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Clebsch–Gordan coefficients for the corepresentations of Shubnikov point groups

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Abstract. The validity of the Racah lemma concerning the relation between the Clebsch–Gordan coefficients of the representations of the groups and their subgroups is shown for corepresentations of anti-unitary groups and their subgroups. A method for calculating Clebsch–Gordan coefficients for all magnetic groups, based on this lemma, is presented. Starting from the Wigner coefficients and using this method, the Clebsch–Gordan coefficients for the single-valued and the double-valued corepresentations of the 90 anti-unitary magnetic (Shubnikov) point groups have been calculated. An example for the calculation of the coefficients for the point groups $41'=C_4\otimes\Theta$, $\bar{4}1'=S_4\otimes\Theta$, $4/m'=C_{4h}(C_4)$, $4'/m=C_{4h}(S_4)$ (as subgroups of $O(3)\otimes\Theta$) is given. A comparison with other possible methods is discussed.

1. Introduction

Recently, generalised crystallographic groups, two-coloured (Shubnikov) (Koptsik 1966, Bradley and Cracknell 1972, Eremenko 1975) and (multi)-coloured (Shubnikov and Koptsik 1974, Kotzev 1975), have been widely used in group-theoretical analysis of different physical properties of crystals with magnetic symmetry. A generalised group is called anti-unitary, if the 'colour load' of the group elements contains the anti-unitary operator of time-inversion Θ (Wigner 1959). The anti-unitary groups consist of unitary, u_i, and anti-unitary, a_i, operators:

$$A=H+Ha_0=\{g_i=u_i,\ g_j=a_j\equiv u_ja_0\}, \tag{1}$$

where $u_i\in H$ form a subgroup of index 2. The wavefunctions and the operators of physical quantities transform in the common way under the action of the operators $g\in A$,

$$g\psi_a^\alpha=\sum_{a'}\psi_{a'}^\alpha D^\alpha(g)_{a'a},\qquad a=1,\ldots,|D^\alpha|, \tag{2}$$

but the mapping $g\to D^\alpha(g)$ is not a homomorphism, i.e. the set of matrices $D^\alpha=\{D^\alpha(g),g\in A\}$ does not form a representation of the group A. Wigner (1959) called this set of matrices a corepresentation. He had proved that for quantum mechanical systems with an anti-unitary symmetry, the irreducible corepresentations (not the ordinary representations) defined the transformation properties of the wavefunctions, the degeneracy of the levels, the correlation between the matrix elements, etc. The need for a further development of the corepresentation theory and, in particular, the

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creation of a generalised theory of the irreducible tensorial sets is obvious. One of the basic elements of such a theory is the set of Clebsch–Gordan Coefficients (CGC).

The CGC for the corepresentations of anti-unitary groups are introduced for the first time in Kotzev (1972) (see also 1974), where equations for the calculation of the coefficients and examples for the applications of the CGC are given. Orthogonality relations for the matrix elements of the corepresentations, projection operators and two generalisations of the Wigner–Eckart theorem are also given in Kotzev (1972). The CGC for the corepresentations are also discussed in the papers by Aviran and Litvin (1973), Rudra (1974), Sacata (1974) and Van den Broek (1979), whose results are in good agreement with those of Kotzev (1972). In recent papers (Rudra and Sikdar 1976, 1977) there are reports about the calculation of the CGC for the Shubnikov point groups, but only in the case of even, under space-inversion, basic functions (the tables of the coefficients are not contained in Rudra and Sikdar (1976, 1977)).

Another method for the calculation of the CGC for the corepresentations, completely different from the methods given in Kotzev (1972, 1974), Aviran and Litvin (1973), Rudra (1974), Sacata (1974), Van den Broek (1979), Rudra and Sikdar (1976, 1977), was proposed in Kotzev and Aroyo (1977) (see also 1978a). The method is based on the generalised Racah lemma, Kotzev and Aroyo (1977), and has the following advantages in comparison with the methods previously used. (a) The phases of the CGC for some different groups are well correlated with those of their common supergroup. (b) In many cases the CGC for the subgroups coincide with the coefficients of the supergroup. (c) Some of the 'intermediate' results in the process of calculation of the CGC (such as isocalar factors, etc) have a self-dependent significance and they are not less useful than the 'main' result. The CGC for the single-valued and double-valued corepresentations of all 90 anti-unitary Shubnikov point groups (58 black–white and 32 grey) were calculated and tabulated by this method. The complete tables are published in Kotzev and Aroyo (1978a, b, c, d, 1979).

In the present work, which is a survey of our papers (Kotzev and Aroyo 1977, 1978a, b, c, d, 1979), the generalised Racah lemma, the calculation method of the CGC for the Shubnikov point groups and some examples for the calculation of the CGC are given.

2. The Racah lemma

The Racah lemma concerns the relation between the CGC for the ordinary representations of groups and their subgroups (Racah 1949). We shall prove that an analogous lemma is valid for the corepresentations.

