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Original investigations

Phase-fixed double-group 3-Γ symbols. I. A novel exposition of the general theory of 3-Γ symbols and coupling coefficients

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The present paper is the first in a series aiming at the establishment of a transparent and readily applicable Wigner–Racah algebra for all the non-commutative double groups.

Starting from the Wigner–Eckart theorem in a very general setting, the theory of the fundamental quantities called here *triple coefficients* – and the closely related coupling coefficients – is developed and leads through a careful discussion of permutational symmetries to the concept of *3-Γ symbols.* By basing the exposition on triple coefficients and by consistently using *matrix* representations, we obtain a notation and a terminology which enable a clear separation of permutational properties and problems concerning complex conjugation, and a more transparent discussion of tensor (Kronecker) product multiplicities.

A particularly elegant formalism is obtained for a situation which generalizes that of the classical rotation-group Wigner–Racah algebra, *viz.*, in which there is a fixed group element effecting (through the inner automorphism it defines) complex conjugation of all the standard irreducible matrix representations.

Key words: three-gamma symbols—coupling coefficients—triple coefficients—complex conjugation of irreducible matrix representations—inner automorphisms—Frobenius–Schur classification—Derome–Sharp matrices—Wigner–Racah algebra.

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1. Introduction

The Wigner–Racah algebra or "the irreducible tensor method" is an indispensable tool in quantum chemistry, in particular for calculations within semiempirical symmetry-based models as, e.g. ligand-field models [1, 2]. In all such models a particularly transparent and rational formulation is envisaged using Wigner–Racah algebra in connection with the formalism of orthonormal operator sets introduced recently [3] and exemplified further in [4]. Calculations in polycentric systems such as oligonuclear transition-metal complexes may be drastically simplified using Wigner–Racah algebra for the rotation group [5] or a suitable point group [6].

The conventional Wigner–Racah algebra of the rotation group and its double group, i.e. the group theory of angular momentum, was well developed almost 25 years ago (see [7, 8, 9], the reprint collection [10], and the useful recent exposition [11]), although quite a few, mostly advanced, topics have been explored since then [12]. A very comprehensive treatise has appeared [13]. Following the famous unpublished 1940 paper by Wigner [14], the 1962 book by Griffith [1] and some general papers in the mid-sixties [15, 16], the seventies have witnessed a substantial output of literature dealing either with general Wigner–Racah algebra or problems related to specific groups or classes of groups – in particular point groups and their double groups, or classical groups, mainly the unitary groups SU(n) and U(n). (For some rather general reviews, see [17, 18, 19]). One of the first papers of the latter type was [20], of which the present work is, in many respects, a continuation. Relevant references will be given as we develop our exposition here and further discussion of the literature will be given in [21]. However, already here, we mention that there is a very extensive series of papers by Butler and co-workers leading up to the recent publication of a book [22] dealing with point- and double-group Wigner–Racah algebra. It might seem superfluous on that background to have another treatment of the subject; however, our description of the general theory and, perhaps more important, our approach to the actual construction of the algebra for the double groups is so different from that of Butler et al. that we think publishing it is justified.

The following papers in the present series will deal with, firstly, general aspects of double groups and their 3-Γ symbols (paper II) and, secondly, the results we have obtained for the series of dihedral double groups (paper III), the tetrahedral double group (paper IV), the octahedral double group (paper V), and, finally, the icosahedral double group (paper VI). Future publications are planned to deal with recoupling coefficients, 6-Γ symbols, and 9-Γ symbols.

The plan of the *present* paper is roughly as follows. A reformulation in Sect. 2 of the Wigner–Eckart theorem leads in Sect. 3.1 to the general convention-free definition of *triple coefficients*, which proves to be a convenient "umbrella" definition for subsequent discussions of coupling (Clebsch–Gordan) coefficients (Sect. 3.3) and of 3-Γ symbols (Sect. 4) and, in particular, of the permutational symmetry phenomena encountered when "subducing" 3-j symbols (this will be described in a precise manner) from the rotation group to its subgroups (papers

II and subsequent papers). Sect. 5 discusses complex conjugation of irreducible matrix representations themselves (Sect. 5.2; the Frobenius–Schur classification) and of representations occurring in 3-Γ symbols. In Sect. 5.5 we describe a particularly important and convenient situation where the Wigner–Racah algebra of a group "mimics" that of the rotation group very closely. Finally, Sect. 6 illustrates the preceding chapters by stating properties of the classical rotation group formalism using the present notation and terminology.

The appendix collects various mathematical comments and proofs of theorems that could be left out of the main text, but which are included because they are either new in the present context or in the way they are presented.

We believe the exposition of 3-Γ symbol theory given here has the additional virtue of being suitable as a *modern* introduction to the subject. The only mathematical prerequisites are elementary concepts from group theory and linear algebra, whereas we manage without explicitly introducing concepts as co- and contragredience, raising and lowering of indices, time-inversion etc.

Although many of the results to be presented are more generally valid, we shall assume our groups to be compact in order not to have an excessive number of reservations and comments in the text regarding the precise validity of particular results.

