1)^{b+c+d+g}\frac{a(a+1)-d(d+1)-b(b+1)+e(e+1)}{\sqrt{(g+1)(2g+1)2g(c+1)(2c+1)2c}}\begin{Bmatrix} a & b & c \\ e & d & g \end{Bmatrix}. \tag{A.43}$$

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

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix}\begin{Bmatrix} c & f & 1 \\ \frac{1}{2} & \frac{1}{2} & g \end{Bmatrix} = \frac{(-1)^{2g}}{3}\begin{Bmatrix} a & b & c \\ \frac{1}{2} & g & e \end{Bmatrix}\begin{Bmatrix} e & d & f \\ \frac{1}{2} & g & a \end{Bmatrix} - \delta_{cf}\frac{(-1)^{b+d-g}}{6(2c+1)}\begin{Bmatrix} a & b & c \\ e & d & \frac{1}{2} \end{Bmatrix}. \tag{A.44}$$

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

$$\sqrt{6(2c+1)(2d+1)(2e+1)}\begin{pmatrix} c & d & e \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} a & b & c \\ d & e & c \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} = \begin{pmatrix} a & b & c \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix}. \tag{A.45}$$

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

$$\begin{pmatrix} c+1 & d & e \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} a & b & c \\ d & e & c+1 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} = (-1)^{b+c+1/2}\begin{pmatrix} a & b & c \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \times \frac{[(d-a)(2a+1)+(e-b)(2b+1)+c+1]}{\sqrt{6(c+1)(2c+1)(2c+3)(2d+1)(2e+1)}}, \tag{A.46a}$$

and

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

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.

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

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

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

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

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

Due to the same argument, the sums over β and γ on the left, and over δ and ρ on the right side are over one term, only.

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

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

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

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

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

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

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 ω about $\hat{\mathbf{n}}$. For an arbitrary rotation about $\hat{\mathbf{n}}$ by an angle ω, we obtain

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

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

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

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

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

where the expansion coefficients

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

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 (α,β,γ); see Fig. B.1.

The Euler angles (α,β,γ) 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:

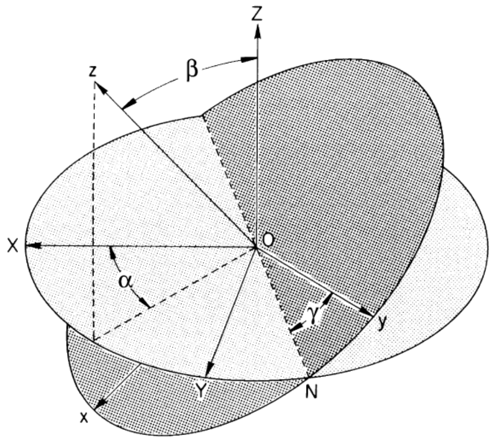

Fig. B.1. The Euler angles α, β, and γ relating the XYZ space-fixed and the xyz body-fixed coordinate frames

1. A counterclockwise rotation α about Z, the vertical axis. This carries the Y axis into the line of nodes N.
2. A counterclockwise rotation β 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 γ 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

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

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 γ about the Z axis, then a rotation β about the Y axis, and finally a rotation α about the same Z axis:

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

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

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

where

$$d^{(J)}_{M'\,M}(\beta) = \langle JM'|\exp(-\mathrm{i}\beta J_Y)|JM\rangle, \tag{B.8}$$

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 $d^{(J)}_{M\,M'}$ satisfy a number of useful symmetry relations:

$$\begin{aligned} d^{(J)}_{M\,M'}(\beta) &= (-1)^{M-M'} d^{(J)}_{M'\,M}(\beta) = d^{(J)}_{-M'\,-M}(\beta) = d^{(J)}_{M'\,M}(-\beta) \\ &= (-1)^{J-M} d^{(J)}_{M\,-M'}(\pi-\beta) = (-1)^{J+M'} d^{(J)}_{M\,-M'}(\pi+\beta). \end{aligned} \tag{B.9}$$

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

Using Zare (1988) we obtain special values:

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

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

$$\begin{aligned} d^{(J)}_{M'\,M}(2\pi) &= (-1)^{J+M'} d^{(J)}_{-M'\,M}(\pi) \\ &= (-1)^{2J}\delta_{M'M} = (-1)^{2J} d^{(J)}_{M'\,M}(0). \end{aligned} \tag{B.11}$$

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

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

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:

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

and

$$\begin{aligned} \sum_{M}\left[\mathcal{D}^{(J)}_{M'\,M}(\omega)\right]^{\dagger}\mathcal{D}^{(J)}_{N'\,M}(\omega) &= \sum_{M} d^{(J)}_{M'\,M}(-\beta) d^{(J)}_{N'\,M}(\beta) \\ &= \sum_{M} d^{(J)}_{M\,M'}(\beta) d^{(J)}_{N'\,M}(\beta) = \delta_{M'N'}. \end{aligned} \tag{B.13b}$$

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*.

$$\mathcal{D}^{(J_1)}_{M_1' M_1}(\omega)\mathcal{D}^{(J_2)}_{M_2' M_2}(\omega) = \sum_J \left(J_1 M_1, J_2 M_2|JM\right)\left(J_1 M_1', J_2 M_2'|JM'\right)\mathcal{D}^{(J)}_{M' M}(\omega). \quad \text{(B.14)}$$

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

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

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

$$\mathcal{D}^{(J)}_{M' M}(\omega) = \sum_{M_1 M_1' M_2 M_2'} \left(J_1 M_1, J_2 M_2|JM\right)\left(J_1 M_1', J_2 M_2'|JM'\right) \times \mathcal{D}^{(J_1)}_{M_1' M_1}(\omega)\mathcal{D}^{(J_2)}_{M_2' M_2}(\omega). \quad \text{(B.16)}$$

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

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

Analogously, we obtain the relations

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

and

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

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

$$\sum_{M M_1 M_2} \mathcal{D}^{(J)}_{M\,M'}(\omega)\mathcal{D}^{(J_1)}_{M_1\,M_1'}(\omega)\mathcal{D}^{(J_2)}_{M_2\,M_2'}(\omega) \begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & M \end{pmatrix} = \begin{pmatrix} J_1 & J_2 & J \\ M_1' & M_2' & M' \end{pmatrix}. \tag{B.19}$$

The closure relation for two consecutive rotations gives

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

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

$$\sum_{M''} d^{(J)}_{M\,M''}(\beta_2) d^{(J)}_{M''\,M'}(\beta_1) = d^{(J)}_{M\,M'}(\beta_1 + \beta_2). \tag{B.21}$$

B.4 Integrals Over Rotation Matrices

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

$$\int \mathrm{d}\Omega\, \mathcal{D}^{(J_1)}_{M_1'\,M_1}(\omega)^* \mathcal{D}^{(J_2)}_{M_2'\,M_2}(\omega) = \frac{8\pi^2}{2J_1+1} \delta_{J_1 J_2} \delta_{M_1' M_2'} \delta_{M_1 M_2}\,. \tag{B.22}$$

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

$$\int \mathrm{d}\Omega\, \mathcal{D}^{(J_3)}_{M_3'\,M_3}(\omega)^* \mathcal{D}^{(J_2)}_{M_2'\,M_2}(\omega)\, \mathcal{D}^{(J_1)}_{M_1'\,M_1}(\omega) = \frac{8\pi^2}{2J_3+1} \big(J_1 M_1,\, J_2 M_2 | J_3 M_3\big)\big(J_1 M_1',\, J_2 M_2' | J_3 M_3'\big)\,, \tag{B.23a}$$

and using (B.15) yields

$$\int \mathrm{d}\Omega\, \mathcal{D}^{(J_3)}_{M_3'\,M_3}(\omega)\, \mathcal{D}^{(J_2)}_{M_2'\,M_2}(\omega)\, \mathcal{D}^{(J_1)}_{M_1'\,M_1}(\omega) = 8\pi^2 \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1' & M_2' & M_3' \end{pmatrix}. \tag{B.23b}$$

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 γ or α 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

$$\mathcal{D}^{(L)}_{M\,0}(\omega) = d^{(L)}_{M\,0}(\theta)\,\mathrm{e}^{-\mathrm{i}M\phi} = C^*_{LM}(\theta, \phi) = \sqrt{\frac{4\pi}{2L+1}}\,Y^*_{LM}(\theta, \phi), \tag{B.24}$$

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

$$\begin{aligned}\mathcal{D}^{(L)}_{0\,M}(\omega) &= d^{(L)}_{0\,M}(\theta)\,\mathrm{e}^{-\mathrm{i}M\chi} = (-1)^M d^{(L)}_{M\,0}(\theta)\,\mathrm{e}^{-\mathrm{i}M\chi} = (-1)^M C^*_{LM}(\theta, \chi)\\ &= C_{L-M}(\theta, \chi) = \sqrt{\frac{4\pi}{2L+1}}\,Y_{L-M}(\theta, \chi),\end{aligned} \tag{B.25}$$

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 $P^M_L(\cos\theta)$ as

$$d^{(L)}_{M\,0}(\theta) = C^*_{LM}(\theta, 0) = \sqrt{\frac{(L-M)!}{(L+M)!}}\,P^M_L(\cos\theta), \tag{B.26}$$

if $M \geq 0$, and

$$d^{(L)}_{0\,M}(\theta) = (-1)^M C^*_{LM}(\theta, 0) = (-1)^M \sqrt{\frac{(L-M)!}{(L+M)!}}\,P^M_L(\cos\theta). \tag{B.27}$$

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

$$\mathcal{D}^{(L)}_{0\,0}(\omega) = d^{(L)}_{0\,0}(\theta) = P_L(\cos\theta). \tag{B.28}$$

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

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

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

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

and for $q = 0$ we obtain

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

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

$$\sum_q C_{kq}(\theta, \phi) C^*_{kq}\left(\theta', \phi'\right) = P_k(\cos\omega), \tag{B.32}$$

where ω is the angle between the two directions (θ, ϕ) and (θ', ϕ').

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

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

where the sum over γ 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

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

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

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

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

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

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 $\theta \longrightarrow -\theta$.

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

$$|Q| \leq 1, \tag{B.37}$$

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 θ and $-\theta$, respectively. I.e., we need to consider expressions of the type $d^{(K)}_{Q'\,Q}(\theta) \pm d^{(K)}_{Q'\,Q}(-\theta)$.

