On the factorisation of matrix elements for systems with anti-unitary symmetry



1986 J. Phys. A: Math. Gen. 19 1279

(http://iopscience.iop.org/0305-4470/19/8/010)

J. Phys. A: Math. Gen. 19 (1986) 1279-1289. Printed in Great Britain

# On the factorisation of matrix elements for systems with anti-unitary symmetry

M N Angelova, M I Aroyo and J N Kotzev
Faculty of Physics, University of Sofia, Sofia 1126, Bulgaria

Received 3 June 1985

**Abstract.** For the case of corepresentations of anti-unitary magnetic groups a new generalisation of the Wigner-Eckart theorem, based on the symmetrised Clebsch-Gordan coefficients, or $3D$-symbols, is given. It is shown that the reduced matrix elements are real for all types of corepresentations. The reduced matrix elements of coupled tensor operators are expressed in terms of the reduced matrix elements of their components.

## 1. Introduction

The central problem in quantum mechanical calculations is how to compute a matrix element of an operator. Such a calculation is simplified if one invokes the Wigner-Eckart theorem, which introduces the concept of a set of operators, transforming according to some irreducible representation of the appropriate symmetry group of the system. The matrix element of such an irreducible tensor operator (ITO) between states belonging to two irreducible representations of the symmetry group is given by the corresponding Clebsch-Gordan coefficients (CGC) up to quantities, describing the physical properties of the operator and known as reduced matrix elements (RME) (see, e.g., Biedenharn and Louck 1981). The next step in that line is the evaluation of matrix elements of products of ITO which are necessary for quantum mechanical calculations in atomic, nuclear, molecular and solid state physics, etc. The relations between RME of such tensor operators are studied in detail for the orthogonal and symmetric groups, as well as for non-simple reducible finite or compact groups (Judd 1963, Vanagas 1971, Butler 1975). When the symmetry group of a system is an anti-unitary (AU) magnetic group, the basis functions and the components of ITO do not transform by the linear representations but by its irreducible corepresentations (coreps) (Wigner 1959, Bradley and Cracknell 1972). It leads to non-trivial difficulties in the computation of matrix elements. The Wigner-Eckart theorem for a case of coreps of finite magnetic groups was generalised for the first time by Kotzev (1967, 1972) and Aviran and Zak (1968), but their results are rather complicated and not very convenient for application.

The aim of the present paper is to factorise the matrix elements of the quantum mechanical operators for coreps of Shubnikov magnetic groups (grey and black-and-white), using the symmetrised coefficients for coreps ($nD$-symbols).

In § 2, we generalise the Wigner-Eckart theorem for coreps on the base of the symmetrised CGC for coreps—$3D$-symbols (in analogy with the Wigner $3j$-symbols). There are some essential advantages of this version of the theorem which are discussed in § 2.

0305-4470/86/081279+11\$02.50  

In § 3 we consider coupled ITO for coreps of magnetic groups. We obtain the RME of coupled tensor operators (CTO) for coreps in terms of the RME of their components for two cases: (i) CTO and its components act in one and the same space; (ii) the components of CTO act independently in different subspaces. The relations are derived using symmetrised coefficients for coreps, such as $6D$- and $9D$-symbols, analogous to the Wigner $6j$- and $9j$-symbols respectively. The peculiarities of the derived relations are discussed.

In the appendix some properties of $1D$-symbols (in analogy with the Wigner $1j$-symbols) and $3D$-symbols, necessary for the derivation of the main results in §§ 2 and 3, are given.

## 2. On the Wigner–Eckart theorem for AU magnetic groups

The generalisation of the Wigner–Eckart theorem for the case of coreps of magnetic groups in terms of the CGC for coreps (we shall refer to it as a 'CGC version') has been given by many authors (Kotzev 1967, 1972, Aviran and Zak 1968, van den Broek 1979). In the general form of the 'CGC version' of the theorem (Kotzev 1972) the matrix elements of ITO $T^{\varkappa}=\{T^{\varkappa}_{q'q}\}$ in the basis $\{|\alpha_i, a'_ia_i\rangle\}$ of the coreps $D^{\alpha_i}\equiv D\Gamma^{\alpha_i}$ of the AU group $\mathrm{G_A}$ are given by the equation

$$\begin{aligned}\langle\alpha_1a'_1a_1|T^{\varkappa}_{q'q}|\alpha_2a'_2a_2\rangle&\\&=2\frac{[\Gamma^{\alpha_1}]}{[D^{\alpha_1}]}\sum_{r_{\alpha_1}p'_1}\left(\sum_{k'_1m'_1}\langle\alpha_1m'_1\|T^{\varkappa}\|\alpha_2\rangle_{r_{\alpha_1}k'_1}Q'(\alpha_1)_{m'_1a'_1k'_1p'_1}\right)\\&\quad\times[\varkappa q'q,\ \alpha_2a'_2a_2|\alpha_1r_{\alpha_1}p'_1a_1]^*\end{aligned}\tag{1}$$

where $[D^{\alpha_1}]$ and $[\Gamma^{\alpha_1}]$ are the dimensions of the corep $D^{\alpha_1}$ and the corresponding irreducible representation $\Gamma^{\alpha_1}$ of the unitary subgroup of $\mathrm{G_A}$, respectively. The matrix elements are expressed in terms of the CGC $[\varkappa q'q,\ \alpha_2a'_2a_2|\alpha_1r_{\alpha_1}p'_1a_1]$, $r_{\alpha_1}=1,\ldots,(\varkappa\alpha_2|\alpha_1)$ where $(\varkappa\alpha_2|\alpha_1)$ is the Kronecker multiplicity of $D^{\alpha_1}$ in $D^{\varkappa}\times D^{\alpha_2}$. Double indices for the row labels of basis functions and operators are introduced for the sake of convenience; the primed indices are equal to 1, 2 for the type 'b' and type 'c' coreps, and are equal to 1 for type 'a' corep; the unprimed indices run from 1 to $[\Gamma^{\alpha}]$.

The definition of RME used in (1) is

$$\begin{aligned}\langle\alpha_1m'_1\|T^{\varkappa}\|\alpha_2\rangle_{r_{\alpha_1}k'_1}=[\Gamma^{\alpha_1}]^{-1}\sum_{q'a'_2qa_1a_2}\langle\alpha_1m'_1a_1|T^{\varkappa}_{q'q}|\alpha_2a'_2a_2\rangle&\\\times[\varkappa q'q,\ \alpha_2a'_2a_2|\alpha_1r_{\alpha_1}k'_1a_1].&\end{aligned}\tag{2}$$

An additional relation between the RME (which considerably decreases their number) can be obtained taking into account the AU operators of $\mathrm{G_A}$:

$$\sum_{m'_1k'_1}\langle\alpha_1m'_1\|T^{\varkappa}\|\alpha_2\rangle_{r_{\alpha_1}k'_1}Q'(\alpha_1)_{m'_1a'_1k'_1p'_1}=\sum_{m''_1k''_1}\langle\alpha_1m''_1\|T^{\varkappa}\|\alpha_2\rangle^*_{r_{\alpha_1}k''_1}Q''(\alpha_1)_{m''_1a'_1k''_1p'_1}\tag{3}$$

where $Q'(\alpha_1)$ and $Q''(\alpha_1)$ take the values $0, \frac{1}{2}, \pm1$ depending on the type of the corep $D^{\alpha_1}$ and the set of indices.