Let B be an arbitrary anti-unitary subgroup of the group A (1). The subduction of the irreducible corepresentation D^α of the group A on the subgroup B

$$(D^\alpha \downarrow B) = \{D^\alpha(g'), g' \in B \subset A\} \tag{3}$$

is a corepresentation of B. It is a reducible corepresentation in the common case. With the help of a unitary reduction matrix S^α, the subduction (3) is decomposed into a direct sum of irreducible corepresentations D^β of the group $B \subset A$:

$$S^{\alpha^{-1}} D^\alpha(g') S^{\alpha(*)} = \bar{D}^\alpha(g') = \bigoplus_{\beta,\tau_\beta} D^{\beta\tau_\beta}(g'), \qquad g' \in B. \tag{4}$$

Here the additional index $\tau_\beta = 1, \ldots, C^\alpha_\beta$ specifies the equivalent corepresentations D^β, which are contained in $(D^\alpha \downarrow B)$ C^α_β times, and S^α are chosen in such a way that the matrices of the equivalent corepresentations in (4) identically coincide, i.e.

$$D^{\beta\tau_\beta}(g') = D^\beta(g'), \qquad g' \in B, \tau_\beta = 1, \ldots, C^\alpha_\beta. \tag{5}$$

In (4), and further on, the asterisk in brackets will be used for a short notation of two equations—the complex conjugation is applied in the case of anti-unitary operators and is not applied in the case of unitary operators.

Applying the transformation (4) to all matrices $D^\alpha(g)$, $g \in A$, we can obtain a corepresentation $\bar{D}^\alpha$ of the group A, which is equivalent to D^α. For $g' \in B$ the matrices $\bar{D}^\alpha(g')$ are diagonal for the indices $\beta\tau_\beta$, $\beta'\tau'_\beta$ i.e. we can write

$$\bar{D}^\alpha(g')_{\beta\tau_b,\beta'\tau'_\beta b'} = \delta_{\beta\tau_\beta,\beta'\tau'_\beta} D^\beta(g')_{bb'}, \qquad g' \in B. \tag{6}$$

The CGC for the corepresentations are defined as the matrix elements

$$U^{\alpha_1\alpha_2}_{a_1a_2,\alpha\rho_\alpha a} \equiv [\alpha_1 a_1, \alpha_2 a_2 | \alpha\rho_\alpha a] \tag{7}$$

of the unitary matrix $U^{\alpha_1\alpha_2}$, which reduces the direct product of the irreducible corepresentations D^{α_1} and D^{α_2} to a quasidiagonal form:

$$(U^{\alpha_1\alpha_2})^{-1} D^{\alpha_1}(g) \otimes D^{\alpha_2}(g) U^{\alpha_1\alpha_2(*)} = \bigoplus_{\alpha\rho_\alpha} D^{\alpha\rho_\alpha}(g), \qquad g \in A. \tag{8}$$

Here the index $\rho_\alpha = 1, \ldots, C^{\alpha_1\alpha_2}_\alpha$ specifies the equivalent D^α, which are contained $C^{\alpha_1\alpha_2}_\alpha$ times in $D^{\alpha_1} \otimes D^{\alpha_2}$, and the matrices $U^{\alpha_1\alpha_2}$ are chosen in such a way that

$$D^{\alpha\rho_\alpha}(g) = D^\alpha(g), \qquad g \in A, \rho_\alpha = 1, \ldots, C^{\alpha_1\alpha_2}_\alpha. \tag{9}$$

The same equations (7)–(9) remain valid for the corepresentation D^β of the subgroup B, after the substitution $A \to B$ and $\alpha \to \beta$, where

$$U^{\beta_1\beta_2}_{b_1b_2,\beta\rho_\beta b} \equiv [\beta_1 b_1, \beta_2 b_2 | \beta\rho_\beta b] \tag{10}$$

are the CGC for the corepresentation D^β of the subgroup B. In order to determine the connection between (7) and (10) it is convenient to write (8) in terms of equivalent corepresentations $\bar{D}^{\alpha_i}$ with the help of (4):

$$\sum_{\substack{\beta_i\tau_{\beta_i}b_i \\ \beta'_i\tau'_{\beta_i}b'_i \\ i=1,2}} [\alpha\rho_\alpha\beta\tau_\beta b | \alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2] \bar{D}^{\alpha_1}(g)_{\beta_1\tau_{\beta_1}b_1,\beta'_1\tau'_{\beta_1}b'_1} \bar{D}^{\alpha_2}(g)_{\beta_2\tau_{\beta_2}b_2,\beta'_2\tau'_{\beta_2}b'_2}$$
$$\times [\alpha_1\beta'_1\tau_{\beta'_1}b'_1, \alpha_2\beta'_2\tau_{\beta'_2}b'_2 | \alpha'\rho'_\alpha\beta'\tau_{\beta'}b']^{(*)}$$
$$= \delta_{\alpha\rho_\alpha,\alpha'\rho'_\alpha} \bar{D}^\alpha(g)_{\beta\tau_\beta b,\beta'\tau_{\beta'}b'}. \tag{11}$$