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

$$d^{(K)}_{0\,0}(\theta) - d^{(K)}_{0\,0}(-\theta) = 0, \tag{B.38}$$

and by using (B.28)

$$d^{(K)}_{0\,0}(\theta) + d^{(K)}_{0\,0}(-\theta) = 2 d^{(K)}_{0\,0}(\theta) = 2 P_K(\cos\theta). \tag{B.39}$$

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

$$\begin{aligned} d^{(K)}_{1\,0}(\theta) - d^{(K)}_{1\,0}(-\theta) &= d^{(K)}_{1\,0}(\theta) - d^{(K)}_{0\,1}(\theta) = 2\, C^{*}_{K\,1}(\theta, 0) \\ &= \frac{2}{\sqrt{K(K+1)}}\, P^{1}_{K}(\cos\theta). \end{aligned} \tag{B.40}$$

The sum yields

$$\begin{aligned} d^{(K)}_{1\,0}(\theta) + d^{(K)}_{1\,0}(-\theta) &= d^{(K)}_{1\,0}(\theta) + d^{(K)}_{0\,1}(\theta) \\ &= C^{*}_{K\,1}(\theta, 0) - C^{*}_{K\,1}(\theta, 0) = 0. \end{aligned} \tag{B.41}$$

For the other occurring differences we simply obtain

$$\begin{aligned} &\left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] - \left[d^{(K)}_{1\,1}(-\theta) \pm d^{(K)}_{-1\,1}(-\theta)\right] \\ &\quad = \left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] - \left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] = 0, \end{aligned} \tag{B.42}$$

and for the summations we eventually get

$$\begin{aligned} &\left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] + \left[d^{(K)}_{1\,1}(-\theta) \pm d^{(K)}_{-1\,1}(-\theta)\right] \\ &\quad = \left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] + \left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right] \\ &\quad = 2\left[d^{(K)}_{1\,1}(\theta) \pm d^{(K)}_{-1\,1}(\theta)\right]. \end{aligned} \tag{B.43}$$

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

$$d^{(1)}_{1\,1}(\theta) + d^{(1)}_{-1\,1}(\theta) = 1, \tag{B.44}$$

and

$$d^{(1)}_{1\,1}(\theta) - d^{(1)}_{-1\,1}(\theta) = \cos\theta, \tag{B.45}$$

and for $K = 2$ we get

$$d^{(2)}_{1\,1}(\theta) + d^{(2)}_{-1\,1}(\theta) = \cos\theta, \tag{B.46}$$

and

$$d^{(2)}_{1\,1}(\theta) - d^{(2)}_{-1\,1}(\theta) = \cos(2\theta). \tag{B.47}$$

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

$$d^{(3)}_{1\,1}(\theta) + d^{(3)}_{-1\,1}(\theta) = \frac{1}{4}\big(5\cos^2\theta - 1\big), \tag{B.48}$$

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

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

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

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}, $Q = -K, \ldots, +K$, are called the *standard components of an irreducible tensor operator* $\mathbf{T}_K$ *of rank* K if they transform under rotation as

$$\mathcal{D}T_{KQ}\mathcal{D}^{-1} = \sum_q T_{Kq}\mathcal{D}^{(K)}_{q\,Q}. \tag{C.1}$$

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

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

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

$$V_+ = \frac{1}{\sqrt{2}}\left(V_x + \mathrm{i}V_y\right), \tag{C.3a}$$

$$V_0 = V_z, \tag{C.3b}$$

$$V_- = \frac{1}{\sqrt{2}}\left(V_x - \mathrm{i}V_y\right). \tag{C.3c}$$

Commutation relations with the angular momentum:

$$\left[J_\pm, T_{kq}\right] = \sqrt{k(k+1) - q(q+1)}\,T_{kq\pm1}, \tag{C.4a}$$

$$\left[J_z, T_{kq}\right] = qT_{kq}. \tag{C.4b}$$

Hermitian conjugate:

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

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

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

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

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

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*

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

and the total angular momentum

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

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

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

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

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

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

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

$$\frac{\mathrm{e}^{\mathrm{i}k\rho}}{\rho} = \mathrm{i}kh_0^{(1)}(k\rho) = \mathrm{i}k\sum_\ell (2\ell+1)\, j_\ell(ka)h_\ell^{(1)}(kb) \times \mathbf{C}_\ell\,(\theta_a\phi_a)\,\mathbf{C}_\ell\,(\theta_b\phi_b)\,, \tag{C.14}$$

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

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

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

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 $T_{k_1q_1}U_{K_2q_2}$. It is a (reducible) tensor operator.

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

$$V_{KQ}(k_1,k_2) = \sum_{q_1q_2}\big(k_1q_1,k_2q_2|KQ\big)T_{k_1q_1}U_{k_2q_2}, \tag{C.17}$$

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

$$V_{KQ}(k_1,k_2) = \sum_{q_1q_2}(-1)^{k_1-k_2+Q}\sqrt{2K+1}\begin{pmatrix} k_1 & k_2 & K\\ q_1 & q_2 & -Q\end{pmatrix}T_{k_1q_1}U_{k_2q_2}. \tag{C.18}$$

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

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

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

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

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 $\big|\tau_1J_1M_1\big\rangle$ and $\big|\tau_2J_2M_2\big\rangle$ 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 $\left\{\tau_1\tau_2\mathbf{J}_1^2\mathbf{J}_2^2\mathbf{J}^2 J_z\right\}$ the matrix elements of $\mathbf{V}_K(k_1,k_2)$ are given as

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

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

$$\left\langle\tau_1\tau_2 J_1 J_2 J\|\mathbf{T}_k\|\tau_1'\tau_2'\mathbf{J}_1'\mathbf{J}_2'\mathbf{J}'\right\rangle = \delta_{\tau_2\tau_2'}\delta_{J_2J_2'}\left\langle\tau_1 J_1\|\mathbf{T}_k\|\tau_1'\mathbf{J}_1'\right\rangle \times (-1)^{J'+J_1+J_2+k}\sqrt{(2J+1)(2J'+1)}\begin{Bmatrix} J_1 & k & J_1' \\ J' & J_2 & J \end{Bmatrix}. \quad (C.22)$$

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

$$\left\langle\tau_1\tau_2 J_1 J_2 J\|\mathbf{U}_k\|\tau_1'\tau_2' J_1' J_2' J'\right\rangle = \delta_{\tau_1\tau_1'}\delta_{J_1J_1'}\left\langle\tau_2 J_2\|\mathbf{U}_k\|\tau_2' J_2'\right\rangle \times (-1)^{J+J_1+J_2'+k}\sqrt{(2J+1)(2J'+1)}\begin{Bmatrix} J_2 & k & J_2' \\ J' & J_1 & J \end{Bmatrix}. \quad (C.23)$$

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

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

Often, the scalar product $\mathbf{T}_k\cdot\mathbf{U}_k$ is used in place of $\left[\mathbf{T}_k\otimes\mathbf{U}_k\right]_0^{(0)}$ 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

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

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 $V_{KQ}(k_1,k_2) = \left[\mathbf{T}_{k_1} \otimes \mathbf{T}_{k_2}\right]_Q^{(K)}$, where $V_{KQ}(k_1,k_2)$ can act only on the set of variables of the system, are obtained as

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

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

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

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

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

Using the renormalized spherical harmonics instead gives a more compact relation

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

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

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

and combining with (A.29) eventually yields

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

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

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

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

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

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)

$$Z^2 < \omega \ll Z\alpha^{-1} , \tag{D.3}$$

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[1]

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

[1] 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

$$\mathbf{e}_\lambda \cdot \mathbf{r}^* = r_\lambda \; . \tag{D.5}$$

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

$$\begin{aligned} \left|\mathbf{p}^{(-)} m_s\right\rangle = \psi^{(-)}_{\mathbf{p}m_s}(\mathbf{r}) = \frac{1}{|\mathbf{p}|} \sum_{\substack{\ell m j m_j \\ m' \mu}} \mathrm{i}^\ell \, \mathrm{e}^{-\mathrm{i}\sigma_\ell^j} \, Y^*_{\ell m}(\hat{\mathbf{p}}) \, R^j_{\varepsilon\ell}(r) Y_{\ell m'}(\hat{\mathbf{r}}) \, \chi_\mu \\ \times \left(\ell m, 1/2 m_s | j m_j\right) \left(\ell m', 1/2 \mu | j m_j\right) , \end{aligned} \tag{D.6}$$

which yields for the expansion coefficients

$$a^j_{\ell m} = \left\langle j \ell m | \mathbf{p}^{(-)} \right\rangle = \frac{1}{|\mathbf{p}|} \mathrm{i}^\ell \, \mathrm{e}^{-\mathrm{i}\sigma_\ell^j} \, Y^*_{\ell m}(\hat{\mathbf{p}}) \; . \tag{D.7}$$

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

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

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

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

With this, we obtain for the dipole matrix element

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

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)

$$\begin{aligned}
\left\langle JM\mathbf{p}_1^{(-)}m_{s_1}\mathbf{p}_2^{(-)}m_{s_2}|V|J_0M_0\mathbf{p}_0^{(+)}m_{s_0}\right\rangle &= \sum_{\substack{\ell_0\ell_1m_1\\ \ell_2m_2}} a_{\ell_1m_1}^{j_1\,*}b_{\ell_2m_2}^{j_2\,*}c_{\ell_0}^{j_0} \\
&\quad\times\left\langle JM\ell_1m_1 1/2m_{s_1}\ell_2m_2 1/2m_{s_2}|V|J_0M_0\ell_0 0 1/2m_{s_0}\right\rangle \\
&= \sum_{\substack{\ell_0\ell_1m_1\ell_2m_2 j_0m_{j_0}\\ j_1m_{j_1}j_2m_{j_2}\\ J_1M_1J_2M_2J_fM_f}} a_{\ell_1m_1}^{j_1\,*}b_{\ell_2m_2}^{j_2\,*}c_{\ell_0}^{j_0} \\
&\quad\times\left\langle([Jj_1]J_1j_2)J_fM_f|V|(J_0j_0)J_2M_2\right\rangle \\
&\quad\times\left(\ell_1m_1,\,1/2m_{s_1}|j_1m_{j_1}\right)\left(\ell_2m_2,\,1/2m_{s_2}|j_2m_{j_2}\right) \\
&\quad\times\left(\ell_0 0,\,1/2m_{s_0}|j_0m_{j_0}\right)\left(JM,\,j_1m_{j_1}|J_1M_1\right) \\
&\quad\times\left(J_1M_1,\,j_2m_{j_2}|J_fM_f\right)\left(J_0M_0,\,j_0m_{j_0}|J_2M_2\right).
\end{aligned} \tag{E.1}$$

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

$$\begin{aligned}
\left\langle J_fM_f|V|J_2M_2\right\rangle &= (-1)^{J_f-M_f}\begin{pmatrix} J_f & 0 & J_2\\ -M_f & 0 & M_2\end{pmatrix}\left\langle J_f\|V\|J_2\right\rangle \\
&= \frac{1}{\sqrt{2J_f+1}}\left\langle J_f\|V\|J_2\right\rangle\,\delta_{J_fJ_2}\,\delta_{M_fM_2}.
\end{aligned} \tag{E.2}$$