We should point out that the Wigner–Eckart theorem, given by equations (1) and (3), is valid for coreps in the canonical form (Wigner 1959). Moreover there are some problems which in principle cannot be solved within the framework of the 'CGC version' of the theorem and which limit its application in the general case: (i) the explicit form of that version of the theorem is different for the different type of the corep $D^{\alpha_1}$; (ii) the RME (2) are not completely independent of the basis functions (as it is in the classical case of linear representations). In what follows we shall show that these problems can be solved using the symmetrised CGC for coreps—3$D$-symbols (Kotzev *et al* 1984a, see also the appendix)—to obtain a new form of the Wigner–Eckart theorem (referred as a '3$D$-symbol version').

In order to find the desired new form of the theorem we act with both unitary and anti-unitary elements of $\mathrm{G_A}$ on the basis functions $\{|\alpha_i a_i\rangle\}$ and the components of ITO $\{T^{\varkappa}_{q}\}$ and obtain

$$\begin{aligned}\langle\alpha_1 a_1|T^{\varkappa}_q|\alpha_2 a_2\rangle^{(*)} &= g\langle\alpha_1 a_1|T^{\varkappa}_q|\alpha_2 a_2\rangle\\ &= \sum_{n_1 n_2} D^{\alpha_1}_{n_1 a_1}(g)^* D^{\varkappa}_{tq}(g) D^{\alpha_2}_{n_2 a_2}(g)\langle\alpha_1 n_1|T^{\varkappa}_t|\alpha_2 n_2\rangle. \end{aligned} \tag{4}$$

Here and everywhere the asterisk in parentheses $(*)$ means that complex conjugation is applied if and only if $g\in\mathrm{G_A}$ is an anti-unitary operator. The matrices $D^{\alpha_1}(g)^*$, $g\in\mathrm{G_A}$ form a corep, which is equivalent to the 'standard' corep $D^{\alpha_1^*}(g)$, $g\in\mathrm{G_A}$. The transformation to the standard corep is carried out by the unitary matrix $K^{\alpha_1^*}$

$$K^{\alpha_1^*-1}D^{\alpha_1}(g)^* K^{\alpha_1^*(*)} = D^{\alpha_1^*}(g), \qquad g\in\mathrm{G_A}. \tag{5}$$

In analogy with the Wigner 1$j$-symbols, we call the matrix elements of $K^{\alpha_1^*}$ the 1$D$-symbols (see the appendix for more details).

After the summation over the unitary and anti-unitary operators of $\mathrm{G_A}$ and taking into account (5) and the definition of 3$D$-symbols (see equation (A5) in the appendix) we get the new form of the Wigner–Eckart theorem for coreps

$$\langle\alpha_1 a_1|T^{\varkappa}_q|\alpha_2 a_2\rangle = \sum_{\rho}\langle\alpha_1\|T^{\varkappa}\|\alpha_2\rangle_\rho \sum_{a_1^*}(K^{\alpha_1^*}_{a_1 a_1^*})^* \begin{pmatrix}\alpha_1^* & \varkappa & \alpha_2\\ a_1^* & q & a_2\end{pmatrix}^*_\rho \tag{6}$$

$$\langle\alpha_1\|T^{\varkappa}\|\alpha_2\rangle_\rho = \langle\alpha_1\|T^{\varkappa}\|\alpha_2\rangle^*_\rho, \qquad \rho = 1,\ldots,(\alpha_1^*\varkappa\alpha_2|\alpha_0). \tag{7}$$

Here, in addition to the replacement of CGC by the 3$D$-symbols, we have also introduced a new definition of RME:

$$\langle\alpha_1\|T^{\varkappa}\|\alpha_2\rangle_\rho = \sum_{a_1 a_1^* q a_2}\langle\alpha_1 a_1|T^{\varkappa}_q|\alpha_2 a_2\rangle K^{\alpha_1^*}_{a_1 a_1^*}\begin{pmatrix}\alpha_1^* & \varkappa & \alpha_2\\ a_1^* & q & a_2\end{pmatrix}_\rho. \tag{8}$$

Now, the RME do not depend on the indices of the corep basis functions. The dependence on the Wigner type of $D^{\alpha_1}$ is included in the multiplicity index $\rho=\rho(r_{\alpha_1}r_0)$, $r_{\alpha_1}=1,\ldots,(\varkappa\alpha_2|\alpha_1)$, $r_0=1,\ldots,(\alpha_1\alpha_1^*|\alpha_0)$ and $(\alpha_1\alpha_1^*|\alpha_0)=1,4,2$ for $D^{\alpha_1}$ of type 'a', 'b', and 'c' respectively.

It is important to stress that as a result of the consideration of both unitary and anti-unitary operators of $\mathrm{G_A}$ and the new definition of RME (8), we obtain real RME (7) for all types of coreps $D^{\alpha_1}$ (not only for type 'a' corep as it is in equation (3)). This result is not surprising as the 3$D$-symbols reduce the triple product $D^{\alpha_1^*}\times D^{\varkappa}\times D^{\alpha_2}$ to the identity corep $D^{\alpha_0}$, which is always from type 'a' (here we choose $D^{\alpha_0}(g)=+1$ for all unitary and anti-unitary $g\in\mathrm{G_A}$).

Let us compare the two definitions of RME, (2) and (8), given by the two versions of the theorem. Equalising the RHS of (1) and (6) and using the relation between 3$D$-symbols and CGC (A8) as well as (A12) and (A13) we obtain

$$\frac{2[\Gamma^{\alpha_1}]}{[D^{\alpha_1}]^{1/2}}\sum_{k_1' m_1'}\langle\alpha_1 m_1'\|T^{\varkappa}\|\alpha_2\rangle_{r_{\alpha_1}k_1'}Q'(\alpha_1)_{m_1' a_1' k_1' p_1'} = \sum_{\rho r_0}\langle\alpha_1\|T^{\varkappa}\|\alpha_2\rangle_\rho \mu^{\alpha_1^*\varkappa\alpha_2}_{r_{\alpha_1}r_0,\rho} Z^{\alpha_1^*}_{p_1' a_1'}(r_0)^*. \tag{9}$$

The unitary matrix $Z^{\alpha_1^*}(r_0)$ depends on the type of the corep $D^{\alpha_1}$ and its form is given in the appendix (A14). The orthogonal matrix of the so-called isoscalar factors (IF) $\mu^{\alpha_1^* \varkappa \alpha_2}$ gives the correspondence between the compound multiplicity index $\rho$ and the pair of indices $(r_{\alpha_1} r_0)$. As is shown in the appendix it can be chosen in a diagonal form (A11) and in this case the sum over $\rho$ in (9) vanishes. The relation (9) shows that the RME of the 'CGC-version' of the theorem (2) are linear combinations of the RME of the '3$D$-symbol version' (8). For example, for the type 'c' corep $D^{\alpha_1}$ we have

$$\langle \alpha_1 1 \| T^\varkappa \| \alpha_2 \rangle_{r_{\alpha_1}1} = \langle \alpha_1 2 \| T^\varkappa \| \alpha_2 \rangle^*_{r_{\alpha_1}2} = z_1[D^{\alpha_1}]^{1/2} \sum_{r_0=1}^{2} \mu(\alpha_1^* \varkappa \alpha_2; r_{\alpha_1} r_0) \langle \alpha_1 \| T^\varkappa \| \alpha_2 \rangle_{r_{\alpha_1} r_0}. \qquad (10)$$

Let us summarise the results of this section: the Wigner–Eckart theorem for coreps, expressed by (6) and (7), gives the factorisation of the matrix elements of the tensor operators in terms of 3$D$-symbols. It has the following advantages in comparison with the 'CGC-version' of the theorem (1) and (3): (i) the RME are real in all cases; (ii) the matrix elements are completely factorised; (iii) the form of the theorem is considerably simplified and it does not depend on the type of corep.