Here the CGC for the corepresentations of the group A are written in a new basis (the index a_i is replaced by the triad $\beta_i\tau_{\beta_i}b_i$),

$$\bar{U}^{\alpha_1\alpha_2}_{\beta_1\tau_{\beta_1}b_1\beta_2\tau_{\beta_2}b_2,\alpha\rho_\alpha\beta\tau_\beta b} \equiv [\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2 | \alpha\rho_\alpha\beta\tau_\beta b]. \tag{12}$$

They are connected with (7) by the transformation

$$[\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2 | \alpha\rho_\alpha\beta\tau_\beta b] = \sum_{a_1a_2a} (\alpha_1 a_1 | \alpha_1\beta_1\tau_{\beta_1}b_1)^* (\alpha_2 a_2 | \alpha_2\beta_2\tau_{\beta_2}b_2)^*$$
$$\times [\alpha_1 a_1, \alpha_2 a_2 | \alpha\rho_\alpha a] (\alpha a | \alpha\beta\tau_\beta b), \tag{13}$$

or, in matrix form,

$$\bar{U}^{\alpha_1\alpha_2} = (S^{\alpha_1} \otimes S^{\alpha_2})^{-1} U^{\alpha_1\alpha_2}\Big(\bigoplus_{\alpha\rho_\alpha} S^{\alpha}\Big), \tag{14}$$

where

$$S^{\alpha}_{a,\beta\tau_\beta b} \equiv (\alpha a|\alpha\beta\tau_\beta b), \qquad (S^{\alpha^{-1}})_{\beta\tau_\beta b_1 a} \equiv (\alpha\beta\tau_\beta b|\alpha a) = (\alpha a|\alpha\beta\tau_\beta b)^*. \tag{15}$$

In the direct sum $\oplus_{\alpha\rho_\alpha} S^{\alpha}$ the matrix S^{α} repeats $C^{\alpha_1\alpha_2}_{\alpha}$ times for every $D^{\alpha} \in D^{\alpha_1} \oplus D^{\alpha_2}$.

Considering (6), (8), the unitarity of the matrices of the CGC, and using (11), it follows that

$$\begin{aligned}\sum_{b'}\Big\{\sum_{b_1b_2}[\beta\rho_\beta b|\beta_1 b_1, \beta_2 b_2][\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta'\tau_{\beta'}b']\Big\}D^{\beta'}(g')_{b'b''}\\ = \sum_{b'} D^{\beta}(g')_{bb'}\Big\{\sum_{b_1b_2}[\beta\rho_\beta b'|\beta_1 b_1, \beta_2 b_2]\\ \times[\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta'\tau_{\beta'}b'']\Big\}^{(*)}.\end{aligned} \tag{16}$$

This equation has the form of the generalised Shur lemma for the corepresentations (Dimmock 1963). The elements of a $d_\beta \times d_{\beta'}$ matrix, commuting with all the matrices of the irreducible corepresentation D^{β}, are separated by braces. The matrix is equal to zero for $\beta' \neq \beta$, while for $D^{\beta} = D^{\beta'}$ it should be Hermitian and a multiple of the unit matrix $D^{\beta}(E)$, i.e.

$$\begin{aligned}\sum_{b_1b_2}[\beta\rho_\beta b|\beta_1 b_1, \beta_2 b_2][\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta'\tau_{\beta'}b']\\ = (\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta)\delta_{\beta b,\beta' b'}.\end{aligned} \tag{17}$$

The quantities in parentheses are known as isoscalar factors.

The requirement of hermiticity for the constant matrix (17) is specific for the corepresentations. From the hermiticity it follows that the matrix elements should be real, so the isoscalar factors can be written in the form

$$\begin{aligned}(\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta)^* = (\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta)\\ \equiv \chi^{\alpha_1\alpha_2\beta}_{\beta_1\tau_{\beta1}\beta_2\tau_{\beta2}\beta\rho_\beta,\alpha\rho_\alpha\beta\tau_\beta}.\end{aligned} \tag{18}$$

If we write all possible equations of the type (16) for a chosen matrix $\bar{U}^{\alpha_1\alpha_2}$, then the corresponding matrix elements (17) will form a unitary matrix

$$X^{\alpha_1\alpha_2} = \Big(\bigoplus_{\beta_i\in\alpha_i} U^{\beta_1\beta_2}\Big)^{-1}\bar{U}^{\alpha_1\alpha_2} \tag{19}$$

which has a quasidiagonal form (see e.g. table 5). The matrix $X^{\alpha_1\alpha_2}$ is an orthogonal matrix because in every block diagonal for the indices βb, $\beta' b'$, there is a submatrix $\chi^{\alpha_1\alpha_2\beta}$ (18) with real elements. So the Racah lemma equation, determining the connection between the CGC for the corepresentations of the group A and its subgroup B, follows directly from (17):

$$\begin{aligned}[\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta\tau_\beta b]\\ = \sum_{\rho_\beta}[\beta_1 b_1, \beta_2 b_2|\beta\rho_\beta b](\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta).\end{aligned} \tag{20}$$