With this, we finally obtain for the transition matrix element

$$\begin{aligned}\left\langle JM\mathbf{p}_1^{(-)}m_{s1}\mathbf{p}_2^{(-)}m_{s2}|V|J_0M_0\mathbf{p}_0^{(+)}m_{s0}\right\rangle = &\sum_{\substack{\ell_0\ell_1m_1\ell_2m_2j_0m_{j_0}\\ j_1m_{j_1}j_2m_{j_2}\\ J_1M_1J_fM_f}} a_{\ell_1m_1}^{j_1*}\\
&\times b_{\ell_2m_2}^{j_2*}c_{\ell_0}^{j_0}\left\langle([Jj_1]J_1j_2)J_f\|V\|(J_0j_0)J_f\right\rangle\\
&\times(-1)^{-\ell_1+1/2-m_{j_1}-\ell_2+1/2-m_{j_2}-\ell_0+1/2-m_{j_0}}\\
&\times(-1)^{-J+j_1-M_1-J_1+j_2-M_f-J_0+j_0-M_f}\\
&\times\sqrt{(2j_1+1)(2j_2+1)(2j_0+1)(2J_1+1)(2J_f+1)}\\
&\times\begin{pmatrix}\ell_1 & 1/2 & j_1\\ m_1 & m_{s_1} & -m_{j_1}\end{pmatrix}\begin{pmatrix}\ell_2 & 1/2 & j_2\\ m_2 & m_{s_2} & -m_{j_2}\end{pmatrix}\begin{pmatrix}\ell_0 & 1/2 & j_0\\ 0 & m_{s_0} & -m_{j_0}\end{pmatrix}\\
&\times\begin{pmatrix}J & j_1 & J_1\\ M & m_{j_1} & -M_1\end{pmatrix}\begin{pmatrix}J_1 & j_2 & J_f\\ M_1 & m_{j_2} & -M_f\end{pmatrix}\begin{pmatrix}J_0 & j_0 & J_f\\ M_0 & m_{j_0} & -M_f\end{pmatrix}.\end{aligned} \tag{E.3}$$

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

$$\begin{aligned}B_e(K'Q',kq) = &\frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1}\int d\mathbf{p}_1\int d\mathbf{p}_2\sum_{\substack{MM'm_{s_1}m_{s_2}\\ m_{s_0}m'_{s_0}M_0}}\\
&\times\sum_{\substack{\ell_0\ell_1m_1\ell_2m_2\\ j_0m_{j_0}j_1m_{j_1}j_2m_{j_2}\\ J_1M_1J_fM_f}}\ \sum_{\substack{\ell'_0\ell'_1m'_1\ell'_2m'_2\\ j_0m'_{j_0}j'_1m'_{j_1}j'_2m'_{j_2}\\ J'_1M'_1J'_fM'_f}}(-1)^{J-M+1/2-m_{s_0}}\\
&\times a_{\ell_1m_1}^{j_1*}b_{\ell_2m_2}^{j_2*}c_{\ell_0}^{j_0}\left\langle([Jj_1]J_1j_2)J_f\|V\|(J_0j_0)J_f\right\rangle\\
&\times a_{\ell'_1m'_1}^{j'_1}b_{\ell'_2m'_2}^{j'_2}c_{\ell'_0}^{j'_0*}\left\langle([Jj'_1]J'_1j'_2)J'_f\|V\|(J_0j'_0)J'_f\right\rangle\\
&\times(-1)^{-\ell_1+1/2-m_{j_1}-\ell_2+1/2-m_{j_2}-\ell_0+1/2-m_{j_0}}\\
&\times(-1)^{-J+j_1-M_1-J_1+j_2-M_f-J_0+j_0-M_f}\\
&\times(-1)^{-\ell'_1+1/2-m'_{j_1}-\ell'_2+1/2-m'_{j_2}-\ell'_0+1/2-m'_{j_0}}\\
&\times(-1)^{-J+j'_1-M'_1-J'_1+j'_2-M'_f-J_0+j'_0-M'_f}\\
&\times\sqrt{(2j_1+1)(2j_2+1)(2j_0+1)(2J_1+1)(2J_f+1)}\\
&\times\sqrt{(2j'_1+1)(2j'_2+1)(2j'_0+1)(2J'_1+1)(2J'_f+1)}\end{aligned}$$

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

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

$$\int \mathrm{d}\mathbf{p}_1\, a^{j_1\,*}_{\ell_1 m_1} a^{j'_1}_{\ell'_1 m'_1} = \mathrm{e}^{\mathrm{i}(\sigma^{j_1}_{\ell_1} - \sigma^{j'_1}_{\ell_1})}\, \delta_{\ell_1 \ell'_1}\, \delta_{m_1 m'_1}\, \Delta E_1 \ , \tag{E.5}$$

and

$$\int \mathrm{d}\mathbf{p}_2\, b^{j_2\,*}_{\ell_2 m_2} b^{j'_2}_{\ell'_2 m'_2} = \mathrm{e}^{\mathrm{i}(\sigma^{j_2}_{\ell_2} - \sigma^{j'_2}_{\ell_2})}\, \delta_{\ell_2 \ell'_2}\, \delta_{m_2 m'_2}\, \Delta E_2 \ . \tag{E.6}$$

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

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

$$\times \sqrt{(2j_1'+1)(2j_2'+1)(2j_0'+1)(2J_1'+1)(2J_f'+1)}$$
$$\times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m_{s_0}' & -q \end{pmatrix} \begin{pmatrix} J & J & K' \\ M & -M' & -Q' \end{pmatrix}$$
$$\times \begin{pmatrix} \ell_1 & 1/2 & j_1 \\ m_1 & m_{s_1} & -m_{j_1} \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j_2 \\ m_2 & m_{s_2} & -m_{j_2} \end{pmatrix} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix}$$
$$\times \begin{pmatrix} \ell_1 & 1/2 & j_1' \\ m_1 & m_{s_1} & -m_{j_1}' \end{pmatrix} \begin{pmatrix} \ell_2 & 1/2 & j_2' \\ m_2 & m_{s_2} & -m_{j_2}' \end{pmatrix} \begin{pmatrix} \ell_0' & 1/2 & j_0' \\ 0 & m_{s_0}' & -m_{j_0}' \end{pmatrix}$$
$$\times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix}$$
$$\times \begin{pmatrix} J & j_1' & J_1' \\ M' & m_{j_1}' & -M_1' \end{pmatrix} \begin{pmatrix} J_1' & j_2' & J_f' \\ M_1' & m_{j_2}' & -M_f' \end{pmatrix} \begin{pmatrix} J_0 & j_0' & J_f' \\ M_0 & m_{j_0}' & -M_f' \end{pmatrix} . \tag{E.7}$$

Now, applying the orthogonality relations of the $3j$-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

$$j_1 = j_1' , \qquad m_{j_1} = m_{j_1}' , \tag{E.8}$$

and

$$j_2 = j_2' , \qquad m_{j_2} = m_{j_2}' . \tag{E.9}$$

Thus, the phase difference disappears which yields

$$B_e(K'Q', kq) = \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{MM'M_0 \\ m_{s_0}m_{s_0}'}} \sum_{\substack{\ell_0\ell_1\ell_2 j_0 m_{j_0} \\ j_1 m_{j_1} j_2 m_{j_2} \\ J_1 M_1 J_f M_f}} \sum_{\substack{\ell_0' j_0' m_{j_0}' \\ J_1' M_1' J_f' M_f'}}$$
$$\times c_{\ell_0}^{j_0} \langle ([Jj_1]J_1 j_2)J_f \| V \| (J_0 j_0) J_f \rangle$$
$$\times c_{\ell_0'}^{j_0'\,*} \langle ([Jj_1]J_1' j_2)J_f' \| V \| (J_0 j_0') J_f' \rangle$$
$$\times (-1)^{J-M+1/2-m_{s_0}+\ell_0'-\ell_0+j_0-j_0'+m_{j_0}-m_{j_0}'}$$
$$\times (-1)^{J_1'-J_1+M_1-M_1'+2M_f-2M_f'}$$
$$\times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)}$$
$$\times \sqrt{(2j_0'+1)(2J_1'+1)(2J_f'+1)}$$
$$\times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m_{s_0}' & -q \end{pmatrix} \begin{pmatrix} J & J & K' \\ M & -M' & -Q' \end{pmatrix}$$
$$\times \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} \ell_0' & 1/2 & j_0' \\ 0 & m_{s_0}' & -m_{j_0}' \end{pmatrix}$$

$$
\times \begin{pmatrix} J & j_1 & J_1 \\ M & m_{j_1} & -M_1 \end{pmatrix} \begin{pmatrix} J_1 & j_2 & J_f \\ M_1 & m_{j_2} & -M_f \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix}
$$
$$
\times \begin{pmatrix} J & j_1 & J_1' \\ M' & m_{j_1} & -M_1' \end{pmatrix} \begin{pmatrix} J_1' & j_2 & J_f' \\ M_1' & m_{j_2} & -M_f' \end{pmatrix} \begin{pmatrix} J_0 & j_0' & J_f' \\ M_0 & m_{j_0}' & -M_f' \end{pmatrix}. \tag{E.10}
$$

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

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

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

$$
B_e(K'Q', kq) = \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \Delta E_{12} \sum_{\substack{\ell_1 \ell_2 j_1 j_2 \\ M_0 m_{s_0} m_{s_0}'}} \sum_{\substack{\ell_0 j_0 m_{j_0} \\ J_1 J_f M_f}} \sum_{\substack{\ell_0' j_0' m_{j_0}' \\ J_1' J_f' M_f'}}
$$
$$
\times c_{\ell_0}^{j_0} \langle ([J j_1] J_1 j_2) J_f \| V \| (J_0 j_0) J_f \rangle
$$
$$
\times c_{\ell_0'}^{j_0'\,*} \langle ([J j_1] J_1' j_2) J_f' \| V \| (J_0 j_0') J_f' \rangle
$$
$$
\times (-1)^{1/2 - m_{s_0} + \ell_0' - \ell_0 + j_0 - j_0' + m_{j_0} - m_{j_0}'}
$$

$$
\begin{aligned}
&\times (-1)^{K'+J_1'-J_1+J-j_1-j_2+2M_f-M_f'}\\
&\times \sqrt{(2j_0+1)(2J_1+1)(2J_f+1)}\\
&\times \sqrt{(2j_0'+1)(2J_1'+1)(2J_f'+1)}\\
&\times \begin{pmatrix} 1/2 & 1/2 & k \\ m_{s_0} & -m_{s_0}' & -q \end{pmatrix} \begin{pmatrix} J_f & J_f' & K' \\ -M_f & M_f' & Q' \end{pmatrix}\\
&\times \begin{Bmatrix} J_1' & J_1 & K' \\ J & J & j_1 \end{Bmatrix} \begin{pmatrix} \ell_0 & 1/2 & j_0 \\ 0 & m_{s_0} & -m_{j_0} \end{pmatrix} \begin{pmatrix} J_0 & j_0 & J_f \\ M_0 & m_{j_0} & -M_f \end{pmatrix}\\
&\times \begin{Bmatrix} J_f & J_f' & K' \\ J_1' & J_1 & j_2 \end{Bmatrix} \begin{pmatrix} \ell_0' & 1/2 & j_0' \\ 0 & m_{s_0}' & -m_{j_0}' \end{pmatrix} \begin{pmatrix} J_0 & j_0' & J_f' \\ M_0 & m_{j_0}' & -M_f' \end{pmatrix} .
\end{aligned}
\tag{E.12}
$$

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

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

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 β.