The above-mentioned proof of the theorem is valid for all kinds of magnetic groups (grey and black-and-white). Similar results, but only for the special case of grey groups, are presented by Newmarch and Golding (1981).

## 3. Factorisation of matrix elements of coupled tensor operators for AU magnetic groups

Using the advantages of the '3$D$-symbol version' of the Wigner–Eckart theorem, we can continue to develop the method of irreducible tensor sets for coreps. In this section we will consider the factorisation of matrix elements of coupled tensor operators (CTO) and the relations between the RME of CTO and its components. Such relations are well known for linear representations (Judd 1963, Butler 1975). However, essential peculiarities appear for the corep case and they result mainly from the generalised Schur lemma for irreducible and reducible coreps (Kotzev and Aroyo 1983). It is convenient to bring these relations into a form which mostly corresponds to the respective relations of the linear representations, taking into account the special features of the coreps. It can be achieved by imposing some reasonable assumptions, which considerably simplify the form of the relations between the RME and facilitate the application of the results.

In order to compare easily our results for the case of coreps with those of the representations, we will follow the scheme proposed by Butler (1975).

In analogy with the representation case, we will use the following definition of a CTO

$$T_q^{\varkappa r_\varkappa} \equiv \{P^{\varkappa_1} Q^{\varkappa_2}\}_q^{\varkappa r_\varkappa} = \sum_{q_1 q_2} P_{q_1}^{\varkappa_1} Q_{q_2}^{\varkappa_2} [\varkappa_1 q_1, \varkappa_2 q_2 | \varkappa r_\varkappa q], \qquad r_\varkappa = 1, \ldots, (\varkappa_1 \varkappa_2 | \varkappa) \qquad (11)$$

where $P_{q_1}^{\varkappa_1}$ and $Q_{q_2}^{\varkappa_2}$ are components of ITO, transforming by the coreps $D^{\varkappa_1}$ and $D^{\varkappa_2}$ of the AU group $G_A$ respectively and $[\varkappa_1 q_1, \varkappa_2 q_2 | \varkappa r_\varkappa q]$ are the corresponding CGC for the coreps.

(1) First of all we shall consider the general case when the CTO $\{P^{\varkappa_1} Q^{\varkappa_2}\}^{\varkappa r_\varkappa}$ as well as its components $P^{\varkappa_1}$ and $Q^{\varkappa_2}$ act in one and the same space with a basis $\{|\alpha_i a_i\rangle\}$. The

matrix elements of $\{P^{\varkappa_1}Q^{\varkappa_2}\}_q^{\varkappa r_\varkappa}$ are expressed by the matrix elements of $P^{\varkappa_1}$ and $Q^{\varkappa_2}$ as follows:

$$\begin{aligned}\langle\alpha_1 a_1|\{P^{\varkappa_1}Q^{\varkappa_2}\}_q^{\varkappa r_\varkappa}|\alpha_2 a_2\rangle &= [D^\varkappa]^{1/2}\sum_{\rho_\varkappa}\mu^{\varkappa_1\varkappa_2\varkappa^*}_{r_\varkappa r_0,\rho_\varkappa}\sum_{q_1q_2q'q^*}\begin{pmatrix}\varkappa_1 & \varkappa_2 & \varkappa^*\\ q_1 & q_2 & q^*\end{pmatrix}_{\rho_\varkappa}K^\varkappa_{q^*q'}N^\varkappa_{qq'}(r_0)^*\\ &\quad\times\sum_{\alpha_3a_3}\langle\alpha_1a_1|P^{\varkappa_1}_{q_1}|\alpha_3a_3\rangle\langle\alpha_3a_3|Q^{\varkappa_2}_{q_2}|\alpha_2a_2\rangle\end{aligned}\tag{12}$$

where on the RHS of (12) the relation between the CGC for coreps and the corresponding $3D$-symbols is used (A15) and the multiplicity index $\rho_\varkappa$ runs from 1 to $(\varkappa_1\varkappa_2\varkappa^*|\alpha_0)$. After the application of the new form of the Wigner–Eckart theorem on both sides of (12) and using the orthogonality relations of $1D$- and $3D$-symbols (A1) and (A7), we get the following relation between the RME:

$$\begin{aligned}\langle\alpha_1\|\{P^{\varkappa_1}Q^{\varkappa_2}\}^{\varkappa r_\varkappa}\|\alpha_2\rangle_{\rho_\alpha} &= [D^\varkappa]^{1/2}\sum_{\alpha_3\rho_1\rho_2}\langle\alpha_1\|P^{\varkappa_1}\|\alpha_3\rangle_{\rho_1}\langle\alpha_3\|Q^{\varkappa_2}\|\alpha_2\rangle_{\rho_2}\\ &\quad\times\sum_{\rho_2'\rho_1'\rho_\varkappa}\begin{Bmatrix}\varkappa_2^* & \varkappa & \varkappa_1^*\\ \alpha_1^* & \alpha_3^* & \alpha_2^*\end{Bmatrix}_{\rho_2'\rho_\alpha\rho_1'\rho_\varkappa}A_{\rho_2'\rho_1'\rho_\varkappa;\rho_2\rho_1,r_\varkappa r_0}\\ \rho_\alpha &= 1,\ldots,(\alpha_1^*\varkappa\alpha_2|\alpha_0).\end{aligned}\tag{13}$$

Equation (13) shows that, as in the representation case, the RME of CTO for coreps are expressed in the form of linear combinations of the RME of its irreducible components. Before starting the detailed discussion of the coefficients in (13) we should point out a very important peculiarity of the result: the RME in (13), defined by (8), are real for the corep case.