It is more convenient to use the reverse equation for the calculation of the coefficients $U^{\beta_1\beta_2}$:

$$[\beta_1 b_1, \beta_2 b_2|\beta\rho_\beta b]$$
$$= \sum_{\alpha\rho_\alpha\tau_\beta} [\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta\tau_\beta b](\alpha\rho_\alpha\beta\tau_\beta|\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta), \quad (21)$$

or, in matrix form,

$$\bigoplus_{\beta_i\in\alpha_i} U^{\beta_1\beta_2} = \bar{U}^{\alpha_1\alpha_2}(X^{\alpha_1\alpha_2})^{-1}, \quad (22)$$

where the matrix $\bar{U}^{\alpha_1\alpha_2}$ is given by the equation (14) and its matrix elements by (13).

The following set of equations, for the calculation of the unknown $X^{\alpha_1\alpha_2}$ elements (18), is derived from (17):

$$\sum_{\rho_\beta} (\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta)(\alpha_1\beta_1\tau'_{\beta_1}, \alpha_2\beta_2\tau'_{\beta_2}; \beta\rho_\beta|\alpha'\rho'_{\alpha'}\beta\tau'_\beta)$$
$$= \sum_{b_1b_2} [\alpha_1\beta_1\tau_{\beta_1}b_1, \alpha_2\beta_2\tau_{\beta_2}b_2|\alpha\rho_\alpha\beta\tau_\beta b][\alpha_1\beta_1\tau'_{\beta_1}b_1, \alpha_2\beta_2\tau'_{\beta_2}b_2|\alpha'\rho'_{\alpha'}\beta\tau'_\beta b]^*. \quad (23)$$

Further, the orthogonality relations for the rows and columns of the matrix (17) should be considered. They follow from the orthogonality of the matrix $X^{\alpha_1\alpha_2}$:

$$\sum_{\beta_i\tau_{\beta_i}\rho_\beta} (\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha\rho_\alpha\beta\tau_\beta)(\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta|\alpha'\rho'_{\alpha'}\beta\tau'_\beta) = \delta_{\alpha\rho_\alpha\tau_\beta,\alpha'\rho'_{\alpha'}\tau'_\beta}$$

$$\sum_{\alpha\rho_\alpha\tau_\beta} (\alpha_1\beta_1\tau_{\beta_1}, \alpha_2\beta_2\tau_{\beta_2}; \beta\rho_\beta(\alpha\rho_\alpha\beta\tau_\beta)(\alpha_1\beta'_1\tau'_{\beta'_1}\alpha_2\beta'_2\tau'_{\beta'_2}; \beta\rho'_\beta|\alpha\rho_\alpha\beta\tau_\beta)$$
$$= \delta_{\beta_1\beta_2\tau_{\beta 1}\tau_{\beta 2}\rho_\beta,\beta'_1\beta'_2\tau'_{\beta'_1},\tau'_{\beta'_2}\rho'_\beta}. \quad (24)$$

So, we prove the validity of the Racah lemma for the corepresentations of anti-unitary groups. But in this case $X^{\alpha_2\alpha_2}$ are orthogonal, i.e. the isoscalar factors (18) *are real.*

Starting with the CGC for the corepresentations of a group A and using the so generalised Racah lemma, the CGC for the corepresentations of all its subgroups B can be determined (Kotzev and Aroyo 1977, 1978a, b, c, d, 1979). It should be noted that the Racah lemma was used for the calculation of CGC for the representations of crystallographic point groups for the first time in Batarunas and Levinson (1960) (see also Baljavichus *et al* 1964). In König and Kremer (1973) is discussed the problem of phase standardisation of the CGC of the point groups considering time inversion symmetry. The authors maintain that all isoscalar factors *can be chosen* (i) real, (ii) positive. It follows from the Racah lemma that for systems with anti-unitary symmetry the isoscalar factors (18) *should be real.* But it is obvious that the condition $\chi \geqslant 0$ is not correct. All the elements of the submatrices $\chi^{\alpha_1\alpha_2\beta}$ are positive only when all $X^{\alpha_1\alpha_2}$ are equivalent to unit matrices (in the opposite case CGC will not form a unitary matrix).

3. The reduction matrix

We can use the equations (24)–(33) in Kotzev (1974), with the corresponding substitution of the symbols, for the calculation of the reduction matrix S^α (4), (15). For the corepresentation D^β of the type 'a' or 'c' (irrespective of the type of D^α corepresentation), we have

$$\frac{|D^\beta|}{|B|}\sum_{u'\in B} D^\alpha(u')_{aa'}D^\beta(u')^*_{bb'} = W_\beta \sum_{\tau_\beta}(\alpha a|\alpha\beta\tau_\beta b)(\alpha a'|\alpha\beta\tau_\beta b')^* \tag{25}$$

where the summation is over the unitary elements only, and $W_\beta = \frac{1}{2}$ for D^β of the type 'a' and $W_\beta = 1$ for the type 'c'.