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

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

$$
q = Q' . \tag{E.15}
$$

With this, the anisotropy parameter can be redefined as

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

Eventually, inserting the expansion coefficient

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

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

$$\begin{aligned}
B_e(K'kq) = {} & \frac{\Delta E_{12}}{4\pi\, |\mathbf{p}_0|^2} \frac{\sqrt{(2k+1)(2K'+1)}}{2J_0+1} \sum_{\substack{b\ell_1 j_1 \\ \ell_2 j_2}} \sum_{\substack{\ell_0 j_0 \ell_0' j_0' \\ J_1 J_f J_1' J_f'}} (2b+1) \\
& \times \mathrm{i}^{\ell_0 - \ell_0'}\, \mathrm{e}^{\mathrm{i}(\sigma_{\ell_0}^{j_0} - \sigma_{\ell_0'}^{j_0'})} \\
& \times \left\langle ([Jj_1]J_1 j_2) J_f \| V \| (J_0 j_0) J_f \right\rangle \\
& \times \left\langle ([Jj_1]J_1' j_2) J_f' \| V \| (J_0 j_0') J_f' \right\rangle \\
& \times (-1)^{J_1 - J_1' - J + j_1 + j_2 + J_f + J_f' + J_0 + \ell_0 - j_0' + 1 - q} \\
& \times \sqrt{(2\ell_0+1)(2j_0+1)(2J_1+1)(2J_f+1)} \\
& \times \sqrt{(2\ell_0'+1)(2j_0'+1)(2J_1'+1)(2J_f'+1)} \\
& \times \begin{pmatrix} K' & b & k \\ q & 0 & -q \end{pmatrix} \begin{pmatrix} b & \ell_0 & \ell_0' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} K' & b & k \\ j_0 & \ell_0 & 1/2 \\ j_0' & \ell_0' & 1/2 \end{Bmatrix} \\
& \times \begin{Bmatrix} J_1' & J_1 & K' \\ J & J & j_1 \end{Bmatrix} \begin{Bmatrix} J_f & J_f' & K' \\ J_1' & J_1 & j_2 \end{Bmatrix} \begin{Bmatrix} j_0' & j_0 & K' \\ J_f & J_f' & J_0 \end{Bmatrix} .
\end{aligned} \tag{E.18}$$

References

Åberg, T., Howat, G. (1982) “Theory of the Auger Effect.” In: S. Flügge, W. Mehlhorn (Eds.), *Handbuch der Physik* **31**, p. 469. Springer, Berlin.
Aksela, H., Mursu, J. (1996). *Phys. Rev. A* **54**, 2882.
Aksela, H., Aksela, S., Jen, J. S., Thomas, T. D. (1977). *Phys. Rev. A* **15**, 985.
Aksela, S., Aksela, H., Thomas, T. D. (1979). *Phys. Rev. A* **19**, 721.
Aksela, S., Kellokumpo, M., Aksela, H., Väyrynen, J. (1981). *Phys. Rev. A* **23**, 2374.
Aksela, H., Aksela, S., Hotokka, M., Jaentti, M. (1983a). *Phys. Rev. A* **28**, 287.
Aksela, S., Harkoma, M., Pohjola, M., Aksela, H. (1983b). *J. Phys. B: At. Mol. Phys.* **17**, 2227.
Aksela, H., Aksela, S., Patana, H. (1984a). *Phys. Rev. A* **30**, 858.
Aksela, H., Aksela, S., Pulkkinen, H. (1984b). *Phys. Rev. A* **30**, 865.
Aksela, H., Aksela, S., Pulkkinen, H. (1984c). Unpublished data, quoted in Tulkki *et al.* (1993).
Aksela, H., Aksela, S., Bancroft, G. M., Tan, K. H. (1986a). *Phys. Rev. A* **33**, 3867.
Aksela, H., Aksela, S., Pulkkinen, H., Bancroft, G. M., Tan, K. H. (1986b). *Phys. Rev. A* **33**, 3876.
Aksela, H., Aksela, S., Pulkkinen, H., Bancroft, G. M., Tan, K. H. (1988a). *Phys. Rev. A* **37**, 1798.
Aksela, S., Sairanen, O. P., Aksela, H., Bancroft, G. M., Tan, K. H. (1988b). *Phys. Rev. A* **37**, 2934.
Aksela, H., Bancroft, G. M., Olsson, B. (1992). *Phys. Rev. A* **46**, 1345.
Aksela, H., Sairanen, O. P., Aksela, S., Kivimäki, A., Naves de Brito, A., Nõmmiste, E. (1995). *Phys. Rev. A* **51**, 1291.
Aksela, H., Mursu J., Jauhiainen, J., Nõmmiste, E., Karvonen, J., Aksela, S. (1997). *Phys. Rev. A* **55**, 3532.
Amusia, M. Y. (1990). “Atomic Photoeffect.” K. T. Taylor. (trans. Ed.), Plenum, New York, London.
Amusia, M. Y., Cherepkov, N. A. (1975). *Case Studies in Atomic Physics* **5**, 47.
Andersen, N., Bartschat, K., Broad, J. T., Hertel, I. V. (1997). *Phys. Rep.* **278**, 107.
Armen, G. B., Larkins, F. P. (1994). Unpublished, data published and cited by Saha (1994).
Asaad, W. N. (1963a). *Nucl. Phys.* **44**, 399.
Asaad, W. N. (1963b). *Nucl. Phys.* **44**, 415.
Asaad, W. N., Burhop, E. H. S. (1958). *Proc. Phys. Soc.* **71**, 369.
Asaad, W. N., Mehlhorn, W. (1968). *Z. Phys.* **217**, 304.
Atkins, P. W. (1970). “Molecular Quantum Mechanics.” Clarendon Press, Oxford.
Auger, P. (1923). *Comm. Royal Acad. Sci. Paris* **177**, 169.

Auger, P. (1924). *Comm. Royal Acad. Sci. Paris* **178**, 929, and 1535.

Auger, P. (1926). *Comm. Royal Acad. Sci. Paris* **182**, 776.

Balashov, V. V., Bodrenko, I. V. (1999). *J. Phys. B: At. Mol. Opt. Phys.* **32**, L687.

Balashov, V. V., Bodrenko, I. V. (2000). *J. Phys. B: At. Mol. Opt. Phys.* **33**, 1473.

Barnett, A. R. (1982). *Comp. Phys. Comm.* **27**, 147.

Bartschat, K. (2003). In: G. F. Hanne, L. Malegat, H. Schmidt-Böcking (Eds.), *AIP Conf. Proc.* **697**, p. 213. Melville, New York.

Bartynski, R. A. (2003). In: G. F. Hanne, L. Malegat, H. Schmidt-Böcking (Eds.), *AIP Conf. Proc.* **697**, p. 111. Melville, New York.

Becker, U. (1990a). "The Physics of Electronic and Atomic Collisions." In: A. Dalgarno, R. S. Freund, P. M. Koch, M. S. Lubell, T. B. Lucatorto (Eds.), *AIP Conf. Proc.* **205**, p. 162. New York.

Becker, U. (1990b). "Synchrotron radiation experiments on atoms and molecules." In: A. Dalgarno, R. S. Freund, P. M. Koch, M. S. Lubell, T. B. Lucatorto (Eds.), *AIP Conf. Proc.* **205**, p. 160. New York.

Becker, U. (1994). Private communication.

Becker, U., Crowe, A. (2001). "Complete Scattering Experiments." Kluwer Academic/Plenum Publishers, New York.

Becker, U., Szostak, D., Kerkhoff, H. G., Kupsch, M., Langer, B., Wehlitz, R., Yagishita, A., Hayaishi, T. (1989). *Phys. Rev. A* **39**, 3902.

Bederson, B. (1969). *Comm. At. Mol. Phys.* **1**, 41, and 65.

Bederson, B., Miller, T. M. (1976). In: H. Kleinpoppen, M. R. C. McDowell (Eds.), "Electron and Photon Interactions with Atoms," p. 191. Plenum Press, New York.

Berezhko, E. G., Kabachnik, N. M. (1977). *J. Phys. B: At. Mol. Phys.* **10**, 2467.

Berezhko, E. G., Ivanov, V. K., Kabachnik, N. M. (1978a). *Phys. Lett. A* **66**, 474.

Berezhko, E. G., Kabachnik, N. M., Rostovsky, V. S. (1978b). *J. Phys. B: At. Mol. Opt. Phys.* **11**, 1749.

Bergmann, L., Schaefer, C. (1992). "Lehrbuch der Experimentalphysik." Vol. 4, "Teilchen." W. de Gruyter, Berlin.

Beyer, H. J., West, J. B., Ross, K. J., Ueda, K., Kabachnik, N. M., Hamdy, H., Kleinpoppen, H. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, L47.

Biedenharn, L. C., Gluckstern, R. L., Hull Jr., M. H., Breit, G. (1955). *Phys. Rev.* **97**, 542.

Blum, K. (1996). "Density Matrix Theory and Applications." 2^{nd} Edn. Plenum Press, New York, London.

Blum, K., Lohmann, B., Taute, E. (1986). *J. Phys. B: At. Mol. Opt. Phys.* **19**, 3815.

Bolognesi, P., Coreno, M., De Fanis, A., Huetz, A., Rioual, S., Rouvellou, B., Avaldi, L. (2003). In: G. F. Hanne, L. Malegat, H. Schmidt-Böcking (Eds.), *AIP Conf. Proc.* **697**, p. 119. Melville, New York.

Bonhoff, K., Nahrup, S., Lohmann, B., Blum, K. (1996). *J. Chem. Phys.* **104**, 7921.