In the derivation of the relation (13) sums of products of four $3D$-symbols and the corresponding $1D$-symbols appear, and these sums can be transformed into the form

$$\begin{aligned}&\begin{Bmatrix}\varkappa_2^* & \varkappa & \varkappa_1^*\\ \alpha_1^* & \alpha_3^* & \alpha_2^*\end{Bmatrix}_{\rho_2'\rho_\alpha\rho_1'\rho_\varkappa}\\ &\quad=\sum_{q_iq_i^*a_ia_i^*}K^{\varkappa_2}_{q_2^*q_2}K^{\varkappa^*}_{qq^*}K^{\varkappa_1}_{q_1^*q_1}K^{\alpha_1}_{a_1^*a_1}K^{\alpha_3}_{a_3^*a_3}K^{\alpha_2}_{a_2^*a_2}\begin{pmatrix}\varkappa_2^* & \alpha_3 & \alpha_2^*\\ q_2^* & a_3 & a_2^*\end{pmatrix}_{\rho_2'}\\ &\quad\quad\times\begin{pmatrix}\alpha_1^* & \varkappa & \alpha_2\\ a_1^* & q & a_2\end{pmatrix}_{\rho_\alpha}\begin{pmatrix}\alpha_1 & \alpha_3^* & \varkappa_1^*\\ a_1 & a_3^* & q_1^*\end{pmatrix}_{\rho_1'}\begin{pmatrix}\varkappa_2 & \varkappa^* & \varkappa_1\\ q_2 & q^* & q_1\end{pmatrix}_{\rho_\varkappa}.\end{aligned}\tag{14}$$

The quantity (14) has symmetry properties under permutations of rows and columns, and under complex conjugations, similar to the corresponding ones of the $6j$-symbols, however, the specific character of the coreps introduces essential peculiarities (Newmarch and Golding 1983). We will call it a $6D$-symbol.

The last factor in equation (13) has the following meaning:

$$\begin{aligned}&A_{\rho_2'\rho_1'\rho_\varkappa;\rho_2\rho_1,r_\varkappa r_0}=(\pi^{\alpha_3\varkappa_2^*\alpha_2^*}\Lambda^{\alpha_3\varkappa_2^*\alpha_2^*-1}\times\pi^{\alpha_1\varkappa_1^*\alpha_3^*}\Lambda^{\alpha_1\varkappa_1^*\alpha_3^*-1}\times\mu^{\varkappa_1\varkappa_2\varkappa^*-1})_{\rho_2'\rho_1'\rho_\varkappa,\rho_2\rho_1r_\varkappa r_0},\\ &\rho_1,\rho_1'=1,\ldots,(\alpha_1\varkappa_1^*\alpha_3^*|\alpha_0),\qquad \rho_2,\rho_2'=1,\ldots,(\alpha_3\varkappa_2^*\alpha_2^*|\alpha_0),\\ &\rho_\varkappa=1,\ldots,(\varkappa_1\varkappa_2\varkappa^*|\alpha_0),\\ &r_\varkappa=1,\ldots,(\varkappa_1\varkappa_2|\varkappa),\qquad r_0=1,\ldots,(\varkappa\varkappa^*|\alpha_0).\end{aligned}\tag{15}$$

It is a product of IF, which appear as a consequence of the application of the Schur lemma for reducible coreps in getting equations (13).

We have already mentioned (see § 2) that the IF realise the correspondence between the multiplicity indices and their meaning is discussed in detail in the appendix. As it is shown there, using sensible assumptions the matrices of the IF can be reduced into a diagonal form, and we get from (15)

$$A_{\rho_2'\rho_1'\rho_\varkappa;\rho_2\rho_1,r_\varkappa r_0} = \pi(\alpha_3\varkappa_2^*\alpha_2^*;\ \rho_2)\pi(\alpha_1\varkappa_1^*\alpha_3^*;\ \rho_1)\mu(\varkappa_1\varkappa_2\varkappa^*;\ r_\varkappa r_0)\delta_{\rho_2'\rho_2}\delta_{\rho_1'\rho_1}\delta_{\rho_\varkappa,r_\varkappa r_0}. \tag{16}$$

We should point out that the above-discussed IF for coreps are real, while in the case of linear representations they can be complex numbers. Taking into account (16), the relation between the RME (13) considerably simplifies and reduces to a form similar to equation (19.5) in Butler (1975).

An important special case for practical applications is when the CTO is a scalar. The corresponding relation between the RME can be obtained either directly from (13), considering the fact that a $6D$-symbol with an identity corep is reduced to a product of dimension factors and a set of IF, or by direct calculations from (12):

$$\begin{aligned}\langle\alpha_1\|(P^{\varkappa_1}Q^{\varkappa_1^*}\}^{\alpha_0 r_0}\|\alpha_2\rangle_{\rho_\alpha} &= \delta_{\alpha_2\alpha_1}[D^{\alpha_1}\times D^{\varkappa_1}]^{-1/2}\\ &\quad\times\sum_{\alpha_3\rho_1}\langle\alpha_1\|P^{\varkappa_1}\|\alpha_3\rangle_{\rho_1}\langle\alpha_3\|Q^{\varkappa_1^*}\|\alpha_1\rangle_{\rho_1}A(\rho_1,\rho_\alpha,r_0),\end{aligned} \tag{17}$$

$$A(\rho_1,\rho_\alpha,r_0) = \pi(\alpha_1\varkappa_1^*\alpha_3^*;\ \rho_1)\pi(\alpha_1\alpha_1^*\alpha_0;\ \rho_\alpha)\mu(\varkappa_1\varkappa_1^*\alpha_0;\ r_0).$$

Here we have taken into account the diagonal choice of the matrices of IF.

(2) Let us consider, now, the modification of equation (13) when the basis $\{|(\beta_i\gamma_i)\alpha_i r_{\alpha_i}a_i\rangle\}$ of the CTO space is a direct product of two subspace bases $\{|\beta_i b_i\rangle\}$ and $\{|\gamma_i c_i\rangle\}$, and each of ITO $P^{\varkappa_1}$ or $Q^{\varkappa_2}$ acts in only one of the component spaces.

It is easy to show that equation (13) now gets the form

$$\begin{aligned}&\langle(\beta_1\gamma_1)\alpha_1 r_{\alpha_1}\|\{P^{\varkappa_1}Q^{\varkappa_2}\}^{\varkappa r_\varkappa}\|(\beta_2\gamma_2)\alpha_2 r_{\alpha_2}\rangle_{\rho_\alpha}\\ &\quad=[D^{\alpha_1}\times D^{\varkappa}\times D^{\alpha_2}]^{1/2}\sum_{\rho_\beta\rho_\gamma}\langle\beta_1\|P^{\varkappa_1}\|\beta_2\rangle_{\rho_\beta}\langle\gamma_1\|Q^{\varkappa_2}\|\gamma_2\rangle_{\rho_\gamma}\\ &\quad\times\sum_{\rho_{\alpha_1}\rho_{\alpha_2}\rho_\varkappa\rho_\beta'\rho_\gamma'}\begin{Bmatrix}\beta_1^* & \gamma_1^* & \alpha_1\\ \varkappa_1 & \varkappa_2 & \varkappa^*\\ \beta_2 & \gamma_2 & \alpha_2^*\end{Bmatrix}\begin{matrix}\rho_{\alpha_1}\\ \rho_\varkappa\\ \rho_{\alpha_2}\end{matrix}\ B_{\rho_{\alpha_1}\rho_\varkappa\rho_{\alpha_2}\rho_\beta'\rho_\gamma';r_{\alpha_1}r_{0_1},r_\varkappa r_0,r_{\alpha_2}r_{0_2},\rho_\beta\rho_\gamma},\\ &\qquad\qquad\qquad\qquad\qquad\qquad\quad\ \rho_\beta'\quad\ \rho_\gamma'\quad\ \rho_\alpha\\ &\quad\rho_\alpha = 1,\ldots,(\alpha_1^*\varkappa\alpha_2|\alpha_0).\end{aligned} \tag{18}$$