For D^β of the type 'b':

$$\frac{|D^\beta|}{|B|}\sum_{u'\in B} D^\alpha(u')_{aa'}D^\beta(u')^*_{bb'}$$

$$= \sum_{\tau_\beta}\{(\alpha a|\alpha\beta\tau_\beta b)(\alpha a'|\alpha\beta\tau_\beta b')^* + (\alpha a|\alpha\beta\tau_\beta \bar{b})(\alpha a'|\alpha\beta\tau_\beta \bar{b}')^*\} \tag{26}$$

where $\bar{b} = ||D^\beta|/2 - b|$, $\bar{b}' = |\frac{1}{2}|D^\beta| - b'|$.

In all these equations only the unitary operators of the subgroup B are considered. The role of the anti-unitary operator is given by the condition

$$(\alpha a'|\alpha\beta\tau_\beta b')^* = \sum_{ab}(\alpha a|\alpha\beta\tau_\beta b)D^\alpha(a_0)^*_{aa'}D^\beta(a_0)_{bb'}, \qquad a_0 \subset B, \tag{27}$$

where a_0 is an arbitrarily chosen, but fixed anti-unitary operator, with which are constructed all $a = ua_0$ (1).

The matrix elements (15) are decomposition coefficients of the basic functions of the corepresentation D^β, expressed in terms of the corresponding functions of the corepresentation D^α:

$$\psi_b^{\beta\tau_\beta} = \sum_a \psi_a^\alpha(\alpha a|\beta\tau_\beta b), \tag{28}$$

i.e. the equations previously mentioned can be used for the construction of bases for corepresentations.

In particular, the matrices S^j, reducing the representations D^j of the rotation group to the crystallographic point groups, are given in the tables of Leushin (1968). As in Leushin (1968) time inversion is considered, so the results of the book are valid for the corepresentations of the anti-unitary group $O(3)\otimes\Theta$ and 32 'grey' Shubnikov groups $G1' = G\otimes\Theta$. The reducing matrices S^α for the 58 'black–white' groups $G' \subset G1'$ can be easily derived from them.

4. Method of calculation for CGC

All the 122 Shubnikov (magnetic) point groups are subgroups of the generalised full rotation group $O(3)\otimes\Theta = \infty\infty\bar{1}1'$. Only 90 of these groups are anti-unitary—32 'grey' $G1' = G\otimes\Theta$ and 58 'black–white' groups $G' \subset G1'$. As was shown in Kotzev (1972, 1974) (see also Kotzev and and Aroyo 1978b), the CGC for the corepresentations of $O(3)\otimes\Theta$ coincided with the well known Wigner coefficients, i.e.

$$[j_1m_1, j_2m_2|j1m] = (j_1m_1, j_2m_2|jm). \tag{29}$$

The CGC for the corepresentations of the Shubnikov point groups can be calculated using the generalised Racah lemma (21), either directly from (29), or by a successive descent down the subgroup chain,

$$\mathrm{O}(3)\otimes\Theta \begin{array}{l} \nearrow\ \mathrm{O_h}\otimes\Theta \supset \mathrm{G}_n \supset \ldots \supset \mathrm{C_1} \\ \\ \searrow\ \mathrm{D_{6h}}\otimes\Theta \supset \mathrm{G}_m \supset \ldots \supset \mathrm{C_1}. \end{array} \tag{30}$$

The generalised Racah lemma (21) and the subgroup chains were used in Kotzev and Aroyo (1978a, b, c, d, 1979), where the complete tables of CGC for the single-valued and the double-valued corepresentations of the 90 anti-unitary Shubnikov groups were published. To save space, the tables (Kotzev and Aroyo 1978b, c, d) give CGC for basic functions, even under space inversion. The CGC for odd corepresentations $D^{\alpha-}$ of the groups $\mathrm{G}\otimes\mathrm{C_i}$ can be determined with the help of the known rule

$$\begin{aligned} [\alpha_1 a_1, \alpha_2 a_2 | \alpha\rho_\alpha a] &= [\alpha_1^{\pm} a_1, \alpha_2^{\pm} a_2 | \alpha^{+}\rho_\alpha a] \\ &= [\alpha_1^{\mp} a_1, \alpha_2^{\pm} a_2 | \alpha^{-}\rho_\alpha a]. \end{aligned} \tag{31}$$

When the unitary subgroup $H \lhd B$ contains improper rotations, and the space-inversion I is not an element of H, it is necessary to calculate the CGC also for basic functions, odd under the space-inversion I. These coefficients are given in Kotzev and Aroyo (1979).