Bonhoff, S., Bonhoff, K., Schimmelpfennig, B., Nestmann, B. (1997). *J. Phys. B: At. Mol. Opt. Phys.* **30**, 2821.

Bonhoff, S. (1998a). *PhD Thesis*, University of Münster, Germany.

Bonhoff, K. (1998b). *PhD Thesis*, University of Münster, Germany.

Born, M., Wolf, E. (1970). "Principles of Optics." Pergamon Press, New York.

Brink, D. M., Satchler, G. R. (1962). "Angular Momentum." Oxford University Press, Oxford.

Buckmaster, H. A. (1964). *Can. J. Phys.* **42**, 386.

Buckmaster, H. A. (1966). *Can. J. Phys.* **44**, 2525.

Burhop, E. H. S., Asaad, W. N. (1972). "The Auger Effect." In: D. R. Bates, I. Estermann (Eds.), *Adv. At. Mol. Phys.* **8**, p. 164. Elsevier Academic Press, New York.

Burnett, G. C., Monroe, T. J., Dunnings, F. B. (1994). *Rev. Sci. Instrum.* **65**, 1893.

Bussert, W., Klar, H. (1983). *Z. Phys. A* **312**, 315.

Caldwell, C. D. (1990). In: T. A. Carlson, M. O. Krause, S. T. Manson (Eds.), "X-ray and Inner-Shell Processes." *AIP Conf. Proc.* **215**, p. 685. Melville, New York.

Caldwell, C. D., Krause, M. O. (1993). *Phys. Rev. A*. **47**, R759.

Carlson, J. A., Mullins, D. R., Beall, C. E., Yates, B. W., Taylor, J. W., Lindle, D. W., Pullen, B. P., Grimm, F. A. (1988). *Phys. Rev. Lett.* **60**, 1382.

Carlson, T. A., Mullin, D. R., Beall, C. E., Yates, B. W., Taylor, J. W., Lindle, D. W., Grimm, F. A. (1989). *Phys. Rev. A* **39**, 1170.

Carravetta, V., Ågren, H. (1987). *Phys. Rev. A* **35**, 1022.

Carre, B., d'Oliveira, P., Ferray, M., Fournier, P., Gounand, F., Cubayanes, D., Bizau, J. M., Wuilleumier, F. J. (1990). *Z. Phys. D* **15**, 117.

Chandra, N. (1989). *Phys. Rev. A* **40**, 752.

Chandra, N., Chakraborty, M. (1992). *J. Chem. Phys.* **97**, 236.

Chattarji, D. (1976). "The Theory of Auger Transitions." Academic Press, London, New York, San Francisco.

Chen, M. H. (1992). *Phys. Rev. A* **45**, 1684.

Chen, M. H. (1993). *Phys. Rev. A* **47**, 3733.

Chen, M. H. (1994). Data published and cited by Saha (1994).

Chen, M. H., Crasemann, B. (1973). *Phys. Rev. A* **8**, 7; and private communication cited by Hillig *et al.* (1974)

Chen, M. H., Larkins, F. P., Crasemann, B. (1990). *Atomic Data and Nuclear Data Tables* **45**, 1.

Cleff, B., Mehlhorn, W. (1971). *Phys. Lett. A* **37**, 3.

Cleff, B., Mehlhorn, W. (1974a). *J. Phys. B: At. Mol. Phys.* **7**, 593.

Cleff, B., Mehlhorn, W. (1974b). *J. Phys. B: At. Mol. Phys.* **7**, 605.

Clenshaw, C. W., Goodwin, E. T., Martin, D. W., Miller, G. F., Olver, F. W. J., Wilkinson, J. H. (1961). *National Physics Laboratory*. "Modern Computing Methods, Notes on Applied Science." 2^{nd} Edn. Her Majesty's Stationary Office (HMSO), London. Vol. 16.

Combet Farnoux, F. (1992). *Phys. Scr. T* **41**, 28.

Condon, E. U., Shortley, G. H. (1935). "Theory of Atomic Spectra." Cambridge University Press, Cambridge.

Coplan, M. A., Cooper, J. W., Moore, J. H., Doering, J. P., van Boeyen, R. W. (2002). In: M. Schulz, D. H. Madison (Eds.), *AIP Conf. Proc.* **604**, p. 103. Melville, New York.

Cooper, J. W. (1989). *Phys. Rev. A* **39**, 3714.

Cowan, R. D. (1981). "The Theory of Atomic Structure and Spectra." University of California Press, Berkeley, Los Angeles, London.

de Gouw, J. A., van Eck, J., Peters, A. C., van der Weg, J., Heideman, H. G. M. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, 2127.

Dill, D., Starace, A. F., Manson, S. T. (1975). *Phys. Rev. A* **11**, 1596.

Dill, D., Swanson, J. R., Wallace, S., Dehmer, J. L. (1980). *Phys. Rev. Lett.* **45**, 1393.

Dorn, A., Nienhaus, J., Wetzstein, M., Winnewisser, C., Eichmann, U., Sandner, W., Mehlhorn, W. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, L225.

Douglas, B. E., Hollingsworth, C. A. (1985). "Symmetry in Bonding and Spectra." Academic Press, London.

Drescher, M., Khalil, T., Müller, N., Fritzsche, S., Kabachnik, N. M., Heinzmann, U. (2003). *J. Phys. B: At. Mol. Opt. Phys.* **36**, 3337.

Dyall, K. G., Grant, I. P., Johnson, C. T., Parpia, F. A., Plummer, E. P. (1989). *Comp. Phys. Comm.* **55**, 425.

Edmonds, A. R. (1974). “Angular Momentum in Quantum Mechanics.” Princeton University Press, Princeton, NJ.

Eichler, J., Fritsch, W. (1976). *J. Phys. B: At. Mol. Opt. Phys.* **9**, 1477.

Einstein, A. (1905). *Ann. Physik* **17**, 132.

Erman, P., Sujkowski, Z. (1961). *Ark. Fys.* **20**, 209.

Fahlman, A., Nordberg, R., Nordling, C., Siegbahn, K. (1966). *Z. Phys.* **192**, 476.

Fano, U. (1957). *Rev. Mod. Phys.* **29**, 74.

Fano, U., Racah, G. (1959). “Irreducible Tensorial Sets.” Academic Press, New York.

Farhat, A., Humphrey M., Langer, B., Berrah, N., Bozek, J. D., Cubaynes, D. (1997). *Phys. Rev. A* **56**, 501.

Ferrett, T. A., Piancastelli, M. N., Lindle, D. W., Heimann, P. A., Shirley, D. A. (1988). *Phys. Rev. A* **38**, 701.

Feuerstein, B., Grum-Grzhimailo, A. N., Bartschat, K., Mehlhorn, W. (1999). *J. Phys. B: At. Mol. Opt. Phys.* **32**, 3727.

Foldy, L., Wouthuysen, W. A. (1950). *Phys. Rev.* **78**, 29.

Frauenfelder, H., Henley, E. M. (1979). “Teilchen und Kerne.” Oldenbourg, München, Wien.

Fritzsche, S. (1991). “RATR: An Input Description.” University of Kassel, Germany.

Fritzsche, S. (1992). *PhD Thesis*, University of Kassel, Germany.

Fritzsche, S. (1993). *Phys. Rev. Lett. A* **180**, 262.

Fritzsche, S. (2001). *J. Electr. Spectr. & Relat. Phen.* **114–116**, 1155.

Fritzsche, S., Zscharnack, G., Musiol, G., Soff, G. (1991). *Phys. Rev. A* **44**, 388.

Fritzsche, S., Froese-Fischer, C., Dong, C. Z. (2000). *Comp. Phys. Comm.* **124**, 340.

Furness, J. B., Mc Carthy, I. E. (1973). *J. Phys. B: At. Mol. Opt. Phys.* **6**, 2280.

Geßner, O., Hikosaka, Y., Zimmermann, B., Hempelmann, A., Lucchese, R. R., Eland, J. H. D., Guyon, P. M., Becker, U. (2002). *Phys. Rev. Lett.* **88**, 193002.

Golovin, A. V. (1991). *Opt. Spectrosc. (USSR)* **71**, 537.

Grant, I. P. (1970). *Advan. Phys.* **19**, 747.

Grant, I. P., Mayers, D. F., Pyper, N. C. (1976). *J. Phys. B: At. Mol. Phys.* **9**, 2777.

Grant, I. P., McKenzie, B. J., Norrington, P. H., Mayers, D. F., Pyper, N. C. (1980). *Comp. Phys. Comm.* **21**, 207.

Grant, I. P. (1988). In: S. Wilson (Ed.), “Methods in Computational Chemistry”, Vol. **2**, p. 1. Plenum Press, New York.

Grant, I. P., Parpia, F. A. (1992). Private communication.

Hahn, U., Semke, J., Merz, H., Kessler, J. (1985). *J. Phys. B: At. Mol. Phys.* **18**, L417.

Haken, H. Wolf, H. C. (1991). “Molekülphysik und Quantenchemie.” Springer, Berlin.

Hanne, G. F., Malegat L., Schmidt-Böcking, H. (Eds.) (2003). *AIP Conf. Proc.* **697**. Melville, New York.

Hansen, J. E., Persson, W. (1987). *Phys. Scr.* **36**, 602.

Harnung, S. E., Schäffer, C. E. (1972). In: J. D. Dunitz, P. Hemmerich, J. A. Ibers, C. K. Jørgensen, J. B. Neilands, D. Reinen, R. J. P. Williams (Eds.), *Structure and Bonding*, Vol. **12**, p. 245. Springer, Berlin.

Heiser, F., Geßner, O., Viefhaus, J., Wieliczek, K., Hentges, R., Becker, U. (1997). *Phys. Rev. Lett.* **79**, 2435.

Hemmers, O., Heiser, F., Eiben, J., Wehlitz, R., Becker, U. (1993). *Phys. Rev. Lett.* **71**, 987.

Hergenhahn, U. (1996). “Winkelverteilung und Spin-Polarisation von Auger-Elektronen.” *PhD Thesis*, Oberhofer, Berlin.

Hergenhahn, U., Becker, U. (1995a). *J. Electr. Spectr. & Relat. Phen.* **72**, 243.

Hergenhahn, U., Becker, U. (1995b). *J. Electr. Spectr. & Relat. Phen.* **76**, 225.

Hergenhahn, U., Kabachnik, N. M., Lohmann, B. (1991). *J. Phys. B: At. Mol. Opt. Phys.* **24**, 4759.

Hergenhahn, U., Lohmann, B., Kabachnik, N. M., Becker, U. (1993). *J. Phys. B: At. Mol. Opt. Phys.* **26**, L117.