The symbol in curly brackets in (18) is given by the following relation:

$$\begin{aligned}&\begin{Bmatrix}\beta_1^* & \gamma_1^* & \alpha_1\\ \varkappa_1 & \varkappa_2 & \varkappa^*\\ \beta_2 & \gamma_2 & \alpha_2^*\end{Bmatrix}\begin{matrix}\rho_{\alpha_1}\\ \rho_\varkappa\\ \rho_{\alpha_2}\end{matrix}\\ &\ \ \rho_\beta'\qquad\rho_\gamma'\qquad\rho_\alpha\\ &\quad=\sum_{\substack{a_i a_i^* b_i b_i^*\\ c_i c_i^* q_i q_i^*}}K^{\beta_1}_{b_1^*b_1}K^{\gamma_1}_{c_1^*c_1}K^{\alpha_1^*}_{a_1a_1^*}K^{\varkappa_1^*}_{q_1q_1^*}K^{\varkappa_2^*}_{q_2q_2^*}K^{\varkappa}_{q^*q}K^{\beta_2^*}_{b_2b_2^*}K^{\gamma_2^*}_{c_2c_2^*}K^{\alpha_2}_{a_2^*a_2}\\ &\quad\times\begin{pmatrix}\beta_1^* & \gamma_1^* & \alpha_1\\ b_1^* & c_1^* & a_1\end{pmatrix}_{\rho_{\alpha_1}}\begin{pmatrix}\varkappa_1 & \varkappa_2 & \varkappa^*\\ q_1 & q_2 & q^*\end{pmatrix}_{\rho_\varkappa}\begin{pmatrix}\beta_2 & \gamma_2 & \alpha_2^*\\ b_2 & c_2 & a_2^*\end{pmatrix}_{\rho_{\alpha_2}}\\ &\quad\times\begin{pmatrix}\beta_1 & \varkappa_1^* & \beta_2^*\\ b_1 & q_1^* & b_2^*\end{pmatrix}_{\rho_\beta'}\begin{pmatrix}\gamma_1 & \varkappa_2^* & \gamma_2^*\\ c_1 & q_2^* & c_2^*\end{pmatrix}_{\rho_\gamma'}\begin{pmatrix}\alpha_1^* & \varkappa & \alpha_2\\ a_1^* & q & a_2\end{pmatrix}_{\rho_\alpha}\end{aligned} \tag{19}$$

where the multiplicity indices $\rho_{\alpha_i}$, $\rho_\varkappa$, $\rho_\beta'$, $\rho_\gamma'$ run from 1 to $(\beta_i^*\gamma_i^*\alpha_i|\alpha_0)$, $(\varkappa_1\varkappa_2\varkappa^*|\alpha_0)$, $(\beta_1\varkappa_1^*\beta_2|\alpha_0)$ and $(\gamma_1\varkappa_2^*\gamma_2^*|\alpha_0)$ respectively.

This quantity has similar symmetry properties to the $9j$-symbol (Butler 1975), and although there are certain differences between them, caused by the corep peculiarities, we will call it the $9D$-symbol.

The last factor in equation (18) is a product of IF and its explicit form is

$$
\begin{aligned}
B_{\rho_{\alpha_1}\rho_\varkappa\rho_{\alpha_2}\rho'_\beta\rho'_\gamma;r_{\alpha_1}r_{0_1},r_\varkappa r_0,r_{\alpha_2}r_{0_2},\rho_\beta\rho_\gamma}
&= [(\mu^{\beta_1\gamma_1\alpha_1^*}\Lambda^{\beta_1^*\gamma_1^*\alpha_1}\times\mu^{\varkappa_1\varkappa_2\varkappa^*}\times\mu^{\beta_2\gamma_2\alpha_2^*}\times\Lambda^{\beta_1\varkappa_1^*\beta_2^*} \\
&\quad\times\Lambda^{\gamma_1\varkappa_2^*\gamma_2^*})^{-1}]_{\rho_{\alpha_1}\rho_\varkappa\rho_{\alpha_2}\rho'_\beta\rho'_\gamma r_{\alpha_1}r_{0_1}r_\varkappa r_0 r_{\alpha_2}r_{0_2}\rho_\beta\rho_\gamma}, \\
&\quad r_{0_1}=1,\ldots,(\alpha_1\alpha_1^*|\alpha_0);\; r_{0_2}=1,\ldots,(\alpha_2\alpha_2^*|\alpha_0);\; r_0=1,\ldots,(\varkappa\varkappa^*|\alpha_0).
\end{aligned}
\tag{20}
$$

It can be simplified considerably using the diagonal choice of the corresponding IF matrices $\mu$ and $\Lambda$ (see the appendix).

Equation (18) which we get for the case of coreps coincides with the analogous Butler relation for the linear representations, but the character features of the coreps lead to: real RME (8), real coefficients $B$ (20) and some differences in the properties of the $9D$-symbols (19).

We note that for the case of grey groups $G_A = G_H \otimes \Theta$ Newmarch and Golding (1983) obtained a relation similar to equation (18), but they used lower-symmetrised 'quasi-$9j$-symbols', constructed by products of three CGC and three symmetrised CGC for coreps.

The following two special cases of equation (18) are of practical interest: (i) one of the operators $P^{\varkappa_1}$ or $Q^{\varkappa_2}$ is the unit one, (ii) the CTO is a scalar operator.

Due to the fact that our $9D$-symbols (19) with one identity corep are reduced to $6D$-symbols and a set of IF, the corresponding relations between the RME for both cases can be obtained directly from (18).

For the first case, if $D^{\varkappa_2} \equiv D^{\alpha_0}$, we obtain

$$
\begin{aligned}
&\langle(\beta_1\gamma_1)\alpha_1 r_{\alpha_1}\|P^{\varkappa_1}\|(\beta_2\gamma_2)\alpha_2 r_{\alpha_2}\rangle_{\rho_\alpha} \\
&\quad= \delta_{\gamma_1\gamma_2}[D^{\alpha_1}\times D^{\alpha_2}]^{1/2}\sum_{\rho_\beta}\langle\beta_1\|P^{\varkappa_1}\|\beta_2\rangle_{\rho_\beta} \\
&\quad\times\begin{Bmatrix}\beta_1^* & \beta_2 & \varkappa_1\\ \alpha_2^* & \alpha_1^* & \gamma_1^*\end{Bmatrix}_{r_{\alpha_1}r_{0_1}r_{\alpha_2}r_{0_2}\rho_\alpha\rho_\beta} B(r_{\alpha_1}r_{0_1},r_0,r_{\alpha_2}r_{0_2},\rho_\beta),
\end{aligned}
\tag{21}
$$

$$
\begin{aligned}
B(r_{\alpha_1}r_{0_1},r_0,r_{\alpha_2}r_{0_2},\rho_\beta) &= \mu(\beta_1\gamma_1\alpha_1^*;\, r_{\alpha_1}r_{0_1})\pi(\beta_1^*\gamma_1^*\alpha_1;\, r_{\alpha_1}r_{0_1}) \\
&\quad\times\mu(\varkappa_1\alpha_0\varkappa_1^*;\, r_0)\mu(\beta_2\gamma_2\alpha_2^*;\, r_{\alpha_2}r_{0_2})\pi(\beta_1\varkappa_1^*\beta_2^*;\, \rho_\beta).
\end{aligned}
$$