As an example of the method stated above, we will discuss the calculation of the CGC for the corepresentations of the anti-unitary group $41' = \mathrm{C_4}\otimes\Theta$ and its isomorphic groups $\bar{4}1' = \mathrm{S_4}\otimes\Theta$, $4/m' = \mathrm{C_{4h}(C_4)}$, $4'/m' = \mathrm{C_{4h}(S_4)}$, considered as subgroups of $\mathrm{O}(3)\otimes\Theta$. These groups do not contain the space inversion I, but for physical applications it is advisable to construct basic functions, even or odd, under space inversion. The CGC for the corepresentations of the four groups coincide for even basic functions. The CGC of the groups $\mathrm{S_4}\otimes\Theta$ and $\mathrm{C_{4h}(S_4)}$ for odd basic functions differ from the coefficients for an even basis. So, for these two groups, it is necessary to calculate in addition the following coefficients: β_1 (odd) $\times\beta_2$ (odd), β_1 (even) $\times\beta_2$ (odd), β_1 (odd) $\times\beta_2$ (even).

The irreducible corepresentations D^β and the basic functions for the four groups are given in table 1 (Leushin 1968). Table 2 is a multiplication table for the corepresentations D^β, and table 3 contains the subductions of the corepresentations $(D^j{\downarrow}41')$. The minimal value of the index j of D^j, whose reductions contain a definite D^β, is the quasimoment $j(\beta)$ of D^β (D^β in reductions specified by the minimal j are shown bold

Table 1. Corepresentations and basic functions

$\mathrm{C_4}\times\Theta = 41'$ $\mathrm{C_{4h}(C_4)} = 4/m'$ $\mathrm{S_4}\times\Theta = \bar{4}1'$ (even) $\mathrm{C_{4h}(S_4)} = 4'/m'$ (even)			$\bar{4}1'$ (odd) $4'/m'$ (odd)	
D_1	Γ_1	$\|0\,0\rangle$	D_2	$\|0\,0\rangle$
D_2	Γ_2	$(1/\sqrt{2})\{\|2\,2\rangle + \|2\,-2\rangle\}$	D_1	$(-1/\sqrt{2})\{\|2\,2\rangle + \|2\,-2\rangle\}$
D_3	$\Gamma_3+\Gamma_4$	$\|1\,1\rangle, \|1\,-1\rangle$	D_3	$\|1\,-1\rangle, \|1\,1\rangle$
D_5	$\Gamma_5+\Gamma_6$	$\|\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$	D_8	$\|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle, -\|\tfrac{1}{2}\,\tfrac{1}{2}\rangle$
D_8	$\Gamma_8+\Gamma_7$	$\|\tfrac{3}{2}\,\tfrac{3}{2}\rangle, \|\tfrac{3}{2}\,-\tfrac{3}{2}\rangle$	D_5	$\|\tfrac{3}{2}\,-\tfrac{3}{2}\rangle, -\|\tfrac{3}{2}\,\tfrac{3}{2}\rangle$

Table 2. Multiplication table

	1	2	3	5	8
1	[1]	2	3	5	8
2	2	[1]	3	8	5
3	3	3	[1+2+2]+{1}	5+8	5+8
5	5	8	5+8	[1+3]+{1}	2+2+3
8	8	5	5+8	2+2+3	[1+3]+{1}

in table 3). For the calculation of the CGC for $41' \subset \infty\infty\bar{1}1'$ it is sufficient to use the Wigner coefficients $U^{j_1j_2}$ with $j_1j_2 = 2, 2; \frac{3}{2}, \frac{3}{2}; 2, \frac{3}{2}; \frac{3}{2}\, 2$ (it follows from table 3). $\bar{U}^{3/2,3/2}$ is given in table 4 (we will note that in many papers the coefficients $\bar{U}^{\alpha_1\alpha_2}$ are called CGC of the subgroup). The full matrix $X^{3/2\ 3/2}$ of the isoscalar factors is given in table 5. The CGC for the corepresentations of the four groups for even bases are written in the form of unitary matrices $U^{\beta_1\beta_2}$ in table 6. The trivial coefficients

$$[11, \beta_2 b_2|\beta_2 1 b_2] = [\beta_1 b_1, 11|\beta_1 1 b_1] = 1 \tag{32}$$

Table 3. Compatibility table

D^j	D^0	D^1	D^2	$D^{1/2}$	$D^{3/2}$
D_β (41′)	$\boldsymbol{D_1}$	$D_1 + \boldsymbol{D_3}$	$D_1 + 2\boldsymbol{D_2} + D_3$	$\boldsymbol{D_5}$	$D_5 + \boldsymbol{D_8}$

are omitted in order to shorten the table. The matrices whose elements are determined by the equation

$$[\beta_2 b_2, \beta_1 b_1|\beta\rho_\beta b] = (-1)^{j(\beta_1)+j(\beta_2)-j(\beta\rho_\beta)}[\beta_1 b_1, \beta_2 b_2|\beta\rho_\beta b] \tag{33}$$

are also not given. It should be noted that the symmetry condition (33) does not follow from group considerations (see for example Kotzev 1972), but it reflects the connection between the coefficients calculated here and Wigner coefficients, for which

$$(j_2 m_2, j_1 m_1|jm) = (-1)^{j_1+j_2-j}(j_1 m_1, j_2 m_2|jm). \tag{34}$$

Contrary to (34), in (33) the quasimoment $j(\beta\rho_\beta)$ depends on β and on ρ_β. This is connected with the fact that the repeated corepresentations of the subgroup B, $D^{\beta\rho_\beta} \equiv D^\beta$, sometimes originate from different corepresentations D^α of the group A, with different quasimoments $j(\alpha)$. For more convenient use of the tables, the columns of every matrix $U^{\beta_1\beta_2}$, whose elements change a sign under the substitution $\beta_1 b_1 \leftrightarrow \beta_2 b_2$ (33), are marked by an asterisk. If the asterisk is absent, the whole column does not change sign.