Hergenhahn, U., Snell, G., Drescher, M., Schmidtke, B., Müller, N., Heinzmann, U., Wiedenhöft, M., Becker, U. (1999). *Phys. Rev. Lett.* **82**, 5020, and private communication.

Hertel, I. V., Stoll, W. (1977). *Adv. At. Mol. Phys.* **13**, 113. Elsevier Academic Press, New York.

Hillig, H., Cleff, B., Mehlhorn, W., Schmitz, W. (1974). *Z. Phys.* **268**, 225.

Hörnfeldt, O. (1962). *Ark. Fys.* **23**, 235.

Hörnfeldt, O., Fahlman, A., Nordling, C. (1962). *Ark. Fys.* **23**, 155.

Howat, G., Åberg, T., Goscinsky, O. (1978). *J. Phys. B: At. Mol. Phys.* **11**, 1575.

Huang, K. N. (1982). *Phys. Rev. A* **26**, 2274.

Huzinaga, S. (1965). *J. Chem. Phys.* **42**, 1293.

Kabachnik, N. M. (1981). *J. Phys. B: At. Mol. Phys.* **14**, L337.

Kabachnik, N. M. (2005). *J. Phys. B: At. Mol. Opt. Phys.* **38**, L19.

Kabachnik, N. M., Grum-Grzhimailo, A. N. (2001). *J. Phys. B: At. Mol. Opt. Phys.* **34**, L63.

Kabachnik, N. M., Lee, O. V. (1989). *J. Phys. B: At. Mol. Opt. Phys.* **22**, 2705.

Kabachnik, N. M., Lee, O. V. (1990a). *Z. Phys. D* **17**, 169.

Kabachnik, N. M., Lee, O. V. (1990b). *J. Phys. B: At. Mol. Opt. Phys.* **23**, 353.

Kabachnik, N. M., Sazhina, I. P. (1976). *J. Phys. B: At. Mol. Phys.* **9**, 1681.

Kabachnik, N. M., Sazhina, I. P. (1984). *J. Phys. B: At. Mol. Phys.* **17**, 1335.

Kabachnik, N. M., Sazhina, I. P. (1986). *Opt. Spectrosc.* **60**, 683.

Kabachnik, N. M., Sazhina, I. P. (1988). *J. Phys. B: At. Mol. Opt. Phys.* **21**, 267.

Kabachnik, N. M., Sazhina, I. P. (2002). *J. Phys. B: At. Mol. Opt. Phys.* **35**, 3591.

Kabachnik, N. M., Schmidt, V. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, 233.

Kabachnik, N. M., Ueda, K. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, 5013.

Kabachnik, N. M., Sazhina, I. P., Lee, I. S., Lee, O. V. (1988). *J. Phys. B: At. Mol. Opt. Phys.* **21**, 3695.

Kabachnik, N. M., Lohmann, B., Mehlhorn, W. (1991). *J. Phys. B: At. Mol. Opt. Phys.* **24**, 2249.

Kabachnik, N. M., Tulkki, J., Aksela, H., Ricz, S. (1994). *Phys. Rev. A* **49**, 4653.

Kämmerling, B., Schmidt, V., Mehlhorn, W., Peatman, W. B., Schaefers, F., Schroeter, T. (1989). *J. Phys. B: At. Mol. Opt. Phys.* **22**, L597.

Kämmerling, B., Krässig, B., Schmidt, V. (1990). *J. Phys. B: At. Mol. Opt. Phys.* **23**, 4487, and private communication.

Kämmerling, B., Krässig, B., Schwarzkopf, O., Ribeiro, J. P., Schmidt, V. (1992). *J. Phys. B: At. Mol. Opt. Phys.* **25**, L5.

Karim, K. R., Crasemann, B. (1985). *Phys. Rev. A* **31**, 709.

Karim, K. R., Chen, M. H., Crasemann, B. (1984). *Phys. Rev. A* **29**, 2605.

Kaur, S., Srivastava, R. (1999). *J. Phys. B: At. Mol. Opt. Phys.* **32**, 2323.

Kessler, J. (1985). "Polarized Electrons." 2^{nd} Edn. Springer, Berlin.

Kettle, S. F. A. (1995). "Symmetry and Structure." Wiley, New York.

Klar, H. (1980). *J. Phys. B: At. Mol. Phys.* **13**, 4741.

Kleiman, U., Becker, U. (2005). *J. Electr. Spectr. & Relat. Phen.* **142**, 45.

Kleiman, U., Lohmann, B. (2003). *J. Electr. Spectr. & Relat. Phen.* **131–132**, 29.

Kleiman, U., Lohmann, B., Blum, K. (1999a). *J. Phys. B: At. Mol. Opt. Phys.* **32**, 309, and 4129.

Kleiman, U., Lohmann, B., Blum, K. (1999b). *J. Phys. B: At. Mol. Opt. Phys.* **32**, L219.

Kleinpoppen, H. (1997). Private communication.

H. Kleinpoppen, M. R. C. McDowell (Eds.) (1976). "Electron and Photon Interactions with Atoms." Plenum Press, New York.

Kleinpoppen, H., Lohmann, B., Grum-Grzhimailo, A., Becker, U. (2005). In: H. H. Stroke (Ed.), *Adv. At. Mol. & Opt. Phys.* **51**, p. 471. Elsevier Academic Press, New York.

Knyr, V. A., Nasyrov, V. V., Popov, Y. V. (2003). In: G. F. Hanne, L. Malegat, Schmidt-Böcking, H. (Eds.), *AIP Conf. Proc.* **697**, p. 76. Melville, New York.

Krause, M. O., Caldwell, C. D., Menzel, A., Benzaid, S., Jiménez-Mier, J. (1996). *J. Electr. Spectr. & Relat. Phen.* **79**, 241.

Kronast, W., Huster, R., Mehlhorn, W. (1986). *Z. Phys. D* **2**, 285.

Kuntze, R., Salzmann, M., Böwering, N., Heinzmann, U. (1993). *Phys. Rev. Lett.* **70**, 3716.

Kuntze, R., Salzmann, M., Böwering, N., Heinzmann, U., Ivanov, V. K., Kabachnik, N. M. (1994). *Phys. Rev. A* **50**, 489.

Lafosse, A., Lebech, M., Brenot, J. C., Guyon, P. M., Jagutzki, O., Spielberger, L., Vervloet, M., Houver, J. C., Dowek, D. (2000). *Phys. Rev. Lett.* **84**, 5987.

Lagutin, B. M., Petrov, I. D., Sukhorukov, V. L., Demekhin, P. V., Zimmermann, B., Mickat, S., Kammer, S., Schartner, K.-H., Ehresmann, A., Shutov, Y. A., Schmoranzer, H. (2003). *J. Phys. B: At. Mol. Opt. Phys.* **36**, 3251.

Landers, A., Weber, Th., Ali, I., Cassimi, A., Hattauss, M., Jagutzki, O., Nauert, A., Osipov, T., Staudte, A., Prior, M. H., Schmidt-Böcking, H., Cocke, C. L., Dörner, R. (2001). *Phys. Rev. Lett.* **87**, 013002.

Langer, B., Berrah, N., Farhat, A., Humphrey, M., Cubaynes, D., Menzel, A., Becker, U. (1997). *J. Phys. B: At. Mol. Opt. Phys.* **30**, 4255.

Larkins, F. P. (1977). *Atomic Data and Nuclear Data Tables* **20**, 311.

Larkins, F. P. (1990). *J. Electr. Spectr. & Relat. Phen.* **51**, 115.

Lee, O. V. (1990). Private communication.

Lehmann, J., Blum, K. (1997). *J. Phys. B: At. Mol. Opt. Phys.* **30**, 633.

Lehmann, J., Bonhoff, K., Bonhoff, S., Lohmann, B., Blum, K. (1997). In: J. L. Duggan, I. L. Morgan (Eds.), "Application of Accelerators in Research and Industry." *AIP Conf. Proc.* **392**, p. 63. New York.

Lindle, D. W., Ferrett, T. A., Heimann, P. A., Shirley, D. A. (1988). *Phys. Rev. A* **37**, 3808.

Löwdin, P. O. (1955). *Phys. Rev.* **97**, 1474.

Lohmann, B. (1984). *Diploma Thesis*, University of Münster, Germany.

Lohmann, B. (1988). *PhD Thesis*, University of Münster, Germany.

Lohmann, B. (1990). *J. Phys. B: At. Mol. Opt. Phys.* **23**, 3147.

Lohmann, B. (1991). *J. Phys. B: At. Mol. Opt. Phys.* **24**, 861.

Lohmann, B. (1992). *J. Phys. B: At. Mol. Opt. Phys.* **25**, 4163.

Lohmann, B. (1993). *J. Phys. B: At. Mol. Opt. Phys.* **26**, 1623.

Lohmann, B. (1996a). *Aust. J. Phys.* **49**, 365, and refs. therein.

Lohmann, B. (1996b). "Spin polarization of Auger electrons; recent developments." In: H. Kleinpoppen, M. C. Campell (Eds.), "Selected Topics in Electron Physics." *Peter-Farago-Symp. Conf. Proc.*, p. 119. Plenum Press, New York.

Lohmann, B. (1996c). "Recent developments in the theory of angular distribution and spin polarization of Auger electrons." In: "VIII. Int. Symp. on Pol. & Corr. in Elec. & Atomic Coll., Vancouver." *Can. J. Phys.* **74**, 962.

Lohmann, B. (1996d). *J. Phys. B: At. Mol. Opt. Phys.* **29**, L521.

Lohmann, B. (1997). "Spin polarization parameters for resonant Auger transitions." In: "IX Int. Symp. on Pol. & Corr. in Elec. & Atomic Coll. and Int. Symp. on (e,2e), Double Phot. & Rel. Topics," Ses. 8. Frascati, Italy.