For the second case we obtain

$$
\begin{aligned}
&\langle(\beta_1\gamma_1)\alpha_1 r_{\alpha_1}\|\{P^{\varkappa_1}Q^{\varkappa_1^*}\}^{\alpha_0 r_0}\|(\beta_2\gamma_2)\alpha_2 r_{\alpha_2}\rangle_{\rho_\alpha} \\
&\quad= \delta_{\alpha_1\alpha_2}[D^{\alpha_1}]^{1/2}[D^{\varkappa_1}]^{-1/2}\sum_{\rho_\beta\rho_\gamma}\langle\beta_1\|P^{\varkappa_1}\|\beta_2\rangle_{\rho_\beta}\langle\gamma_1\|Q^{\varkappa_1^*}\|\gamma_2\rangle_{\rho_\gamma} \\
&\quad\times\begin{Bmatrix}\beta_1^* & \beta_2 & \varkappa_1\\ \gamma_2 & \gamma_1 & \alpha_1\end{Bmatrix}_{r_{\alpha_1}r_{0_1}r_{\alpha_2}r_{0_2}\rho_\gamma\rho_\beta} B(r_{\alpha_1}r_{0_1},\, r_0,\, r_{\alpha_2}r_{0_2},\, \rho_\beta,\, \rho_\alpha)
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
B(r_{\alpha_1}r_{0_1},\, r_0,\, r_{\alpha_2}r_{0_2},\, \rho_\beta,\, \rho_\alpha) &= \mu(\beta_1\gamma_1\alpha_1^*;\, r_{\alpha_1}r_{0_1})\mu(\varkappa_1\varkappa_1^*\alpha_0;\, r_0) \\
&\quad\times\mu(\beta_2\gamma_2\alpha_2^*;\, r_{\alpha_2}r_{0_2})\pi(\beta_2\gamma_2\alpha_2^*;\, r_{\alpha_2}r_{0_2})\pi(\beta_1\beta_2^*\varkappa_1^*;\, \rho_\beta)\pi(\alpha_1\alpha_1^*\alpha_0;\, \rho_0).
\end{aligned}
$$

In both relations we have used diagonal IF matrices.

## 4. Conclusion

In this paper, as a next step in the generalisation of the method of irreducible tensorial sets for the case of corepresentations of anti-unitary magnetic groups, we get the new form of Wigner–Eckart theorem and we factorise the reduced matrix elements of coupled tensor operators. We reach it using highly symmetrical coefficients for corepresentations ($3D$-, $6D$- and $9D$-symbols). The complete factorisation of matrix elements is achieved using real reduced matrix elements for all Wigner types of corepresentations and real isoscalar factors.

We show that it is possible to reduce all obtained formulae to a form closely related to the classical ones for the case of linear representations, although there are peculiarities in the corepresentation theory.

Finally, we want to note that our results are valid for all types of magnetic anti-unitary groups (black-and-white and grey). They can be applied in the treatment of various quantum mechanical problems in magnetic and non-magnetic systems (e.g. crystal field theory, spin–orbit interactions, exchange interactions, etc).

In our next paper we will discuss the effect of the group-subgroup relations on the reduced matrix elements and some examples for the application of obtained results will be considered.

## Appendix. On $1D$-symbols and $3D$-symbols

(1) In § 2 we define the unitary matrix $K^{\alpha^*} = \|K^{\alpha^*}_{aa^*}\|$, transforming the corep $D^\alpha(g)^*$ to the equivalent corep $D^{\alpha^*}(g)$, belonging to the standard set. By 'standard set' of coreps of $G_A$ we mean a set of matrices of all coreps $D^\alpha$ of the group, which are chosen in advance and fixed. In analogy with the linear representation case the matrix $K^{\alpha^*}$ is called the metric (Wigner) tensor for coreps and its matrix elements—the $1D$-symbols: they play the role of $1j$-symbols for coreps (Derome and Sharp 1965, Butler 1975, Newmarch and Golding 1981).

It is worth mentioning that the corep Wigner tensor is determined up to a unitary matrix $M^{\alpha^*}$, commuting with all matrices of the corep $D^{\alpha^*}$, while in the linear case the arbitrariness of this type is reduced to a phase factor only (Newmarch and Golding 1981, Kotzev and Aroyo 1983).

The orthogonality relations of $1D$-symbols follow directly from the unitarity of $K^{\alpha^*}$ matrices, i.e.

$$\sum_{a^*} K^{\alpha^*}_{aa^*}(K^{\alpha^*}_{a'a^*})^* = \delta_{aa'}, \qquad a, a' = 1, \ldots, [D^\alpha] \tag{A1}$$

and similar relations hold for the columns.

The Wigner tensor $K^\alpha$, transforming $D^{\alpha^*}(g)^*$ to $D^\alpha(g)$, $g \in G_A$ is related to $K^{\alpha^*}$ (as a corollary of the Schur lemma for coreps) through the equation

$$K^\alpha = \tilde{K}^{\alpha^*} M^\alpha \tag{A2}$$

where the tilde means transposition. The matrix $M^\alpha$ commuting with $D^\alpha(g)$, $g \in G_A$ is related to $M^{\alpha^*}$:

$$M^{\alpha^*} = K^{\alpha^*-1}(M^\alpha)^* K^{\alpha^*}. \tag{A3}$$

In the case of linear representations $M^\alpha = \phi_\alpha E^\alpha$, and the phase factor $\phi_\alpha$ is known as $1j$-phase, satisfying $\phi_{\alpha^*} = (\phi_\alpha)^*$.

The above-defined $1D$-symbols play an important role in the generalisation of the Derome–Sharp lemma for coreps and in the relations between the CGC, $6D$-symbols and $9D$-symbols by the corresponding $3D$-symbols.

(2) Let us discuss some properties of the $3D$-symbols, the symmetrised CGC for coreps (Kotzev *et al* 1984a), which will be necessary in the derivation of the results of §§ 2 and 3.

(i) We define the $3D$-symbols as matrix elements of the rectangular matrix

$$V^{\alpha_1\alpha_2\alpha_3} = \| V^{\alpha_1\alpha_2\alpha_3}_{a_1a_2a_3,\alpha_0\rho a_0} \| = \left\| \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_\rho \right\|. \tag{A4}$$

It is constructed by the first $(\alpha_1\alpha_2\alpha_3|\alpha_0)$ columns of the matrix $U^{\alpha_1\alpha_2\alpha_3}$ of the generalised CGC for coreps, which reduce the triple Kronecker product of coreps $D^{\alpha_1}\times D^{\alpha_2}\times D^{\alpha_3}$ to the identity one $D^{\alpha_0}\in D^{\alpha_1}\times D^{\alpha_2}\times D^{\alpha_3}$. We can write

$$V^{\alpha_1\alpha_2\alpha_3+}D^{\alpha_1}(g)\times D^{\alpha_2}(g)\times D^{\alpha_3}(g)\,V^{\alpha_1\alpha_2\alpha_3(*)} = e^{\alpha_1\alpha_2\alpha_3}_{\alpha_0}\times D^{\alpha_0}(g), \qquad g\in \mathrm{G_A} \tag{A5}$$

where $e^{\alpha_1\alpha_2\alpha_3}_{\alpha_0}$ is an identity matrix, $\dim e^{\alpha_1\alpha_2\alpha_3}_{\alpha_0} = (\alpha_1\alpha_2\alpha_3|\alpha_0)$. The specific arbitrariness of the CGC for coreps is used for the symmetrisation of the corresponding $(\alpha_1\alpha_2\alpha_3|\alpha_0)$ columns of $U^{\alpha_1\alpha_2\alpha_3}$ so that the above-defined $3D$-symbols satisfy symmetry relations similar to those of the $3j$-symbols.