When one or both basic functions in the Kronecker product $D^{\beta_1} \times D^{\beta_2}$ are odd, then the CGC for $S_4 \times \Theta$ and $C_{4h}(S_4)$ differ from those given in table 6 by the multiple ± 1. Table 7 is a version of the multiplication table, when the barred indices $\bar{\beta}$ of the corepresentations D^β mean that the CGC can be determined by multiplying the correspondent CGC in table 6 by (-1). In the opposite case the coefficients coincide. The CGC for the corepresentations of the group $4/m1' = C_{4h} \otimes \Theta = 41' \times \bar{1}$ can be

Table 4. Matrix $U^{3/2\,3/2}$

			β	1				2				3							
			j	0	1	2	3	2		3		1		2		3			
			τ_β	1	1	1	1	1	2	1	2	1	1	1	1	1	1	2	2
α_1	$\beta_1\tau_1 b_1$	α_2	$\beta_2\tau_2 b_2$ $\underline{b}$	1	1	1	1	1	1	1	1	1	2	1	2	1	2	1	2
3/2	511	3/2	511									$-\sqrt{2/5}$				$3/\sqrt{40}$		$\sqrt{3/8}$	
3/2	511	3/2	512	1/2	$i/\sqrt{20}$	−1/2	$-3i/\sqrt{20}$												
3/2	512	3/2	511	−1/2	$i/\sqrt{20}$	1/2	$-3i/\sqrt{20}$												
3/2	512	3/2	512										$-\sqrt{2/5}$				$3/\sqrt{40}$		$\sqrt{3/8}$
3/2	811	3/2	811														$\sqrt{5/8}$		$-\sqrt{3/8}$
3/2	811	3/2	812	1/2	$3i/\sqrt{20}$	1/2	$i/\sqrt{20}$												
3/2	812	3/2	811	−1/2	$3i/\sqrt{20}$	−1/2	$i/\sqrt{20}$												
3/2	812	3/2	812													$\sqrt{5/8}$		$-\sqrt{3/8}$	
3/2	511	3/2	811					−1/2	−i/2	1/2	i/2								
3/2	511	3/2	812										$\sqrt{3/10}$		$\sqrt{1/2}$		$\sqrt{3/40}$		$\sqrt{1/8}$
3/2	512	3/2	811									$-\sqrt{3/10}$		$-\sqrt{1/2}$		$-\sqrt{3/40}$		$-\sqrt{1/8}$	
3/2	512	3/2	812					−1/2	i/2	1/2	−i/2								
3/2	811	3/2	511					1/2	i/2	1/2	i/2								
3/2	811	3/2	512									$-\sqrt{3/10}$		$\sqrt{1/2}$		$-\sqrt{3/40}$		$-\sqrt{1/8}$	
3/2	812	3/2	511										$\sqrt{3/10}$		$-\sqrt{1/2}$		$\sqrt{3/40}$		$\sqrt{1/8}$
3/2	812	3/2	512					1/2	−i/2	1/2	−i/2								

Table 5. Matrix of the isoscalar factors $X^{3/2\;3/2} = \chi^{3/2\;3/2\;1} \oplus \chi^{3/2\;3/2\;2} \oplus 2\chi^{3/2\;3/2\;3}$