Lohmann, B. (1998). *Habilitation Thesis*, University of Münster, Germany.
Lohmann, B. (1999a). *J. Phys. B: At. Mol. Opt. Phys.* **32**, L643.
Lohmann, B. (1999b). *Aust. J. Phys.* **52**, 397.
Lohmann, B., Fritzsche, S. (1994). *J. Phys. B: At. Mol. Opt. Phys.* **27**, 2919.
Lohmann, B., Fritzsche, S. (1996). *J. Phys. B: At. Mol. Opt. Phys.* **29**, 5711.
Lohmann, B., Larkins, F. P. (1994). *J. Phys. B: At. Mol. Opt. Phys.* **27**, L143.
Lohmann, B., Kleiman, U. (2001). In: J. Berakdar, J. Kirschner (Eds.), "Many Particle Spectroscopy of Atoms, Molecules, Clusters, and Surfaces." p. 173. Kluwer/Plenum, New York, London.
Lohmann, B., Kleiman, U. (2006). *J. Phys. B: At. Mol. Opt. Phys.* **39**, 271.
Lohmann, B., Hergenhahn, U., Kabachnik, N. M. (1993). *J. Phys. B: At. Mol. Opt. Phys.* **26**, 3327.
Lohmann, B., Fritzsche, S., Larkins, F. P. (1996). *J. Phys. B: At. Mol. Opt. Phys.* **29**, 1191.
Lohmann, B., Bonhoff, S., Bonhoff, K., Lehmann, J., Blum, K. (1997). In: J. L. Duggan, I. L. Morgan (Eds.), "Application of Accelerators in Research and Industry." *AIP Conf. Proc.* **392**, p. 59. New York.
Lohmann, B., Fritzsche, S., Andrä, H. J. (1998). "Absolut transition rates for Auger neutralization processes." Unpublished data. University of Münster, University of Kassel, Germany.
Lohmann, B., Srivastava, R., Kleiman, U., Blum, K. (2002). In: D. H. Madison, M. Schulz (Eds.), *AIP Conf. Proc.* **604**, p. 229. Melville, New York.
Lohmann, B., Zimmermann, B., Kleinpoppen, H., Becker, U. (2003a). In: B. Bederson, H. Walther (Eds.), *Adv. At. Mol. & Opt. Phys.* **49**, p. 217. Elsevier Academic Press, New York.
Lohmann, B., Langer, B., Snell, G., Kleiman, U., Canton, S., Martins, M., Becker, U., Berrah, N. (2003b). In: G. F. Hanne, L. Malegat, H. Schmidt-Böcking (Eds.), *AIP Conf. Proc.*, vol. **697**, p. 133. Melville, New York.
Lohmann, B., Langer, B., Snell, G., Kleiman, U., Canton, S., Martins, M., Becker, U., Berrah, N. (2005). *Phys. Rev. A* **71**, 020701(R).
Lombardi, M. (1975). *Phys. Rev. Lett.* **35**, 1172.
Lower, J., Panajotovic, R., Weigold, E. (2004). *Phys, Scr. T* **110**, 216.
Mayer-Kuckuk, T. (1977). "Atomphysik." Teubner, Stuttgart.
Mayer-Kuckuk, T. (1979). "Kernphysik." Teubner, Stuttgart.
McGuire, E. J. (1969). *Phys. Rev.* **185**, 1.
McGuire, E. J. (1970). *Phys. Rev. A* **2**, 273.
McGuire, E. J. (1975). *Sandia Research Lab.* Research report no. SAND-75-0443.
McKenzie, B. J., Grant, I. P., Norrington, P. H. (1980). *Comp. Phys. Comm.* **21**, 233.
Mehlhorn, W. (1968). *Phys. Lett. A* **26**, 166.
Mehlhorn, W. (1985). "Auger-Electron Spectrometry of Core Levels of Atoms." In: B. Crasemann (Ed.), "Atomic Inner Shell Physics." Plenum Press, New York.
Mehlhorn, W. (1990). In: T. A. Carlson, M. O. Krause, S. T. Manson (Eds.), "X-ray and Inner Shell Processes." *AIP Conf. Proc.* **215**, p. 465. New York.
Mehlhorn, W., Stalherm, D. (1968). *Z. Phys.* **217**, 294.
Mehlhorn, W., Taulbjerg, K. (1980). *J. Phys. B: At. Mol. Phys.* **13**, 445.
Meister, H. J., Weiss, H. F. (1968). *Z. Phys.* **216**, 165.
Menzel, A. (1994). *PhD Thesis*, Technical University of Berlin, Germany.
Menzel, A., Hemmers, O., Langer, B., Wehlitz, R., Becker, U. (1993). "BESSY annual report.", and private communication.
Merz, H. (1991). Private communication.

Merz, H., Semke, J. (1990). In: T. A. Carlson, M. O. Krause, S. T. Manson (Eds.), “X-ray and Inner Shell Processes.” *AIP Conf. Proc.* **215**, p. 719. New York.

Messiah, A. (1979). “Quantenmechanik.” de Gruyter, Berlin.

Meyer, M., von Raven, E., Sonntag, B., Hansen, J. E. (1991). *Phys. Rev. A* **43**, 177.

Meyer, M., Marquette, A., Grum-Grzhimailo, A. N., Kleiman, U., Lohmann, B. (2001). *Phys. Rev. A* **64**, 022703.

Michl, J., Thulstrup, E. W. (1986). “Spectroscopy with Polarized Light.” V.C.H. Wiley, New York.

Moore, C. E. (1976). “Atomic energy levels.” *Natl. Bur. Stand., U.S. Circ.* No. **467**, Vol. **1**. U.S. GPO, Washington, DC.

Motoki, S., Adachi, J., Hikosaka, Y., Ito, K., Sano, M., Soejima, K., Yagishita, A., Raseev, G., Cherepkov, N. A. (2000). *J. Phys. B: At. Mol. Opt. Phys.* **33**, 4193.

Mott, N. F., Massey, H. S. W. (1965). “The Theory of Atomic Collisions.” 3^{rd} Edn, Chap. **IX. 4**. Clarendon Press, Oxford.

Müller, N., David, R., Snell, G., Kuntze, R., Drescher, M., Böwering, N., Stoppmanns, P., Yu, S. W., Heinzmann, U., Viefhaus, J., Hergenhahn, U., Becker, U. (1995). *J. Electr. Spectr. & Relat. Phen.* **72**, 187.

Mursu, J., Aksela, H., Sairanen, O. P., Kivimäki, A., Nõmmiste, E., Ausmees, A., Svensson, S., Aksela, S. (1996). *J. Phys. B: At. Mol. Opt. Phys.* **29**, 4387.

Nahrup, S. (1995). *Diploma Thesis*, University of Münster, Germany.

Oenning, R. (1989). *Diploma Thesis*, University of Münster, Germany.

O’Keeffe, P., Aloïse, S., Meyer, M., Grum-Grzhimailo, A. N. (2003). *Phys. Rev. Lett.* **90**, 023002.

O’Keeffe, P., Aloïse, S., Fritzsche, S., Lohmann, B., Kleiman, U., Meyer, M., Grum-Grzhimailo, A. N. (2004). *Phys. Rev. A* **70**, 012705.

Ong, W., Russek, A. (1978). *Phys. Rev. A* **17**, 120.

Paripás, B., Víkor, G., Ricz, S. (1997). *J. Phys. B: At. Mol. Opt. Phys.* **30**, 403.

Parpia, F. A., Grant, I. P. (1992). Private communication.

Paulus, G. G., Lindner, F., Walther, H., Baltuska, A., Goulielmakis, E., Lezius, M., Krausz, F. (2003). *Phys. Rev. Lett.* **91**, 253004.

Persson, W., Wahlström, C.-G., Bertucelli, G., Di Rocco, H. O., Reyna Almandos, J. G., Gallardo, M. (1988). *Phys. Scr.* **38**, 347.

Petrini, D., Araújo, F. X. (1994). *Astron. Astrophys.* **282**, 315.

Racah, G. (1942). *Phys. Rev.* **62**, 438.

Ridder, D., Dieringer, J., Stolterfoht, N. (1976). *J. Phys. B: At. Mol. Phys.* **9**, L307.

Rose, M. E. (1957). “Elementary Theory of Angular Momentum.” J. Wiley & Sons, New York.

Rotenberg, M., Bivins, R., Metropolis, N., Wooten Jr., J. K. (1959). “The *3-j* and *6-j* Symbols.” Technology Press, Cambridge, MA.

Saha, H. P. (1994). *Phys. Rev. A* **49**, 894.

Sandner, W. (1985). “New Application of Electron-Electron Coincidences.” In: H. Kleinpoppen, J. S. Briggs, H. O. Lutz (Eds.), “Fundamental Processes in Atomic Collision Physics.” *NATO ASI Series B: Physics* **134**, p. 453. New York.

Sarkadi, L., Vajnai, T., Pálinkás, J., Kövér, A., Végh, J., Mukoyama, T. (1990). *J. Phys. B: At. Mol. Opt. Phys.* **23**, 3643.

Schimmelpfennig, B. (1994). *PhD Thesis*, University of Bonn, Germany.

Schimmelpfennig, B., Nestmann, B., Peyerimhoff, S. D. (1992). *J. Phys. B: At. Mol. Opt. Phys.* **25**, 1217.

Schimmelpfennig, B., Nestmann, B., Peyerimhoff, S. D. (1995). *J. Electr. Spectr. & Relat. Phen.* **74**, 173.

Schmidt, V. (1992). *Rep. Prog. Phys.* **55**, 1483.

Schmidt, V. (1997). "Electron Spectrometry of Atoms using Synchrotron Radiation." Cambridge University Press, Cambridge, MA.

Schmidtke, B., Drescher, M., Cherepkov, N. A., Heinzmann, U. (2000a). *J. Phys. B: At. Mol. Opt. Phys.* **33**, 2451.

Schmidtke, B., Khalil, T., Drescher, M., Müller, N., Kabachnik, N. M., Heinzmann, U. (2000b). *J. Phys. B: At. Mol. Opt. Phys.* **33**, 5225.

Schmidtke, B., Khalil, T., Drescher, M., Müller, N., Kabachnik, N. M., Heinzmann, U. (2001). *J. Phys. B: At. Mol. Opt. Phys.* **34**, 4293.

Schpolski, E. W. (1983). "Atomphysik." 12^{th} Edn., VEB Deutscher Verlag der Wissenschaften, Berlin.

Schuch, R., Cederquist, M., Larsson, E., Lindroth, S., Schmidt, H. (Eds.) (2004). *Phys. Scr.* **T110**.

Shampine, L. F., Gordon, M. K. (1975). "Computer Solution of Ordinary Differential Equations: The Initial Value Problem." W. H. Freeman and Co., San Francisco.

Shaw Jr., R. W., Thomas, T. D. (1975). *Phys. Rev. A* **11**, 1491.

Shirley, D. A. (1973). *Phys. Rev. A* **7**, 1520.

Siegbahn, K., Nordling, C., Fahlman, A., Nordberg, R., Hamrin, K., Hedman, J., Johansson, G., Bergmark, T., Karlsson, S.-E., Lindgren, T., Lindberg, B. (1967). "ESCA – Atomic, Molecular and Solid State Structure Studied by Means of Electron Spectroscopy." *Nova Acta Regiae Soc. Sci. Upsaliensis* Ser. **IV**, Vol. **20**.

Siegbahn, K., Nordling, C., Johansson, G., Hedman, J., Heden, P. F., Hamrin, K., Gelius, U., Bergmark, T., Werme, L. O., Manne, R., Baer, Y. (1969). "ESCA Applied to Free Molecules." North-Holland, Amsterdam.