Viewing the $3D$-symbols as vector coupling coefficients, they can be defined as coefficients in a linear combination of orthogonal basis functions $\{|\alpha_i a_i\rangle\}$ (transforming by the corep $D^{\alpha_i}$), which forms a $\mathrm{G_A}$ invariant

$$|(\alpha_1\alpha_2\alpha_3)\alpha_0\rho a_0\rangle = \sum_{a_1a_2a_3} |\alpha_1a_1\rangle|\alpha_2a_2\rangle|\alpha_3a_3\rangle \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_\rho. \tag{A6}$$

From the unitarity of the matrix $U^{\alpha_1\alpha_2\alpha_3}$ and the definition (A5) it follows that the orthogonality relations for $3D$-symbols hold only for the columns of $V^{\alpha_1\alpha_2\alpha_3}$, i.e.

$$\sum_{a_1a_2a_3} \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}^*_\rho \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_{\rho'} = \delta_{\rho\rho'}, \qquad \rho,\rho' = 1,\ldots,(\alpha_1\alpha_2\alpha_3|\alpha_0). \tag{A7}$$

(ii) Using the Schur lemma for reducible coreps, we obtain a relation between the $3D$-symbols and the corresponding CGC, which 'step by step' reduce $D^{\alpha_1}\times D^{\alpha_2}\times D^{\alpha_3}$ to $D^{\alpha_0}$

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_\rho = \sum_{r_{\alpha_3^*}r_0} \sum_{a_3^*} [\alpha_1a_1, \alpha_2a_2|\alpha_3^* r_{\alpha_3^*} a_3^*][\alpha_3^* a_3^*, \alpha_3a_3|\alpha_0r_0a_0]\mu^{\alpha_1\alpha_2\alpha_3}_{r_{\alpha_3^*}r_0,\rho}. \tag{A8}$$

Here the sums over the multiplicity indices $r_{\alpha_3^*}$ and $r_0$ are up to $(\alpha_1\alpha_2|\alpha_3^*)$ and $(\alpha_3^*\alpha_3|\alpha_0)$ respectively. We should remind ourselves that the multiplicity of the identity corep $D^{\alpha_0}$ in $D^{\alpha_3^*}\times D^{\alpha_3}$ is equal to 1, 4, and 2 for coreps of the Wigner type 'a', 'b' and 'c' respectively, while for linear representations it is always equal to 1. In order to clear the meaning of the orthogonal matrix $\mu^{\alpha_1\alpha_2\alpha_3}$, $\dim \mu^{\alpha_1\alpha_2\alpha_3} = (\alpha_1\alpha_2\alpha_3|\alpha_0) = (\alpha_1\alpha_2|\alpha_3^*)(\alpha_3^*\alpha_3|\alpha_0)$ we shall construct two equivalent sets of invariants, using the $3D$-symbols on the LHS and the CGC on the RHS of equation (A8):

$$|(\alpha_1\alpha_2)\alpha_3^* r_{\alpha_3^*}(\alpha_3^*\alpha_3)\alpha_0r_0a_0\rangle \equiv |(\alpha_1\alpha_2, \alpha_3)\alpha_0 r_{\alpha_3^*} r_0 a_0\rangle,$$

$$r_{\alpha_3^*} = 1,\ldots,(\alpha_1\alpha_2|\alpha_3^*), \qquad r_0 = 1,\ldots,(\alpha_3^*\alpha_3|\alpha_0) \tag{A9}$$

$$|(\alpha_1\alpha_2\alpha_3)\alpha_0\rho a_0\rangle, \qquad \rho = 1,\ldots,(\alpha_1\alpha_2\alpha_3|\alpha_0) = (\alpha_1\alpha_2|\alpha_3^*)(\alpha_3^*\alpha_3|\alpha_0).$$

It is obvious that the matrix elements of $\mu^{\alpha_1\alpha_2\alpha_3}$ are the coefficients of the linear combination, expressing one of the invariant sets in terms of the other:

$$|(\alpha_1\alpha_2\alpha_3)\alpha_0\rho a_0\rangle = \sum_{r_{\alpha_3^*}r_0} |(\alpha_1\alpha_2, \alpha_3)\alpha_0 r_{\alpha_3^*} r_0 a_0\rangle \mu^{\alpha_1\alpha_2\alpha_3}_{r_{\alpha_3^*}r_0,\rho}. \tag{A10}$$

These coefficients do not depend on the partners of the basis and they are called isoscalar factors (IF). For the corep case IF are real, while for linear representations they can be complex in the general case. The CGC in (A8) are chosen in such a way, so that every invariant from one set is mapped on only one invariant from the other set and vice versa, i.e. the matrix $\mu^{\alpha_1\alpha_2\alpha_3}$ is of a diagonal form.

$$\mu^{\alpha_1\alpha_2\alpha_3}_{r_{\alpha_3^*}r_0,\rho} = \mu(\alpha_1\alpha_2\alpha_3;\, r_{\alpha_3^*}r_0)\, \delta_{r_{\alpha_3^*}r_0,\rho}, \qquad \mu(\alpha_1\alpha_2\alpha_3;\, r_{\alpha_3^*}r_0) = \pm 1. \tag{A11}$$

The following equation, which is fulfilled for a fixed value of the multiplicity index $r_0 = 1, \ldots, (\alpha_3^*\alpha_3|\alpha_0)$, gives the relation between the second CGC in (A8) and the $1D$-symbols (Aroyo and Kotzev 1984):

$$[D^{\alpha_3}]^{1/2} \sum_{a_3} [\alpha_3^* a_3^*, \alpha_3 a_3|\alpha_0 r_0 a_0] K^{\alpha_3^*}_{a_3 b_3^*} = N^{\alpha_3^*}_{a_3^* b_3^*}(r_0), \qquad r_0 = 1, \ldots, (\alpha_3^*\alpha_3|\alpha_0) \tag{A12}$$

where the unitary matrix $N^{\alpha_3^*}(r_0)$ belongs to the commuting algebra on the corep $D^{\alpha_3^*}$. From the Schur lemma for reducible coreps it follows that

$$N^{\alpha_3^*}(r_0) = Z^{\alpha_3^*}(r_0) \times E^{\alpha_3^*}. \tag{A13}$$

Here $E^{\alpha_3^*}$ is the identity matrix, whose dimension equals the dimension of the irreducible representation $\Gamma^{\alpha_3^*}$ of the unitary subgroup of $G_A$ and the unitary matrix $Z^{\alpha_3^*}(r_0)$ depends on the Wigner type of the corep $D^{\alpha_3^*}$ (van den Broek 1979, Kotzev and Aroyo 1983):

| type $a$: $r_0 = 1$ | type $b$: $r_0 = 1, \ldots, 4$ | type $c$: $r_0 = 1, 2$ | |
|---|---|---|---|
| $Z^{\alpha_3^*}(r_0) = \pm 1$ | $Z^{\alpha_3^*}(r_0) = \begin{pmatrix} z_1 & z_2 \\ -z_2^* & z_1^* \end{pmatrix}$ | $Z^{\alpha_3^*}(r_0) = \begin{pmatrix} z_1 & 0 \\ 0 & z_1^* \end{pmatrix}$ | $z_1, z_2 \in \mathbb{C}$. |