				β	1				2				3							
				b	1				1				1				2			
				j	0	2	1	3	2	3	2	3	1	2	3	3	1	2	3	3
$\beta b \rho_\beta \alpha_1$	β_1	τ_{β_1}	α_2	$\beta_2 \tau_{\beta_2}$ τ_β	1	1	1	1	1	1	2	2	1	1	1	2	1	1	1	2
111	3/2	51	3/2	51	$1/\sqrt{2}$	$-1/\sqrt{2}$														
	3/2	81	3/2	81	$1/\sqrt{2}$	$1/\sqrt{2}$														
112	3/2	51	3/2	51			$1/\sqrt{10}$	$-3/\sqrt{10}$												
	3/2	81	3/2	81			$3/\sqrt{10}$	$1/\sqrt{10}$												
211	3/2	51	3/2	81					$-1/\sqrt{2}$	$1/\sqrt{2}$										
	3/2	81	3/2	51					$-1/\sqrt{2}$	$1/\sqrt{2}$										
212	3/2	51	3/2	81							$-1/\sqrt{2}$	$1/\sqrt{2}$								
	3/2	81	3/2	51							$-1/\sqrt{2}$	$1/\sqrt{2}$								
31	3/2	51	3/2	51									$-\sqrt{2/5}$	0	$3/\sqrt{40}$	$\sqrt{3/8}$				
	3/2	81	3/2	81									0	0	$\sqrt{5/8}$	$-\sqrt{3/8}$				
	3/2	51	3/2	81									$\sqrt{3/10}$	$1/\sqrt{2}$	$\sqrt{3/40}$	$\sqrt{1/8}$				
	3/2	81	3/2	51									$-\sqrt{3/10}$	$1/\sqrt{2}$	$-\sqrt{3/40}$	$-\sqrt{1/8}$				
321	3/2	51	3/2	51													$-\sqrt{2/5}$	0	$3/\sqrt{40}$	$\sqrt{3/8}$
	3/2	81	3/2	81													0	0	$\sqrt{5/8}$	$-\sqrt{3/8}$
	3/2	51	3/2	81													$\sqrt{3/10}$	$1/\sqrt{2}$	$\sqrt{3/40}$	$\sqrt{1/8}$
	3/2	81	3/2	51													$-\sqrt{3/10}$	$1/\sqrt{2}$	$-\sqrt{3/40}$	$-\sqrt{1/8}$

Table 6. Clebsch–Gordan coefficients $U^{\beta_1\beta_2}$

U^{33}				
		*		
	1	1	2	2
	1	2	1	2
	1	1	1	1
31 31			$1/\sqrt{2}$	$i\sqrt{1/2}$
31 32	$1/\sqrt{2}$	$i\sqrt{1/2}$		
32 31	$1/\sqrt{2}$	$-i\sqrt{1/2}$		
32 32			$\sqrt{1/2}$	$-i\sqrt{1/2}$

U^{55}				
	*			
	1	1	3	3
	1	2	1	1
	1	1	1	2
51 51			1	
51 52	$\sqrt{1/2}$	$i\sqrt{1/2}$		
52 51	$-\sqrt{1/2}$	$i\sqrt{1/2}$		
52 52				1

U^{88}				
	*			
	1	1	3	3
	1	2	1	1
	1	1	1	2
81 81				1
81 82	$\sqrt{1/2}$	$i\sqrt{1/2}$		
82 81	$-\sqrt{1/2}$	$i\sqrt{1/2}$		
82 82			1	

U^{35}				
	*	*		
	5	5	8	8
	1	1	1	1
	1	2	1	2
31 51			1	
31 52	1			
32 51		−1		
32 52				1

U^{38}				
			*	*
	5	5	8	8
	1	1	1	1
	1	2	1	2
31 81				−1
31 82		1		
32 81	1			
32 82			1	

U^{58}				
			*	*
	2	2	3	3
	1	2	1	1
	1	1	1	2
51 81	$\sqrt{1/2}$	$i\sqrt{1/2}$		
51 82				1
52 81			−1	
52 82	$\sqrt{1/2}$	$-i\sqrt{1/2}$		

U^{28}		
	*	*
	5	5
	1	1
	1	2
21 81		−1
21 82	1	

U^{25}		
	*	*
	8	8
	1	1
	1	2
21 51		−1
21 52	1	

U^{23}		
	3	3
	1	1
	1	2
21 31		1
21 32	1	

Table 7. CGC for $\bar{4}1'$ and $4'/m'$ – odd bases

$\beta_1\beta_2$	$\beta_1^o \times \beta_2^o$	$\beta_1^e \times \beta_2^o$	$\beta_1^o \times \beta_2^e$	$\beta_1\beta_2$	$\beta_1^o \times \beta_2^o$	$\beta_1^e \times \beta_2^o$	$\beta_1^o \times \beta_2^e$
22	1	$\bar{1}$	$\bar{1}$	25	$\bar{8}$	8	8
33	$1_1, \bar{1}_2, 2_1. \bar{2}_2$	$\bar{1}_1, \bar{1}_2, 2_1, 2_2$	$\bar{1}_1, 1_2, 2_1, \bar{2}_2$	28	$\bar{5}$	5	5
55	$1_1, \bar{1}_2, 3$	$1_1, 1_2, 3$	$\bar{1}_1, 1_2, \bar{3}$	35	$\bar{5}, 8$	$5, 8$	$5, \bar{8}$
88	$1_1, \bar{1}_2, 3$	$1_1, 1_2, 3$	$\bar{1}_1, 1_2, \bar{3}$	38	$5, \bar{8}$	$5, 8$	$\bar{5}, 8$
23	3	3	3	58	$2_1, \bar{2}_2, 3$	$2_1, 2_2, \bar{3}$	$\bar{2}_1, 2_2, 3$

determined from table 6 using the rule (31). In a similar way the double magnetic groups are classified by isomorphism and the CGC for them are calculated in Kotzev and Aroyo (1978b, c, d, 1979).

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