Slater, J. C. (1951). *Phys. Rev.* **81**, 385.

Snell, G., Hergenhahn, U., Drescher, M., Schmidtke, B,. Müller, N., Wiedenhöft, M., Becker, U., Heinzmann, U. (1996a). "BESSY annual report."

Snell, G., Drescher, M., Müller, N., Heinzmann, U., Hergenhahn, U., Viefhaus, J., Heiser, F., Becker, U., Brookes, N. B. (1996b). *Phys. Rev. Lett.* **76**, 3923.

Snell, G., Langer, B., Drescher, M., Müller, N., Zimmermann, B., Hergenhahn, U., Viefhaus, J., Heinzmann, U., Becker, U. (1999). *Phys. Rev. Lett.* **82**, 2480.

Snell, G., Viefhaus, J., Dunnings, F. B., Berrah, N. (2000). *Rev. Sci. Instrum.* **71**, 2608.

Snell, G., Hergenhahn, U., Müller, N., Drescher, M., Viefhaus, J., Becker, U., Heinzmann, U. (2001). *Phys. Rev. A* **63**, 032712.

Snell, G., Langer, B., Young, A. T., Berrah, N. (2002). *Phys. Rev. A* **66**, 022701.

Southworth, S., Becker, U., Truesdale, C. M., Kobrin, P. H., Lindle, D. W., Owaki, S., Shirley, D. A. (1983). *Phys. Rev. A* **28**, 261.

Srivastava, R., Blum, K., McEachran, R. P., Stauffer, A. D. (1996a). *J. Phys. B: At. Mol. Opt. Phys.* **29**, 3513.

Srivastava, R., Blum, K., McEachran, R. P., Stauffer, A. D. (1996b). *J. Phys. B: At. Mol. Opt. Phys.* **29**, 5947.

Starace, A. F. (1982). In: S. Flügge, W. Mehlhorn (Eds.), *Encyclopedia of Physics* **31**, p. 1. Springer, New York.

Stoppmanns, P., Schmiedeskamp, B., Vogt, B., Müller, N., Heinzmann, U. (1992). *Phys. Scr.* **T41**, 190.

Takahashi, M., Cave, J. P., Eland, J. H. D. (2000). *Rev. Sci. Instrum.* **71**, 1337.

Taouil, L., Duguet, A., Lahman-Bennani, A., Lohmann, B., Rasch, J., Whelan, C. T., Walters, H. R. J. (1999). *J. Phys. B: At. Mol. Opt. Phys.* **32**, L5.

Taylor, J. R. (1972). "Scattering Theory." J. Wiley & Sons, New York, London, Sydney, Toronto.

Theodosiou, C. E. (1987). *Phys. Rev. A* **36**, 3138.

Tinkham, M. (1964). "Group Theory and Quantum Mechanics." McGraw-Hill, New York.

Tulkki, J., Kabachnik, N. M., Aksela, H. (1993). *Phys. Rev. A* **48**, 1277, and private communication.

Tulkki, J., Aksela, H., Kabachnik, N. M. (1993). *Phys. Rev. A* **48**, 2957.

Turri, G., Lohmann, B., Langer, B., Snell, G., Becker, U., Berrah, N. (2007). *J. Phys. B: At. Mol. Opt. Phys.* **40**, 3453.

Ueda, K., West, J. B., Ross, K. J., Beyer, H. J., Kabachnik, N. M. (1998). *J. Phys. B: At. Mol. Opt. Phys.* **31**, 4801.

Varshalovich, D. A., Moskalev, A. N., Khersonskii, V. K. (1988). "Quantum Theory of Angular Momentum." World Scientific, Singapore.

Vanderpoorten, R. (1975). *J. Phys. B: At. Mol. Phys.* **8**, 926.

Väyrynen, J., Aksela, S. (1979). *J. Electr. Spectr. & Relat. Phen.* **16**, 423.

van der Laan, G., Thole, B. T. (1995). *Phys. Rev. B* **52**, 15355.

Viefhaus, J., Avaldi, L., Hentges, R., Wiedenhöft, M., Wieliczek, K., Becker, U. (1996). In: "17th Int. Conf. X-ray and Inner-Shell Processes." *Book of Abstracts*, p. 220. Hamburg.

Viefhaus, J., Zimmermann, B., Kleinpoppen, H., Becker, U. (1998). Private communication.

Vollmer, R., Etzkorn, M., Anilkumar, P. S., Ibach, H., Kirschner, J. (2003). *Phys. Rev. Lett.* **91**, 147201.

von Raven, E., Meyer, M., Pahler, M., Sonntag, B. (1990). *J. Electr. Spectr. & Relat. Phen.* **52**, 677.

Wagner, C. D. (1975). *Faraday Discuss. Chem. Soc.* **60**, 291.

Walters, D. L., Bhalla, C. P. (1971). *Atomic Data* **3**, 301.

Wehlitz, R., Pibida, L. S., Levin, J. C., Sellin, I. A. (1999). *Phys. Rev. A* **59**, 421.

Weigold, E., Lower, J., Berakdar, J., Mazevet, S. (2002). In: M. Schulz, D. H. Madison (Eds.), *AIP Conf. Proc.* **604**, p. 32. Melville, New York.

Wentzel, G. (1927). *Z. Phys.* **43**, 524.

Werme, L. O., Bergmark, T., Siegbahn, K. (1972). *Phys. Scr.* **6**, 141.

Werme, L. O., Bergmark, T., Siegbahn, K. (1973). *Phys. Scr.* **8**, 149.

Wigner, E. P. (1959). "Group Theory and its Application to the Quantum Mechanics of Atomic Spectra." Academic Press, New York.

Wöste, G., Fullerton, C., Blum, K., Thompson, D. (1994). *J. Phys. B: At. Mol. Opt. Phys.* **27**, 2625.

Ying-Nan, C. (1966). *J. Chem. Phys.* **45**, 2969.

Young, A. T., Feng, J., Arenholz, E., Padmore, H. A., Henderson, T., Marks, S., Hoyer, E., Schlueter, R., Kortright, J. B., Martynov, V., Steier, C., Portmann, G. (2001). *Nucl. Instrum. & Methods A* **467**, 549.

Zare, R. N. (1988). "Angular Momentum." J. Wiley & Sons, New York.

Zähringer, K., Meyer, H. D., Cederbaum, L. S. (1992). *Phys. Rev. A* **46**, 5643.

Zähringer, K., Meyer, H. D., Cederbaum, L. S., Tarantelli, F., Sgamellotti, A. (1993). *Chem. Phys. Lett.* **206**, 247.

Zheng, Q., Edwards, A. K., Wood, R. M., Mangan, M. A. (1995a). *Phys. Rev. A* **52**, 3940.

Zheng, Q., Edwards, A. K., Wood, R. M., Mangan, M. A. (1995b). *Phys. Rev. A* **52**, 3945.

Zimmermann, B. (2000). "Vollständige Experimente in der atomaren und molekularen Photoionisation." In: U. Becker (Ed.), *Studies of Vacuum Ultraviolet and X-Ray Processes* **13**. Wissenschaft und Technik Verlag, Berlin.

Zimmermann, B., Wilhelmi, O., Schartner, K.-H., Vollweiler, F., Liebel, H., Ehresmann, A., Lauer, S., Schmoranzer, B. M., Lagutin, B. M., Petrov, I. D., Sukhorukov, V. L. (2000). *J. Phys. B: At. Mol. Opt. Phys.* **33**, 2467.

Index

Springer Series on
ATOMIC, OPTICAL, AND PLASMA PHYSICS

Springer Series on

ATOMIC, OPTICAL, AND PLASMA PHYSICS

20 **Electron Emission in Heavy Ion–Atom Collision**
By N. Stolterfoht, R.D. DuBois, and R.D. Rivarola

21 **Molecules and Their Spectroscopic Properties**
By S.V. Khristenko, A.I. Maslov, and V.P. Shevelko

22 **Physics of Highly Excited Atoms and Ions**
By V.S. Lebedev and I.L. Beigman

23 **Atomic Multielectron Processes**
By V.P. Shevelko and H. Tawara

24 **Guided-Wave-Produced Plasmas**
By Yu.M. Aliev, H. Schlüter, and A. Shivarova

25 **Quantum Statistics of Nonideal Plasmas**
By D. Kremp, M. Schlanges, and W.-D. Kraeft

26 **Atomic Physics with Heavy Ions**
By H.F. Beyer and V.P. Shevelko

27 **Quantum Squeezing**
By P.D. Drumond and Z. Ficek

28 **Atom, Molecule, and Cluster Beams I**
Basic Theory, Production and Detection of Thermal Energy Beams
By H. Pauly

29 **Polarization, Alignment and Orientation in Atomic Collisions**
By N. Andersen and K. Bartschat

30 **Physics of Solid-State Laser Physics**
By R.C. Powell
(Published in the former Series on Atomic, Molecular, and Optical Physics)

31 **Plasma Kinetics in Atmospheric Gases**
By M. Capitelli, C.M. Ferreira, B.F. Gordiets, and A.I. Osipov

32 **Atom, Molecule, and Cluster Beams II**
Cluster Beams, Fast and Slow Beams, Accessory Equipment and Applications
By H. Pauly

33 **Atom Optics**
By P. Meystre

34 **Laser Physics at Relativistic Intensities**
By A.V. Borovsky, A.L. Galkin, O.B. Shiryaev, and T. Auguste

35 **Many-Particle Quantum Dynamics in Atomic and Molecular Fragmentation**
Editors: J. Ullrich and V.P. Shevelko

36 **Atom Tunneling Phenomena in Physics, Chemistry and Biology**
Editor: T. Miyazaki

37 **Charged Particle Traps**
Physics and Techniques of Charged Particle Field Confinement
By V.N. Gheorghe, F.G. Major, and G. Werth

38 **Plasma Physics and Controlled Nuclear Fusion**
By K. Miyamoto

39 **Plasma-Material Interaction in Controlled Fusion**
By D. Naujoks

40 **Relativistic Quantum Theory of Atoms and Molecules**
Theory and Computation
By I.P. Grant

41 **Turbulent Particle-Laden Gas Flows**
By A.Y. Varaksin

42 **Phase Transitions of Simple Systems**
By B.M. Smirnov and S.R. Berry

43 **Collisions of Charged Particles with Molecules**
By Y. Itikawa

44 **Plasma Polarization Spectroscopy**
Editors: T. Fujimoto and A. Iwamae

45 **Emergent Non-Linear Phenomena in Bose–Einstein Condensates**
Theory and Experiment
Editors: P.G. Kevrekidis, D.J. Frantzeskakis, and R. Carretero-González

46 **Angle and Spin Resolved Auger Emission**
Theory and Applications to Atoms and Molecules
By B. Lohmann