(A14)

Taking into account (A8) and (A12), we obtain the equation which expresses the CGC in terms of $3D$-symbols and $1D$-symbols,

$$[\alpha_1 a_1, \alpha_2 a_2|\alpha_3^* r_{\alpha_3^*} a_3^*] = [D^{\alpha_3}]^{1/2} \sum_{\rho} \mu^{\alpha_1\alpha_2\alpha_3}_{r_{\alpha_3^*}r_0,\rho} \sum_{a_3 b_3^*} \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_{\rho} K^{\alpha_3}_{a_3 b_3^*} N^{\alpha_3^*}_{a_3^* b_3^*}(r_0)^*$$

$$r_0 = 1, \ldots, (\alpha_3^*\alpha_3|\alpha_0). \tag{A15}$$

(iii) Under complex conjugation the $3D$-symbols transform in accordance with the generalised Derome–Sharp lemma (Kotzev *et al* 1984b)

$$\begin{pmatrix} \alpha_1^* & \alpha_2^* & \alpha_3^* \\ a_1^* & a_2^* & a_3^* \end{pmatrix}_{\rho} = \sum_{\rho'} \sum_{a_1 a_2 a_3} (K^{\alpha_1^*}_{a_1 a_1^*} K^{\alpha_2^*}_{a_2 a_2^*} K^{\alpha_3^*}_{a_3 a_3^*})^* \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}^*_{\rho'} \Lambda^{\alpha_1^*\alpha_2^*\alpha_3^*}_{\rho'\rho}. \tag{A16}$$

As in (A8) the orthogonal matrix of IF $\Lambda^{\alpha_1^*\alpha_2^*\alpha_3^*}$ is a corollary of the application of the generalised Schur lemma and it expresses the multiplicity arbitrariness.

The $3D$-symbols for magnetic point groups calculated and tabulated in our paper (Kotzev *et al* 1984a) are chosen in such a way that there is a 'one-to-one' correspondence between the invariants of the two sets, i.e. we can set $\Lambda^{\alpha_1^*\alpha_2^*\alpha_3^*} = e^{\alpha_1\alpha_2\alpha_3}_{\alpha_0}$.

(iv) One of the most important properties of the $3D$-symbols concerns their behaviour under permutations. Using the generalised Schur lemma for reducible coreps we get the following relation between the permuted $3D$-symbols:

$$\begin{pmatrix} \alpha_a & \alpha_b & \alpha_c \\ a_a & a_b & a_c \end{pmatrix}_\rho = \sum_{\rho'} \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_{\rho'} \pi^{\alpha_a\alpha_b\alpha_c}_{\rho'\rho} \tag{A17}$$

where $\left(\begin{smallmatrix} 1 & 2 & 3 \\ a & b & c \end{smallmatrix}\right)$ is a permutation of the columns of the $3D$-symbols. The orthogonal matrix $\pi^{\alpha_a\alpha_b\alpha_c}$, $\dim \pi^{\alpha_a\alpha_b\alpha_c} = (\alpha_a\alpha_b\alpha_c|\alpha_0) = (\alpha_1\alpha_2\alpha_3|\alpha_0)$ is of the same type as the above-discussed $\mu^{\alpha_1\alpha_2\alpha_3}$ and $\Lambda^{\alpha_1^*\alpha_2^*\alpha_3^*}$. Its matrix elements contain the information for the permutation properties of the $3D$-symbols. The ambiguity in their determination helps us to obtain $3D$-symbols for all 90 magnetic point groups with permutational properties, similar to those of $3j$-symbols: under an odd permutation of their columns they differ almost in a sign (no change under even permutations),

$$\pi^{\alpha_a\alpha_b\alpha_c}_{\rho'\rho} = \pi(\alpha_a\alpha_b\alpha_c;\rho)\,\delta_{\rho'\rho}, \qquad \pi(\alpha_a\alpha_b\alpha_c;\rho) = \pm 1. \tag{A18}$$

(v) In the derivation of the relations of § 3 we use a special type of $3D$-symbol transformation to the so-called $G_A$-equivalent basis (Haase and Butler 1984), defined in the following way

$$\overline{\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1' & a_2' & a_3' \end{pmatrix}}_\rho = \sum_{a_1a_2a_3} (M^{\alpha_1}_{a_1a_1'} M^{\alpha_2}_{a_2a_2'} M^{\alpha_3}_{a_3a_3'})^* \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ a_1 & a_2 & a_3 \end{pmatrix}_\rho. \tag{A19}$$

This transformation is carried out by the matrices $M^{\alpha i}$, belonging to the commuting algebra of $D^{\alpha i}$ coreps, i.e. the explicit form of the matrices $D^{\alpha i}(g)$, $g \in G_A$ do not change under such a transformation.

## References


Aroyo M I and Kotzev J N 1984 *Proc. 13th Int. Colloq. on Group-Theoretical Methods in Physics, Maryland, 1984* ed W W Zachary (Singapore: World Scientific) p 360

Aviran A and Zak J 1968 *J. Math. Phys.* **9** 2138

Biedenharn L C and Louck J D 1981 *Encyclopedia of Mathematics and its Applications* vol 8, ed G C Rota (Reading, MA: Addison-Wesley)

Bradley C J and Cracknell A P 1972 *The Mathematical Theory of Symmetry in Solids* (Oxford: OUP)

Butler P H 1975 *Phil. Trans. R. Soc.* A **277** 545

Derome J R and Sharp W T 1965 *J. Math. Phys.* **6** 1584

Haase R W and Butler P H 1984 *J. Phys. A: Math. Gen.* **17** 47

Judd B R 1963 *Operator Techniques in Atomic Spectroscopy* (New York: McGraw Hill)

Kotzev J N 1967 *On the Wigner-Eckart Theorem for Corepresentations* Kharkov University

—— 1972 *On the Theory of Corepresentations of Magnetic Groups* (Kharkov: IRE AN USSR)

Kotzev J N and Aroyo M I 1983 *Group-Theoretical Methods in Physics, Zvenigorod, 1982* vol 1, ed M A Markov (Moscow: Nauka) p 362

Kotzev J N, Aroyo M I and Angelova M N 1984a *J. Mol. Struct.* **115** 123

—— 1984b *Lecture Notes Phys.* **201** 416

Newmarch J D and Golding R M 1981 *J. Math. Phys.* **22** 233

—— 1983 *J. Math. Phys.* **24** 441

Vanagas V B 1971 *Algebraic Methods in Nuclear Theory* (Vilnus: Mintis)

van den Broek P M 1979 *J. Math. Phys.* **20** 2028

Wigner E P 1959 *Group Theory* (New York: Academic)