Notation

We shall use the abbreviations "*rep*" and "*irrep*" for "representation" and "irreducible representation", respectively; thus, a rep is not necessarily irreducible. In this language, "rep matrix" is just what has often been called "matrix representative" of or corresponding to a certain group element in a specified group representation. *Matrix* reps will be given special Roman type letters, $\mathbb{\Gamma}$ say, the rep matrices corresponding to group elements R denoted by $\mathbb{\Gamma}(R)$ and their matrix elements by $\mathbb{\Gamma}(R)_{ij}$. Ordinary letters will, as is customary, denote reps without specific reference to a certain matrix form, i.e. will denote equivalence classes of reps. In general contexts, the totally symmetric (trivial 1-dimensional) irrep of a group G will be denoted 1_G and its component 0. If $\mathbb{\Gamma}$ is a matrix rep, $\dim \mathbb{\Gamma}$ denotes its dimension and $\bar{\mathbb{\Gamma}}$ is the complex conjugate rep defined by

$$\bar{\mathbb{\Gamma}}(R) = \overline{\mathbb{\Gamma}(R)}$$

for all group elements R. The bar denotes complex conjugation.

For matrices, the right superscript symbol "T" denotes transposition (interchange of rows and columns), while † denotes formation of the adjoint (the Hermitian conjugate), i.e., $\mathbb{A}^\dagger = \bar{\mathbb{A}}^\mathrm{T}$. By $\mathbb{1}$ and $\mathbb{0}$ are meant the unit and zero matrix, respectively (in any dimension).

Regarding the rotation group R_3 (alternatively denoted $SO(3)$, $\boldsymbol{d}_3$ or K), we use for its irreps the notation D_l; $l = 0, 1, 2, \ldots$ (i.e., the dimension of D_l is $2l+1$). The rotation double group is denoted R_3^* here (other designations are $SU(2)$, $\boldsymbol{u}_2$, and K'), and its irreps are $D_j; j=0, 1/2, 1, 3/2, \ldots$ (dim $D_j=2j+1$). By R_{3i} is meant the direct product $R_3 \times C_i = R_3 \times S_2$.

2. The Wigner–Eckart theorem

The Wigner–Eckart theorem compactly expresses the essence of the application of group representations to the simplification and standardized parametrization of matrices of quantum-chemical operators. Various versions of the statement are presented in many of the standard textbooks in this area (e.g. [7] pp. 303–305; [8] pp. 78–79; [11] pp. 67–69; [23] pp. 73–75; [24] pp. 191–192; [25] pp. 224–230; [26] pp. 131–132; [27] pp. 56–57; [28] pp. 273–276; [29] pp. 64–68; [30] pp. 230–232; [31] pp. 273–275) so it should need no lengthy introduction. Nevertheless we shall discuss the derivation and formulation of the theorem in some detail here, mainly for the reason that this will provide the natural background for the introduction of the concept of *triple coefficients* in Sect. 3.

We shall assume the following rather general set-up for the Wigner–Eckart theorem:
* A *group* G and a *unitary operator rep* $\mathcal{T}$ of G on a Hilbert space V.
* Vector sets $(\varphi_1, \ldots, \varphi_{d_1})$ and $(\psi_1, \ldots, \psi_{d_3})$ in V *transforming* under $\mathcal{T}$ *as* certain *unitary matrix reps* Γ_1 and Γ_3 of G (of dimensions d_1 and d_3, respectively). We recall that this means that for any index γ_1 we have

$$\mathcal{T}(R)\varphi_{\gamma_1} = \sum_{\gamma_1'} \Gamma_1(R)_{\gamma_1'\gamma_1}\varphi_{\gamma_1'} \quad \text{for all } R \in G, \tag{2.1}$$

the sum being extended over the components $1, \ldots, d_1$ of Γ_1 (and analogously for the ψ's).
* A set $(\mathcal{O}_1, \ldots, \mathcal{O}_{d_2})$ of operators on V transforming under $\mathcal{T}$ as a certain unitary matrix rep Γ_2 (of dimension d_2) of G. Recall that this means that for any index γ_2 we have

$$\mathcal{T}(R)\mathcal{O}_{\gamma_2}\mathcal{T}(R)^{-1} = \sum_{\gamma_2'} \Gamma_2(R)_{\gamma_2'\gamma_2}\mathcal{O}_{\gamma_2'} \quad \text{for all } R \in G. \tag{2.2}$$

An operator set of this kind is sometimes called a *tensor operator transforming* as Γ_2 (an *irreducible* tensor operator if Γ_2 is irreducible).

We are interested in matrix elements of the form $\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle$ of the operators $\mathcal{O}_{\gamma_2}$. Since $\mathcal{T}$ is unitary, we have

$$\begin{aligned}\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle &= \langle\mathcal{T}(R)\varphi_{\gamma_1}|\mathcal{T}(R)\mathcal{O}_{\gamma_2}\mathcal{T}(R)^{-1}|\mathcal{T}(R)\psi_{\gamma_3}\rangle \\ &= \left\langle \sum_{\gamma_1'} \Gamma_1(R)_{\gamma_1'\gamma_1}\varphi_{\gamma_1'} \middle| \sum_{\gamma_2'} \Gamma_2(R)_{\gamma_2'\gamma_2}\mathcal{O}_{\gamma_2'} \middle| \sum_{\gamma_3'} \Gamma_3(R)_{\gamma_3'\gamma_3}\psi_{\gamma_3'} \right\rangle \\ &= \sum_{\gamma_1'\gamma_2'\gamma_3'} \bar{\Gamma}_1(R)_{\gamma_1'\gamma_1}\Gamma_2(R)_{\gamma_1'\gamma_2}\Gamma_3(R)_{\gamma_3'\gamma_3}\langle\varphi_{\gamma_1'}|\mathcal{O}_{\gamma_2'}|\psi_{\gamma_3'}\rangle \quad \text{for all } R \in G.\end{aligned} \tag{2.3}$$

If the matrix elements $\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle$ are ordered suitably in a row matrix $\mathbb{r}$, eq. (2.3) may be written compactly as

$$\mathbb{r}=\mathbb{r}[\bar{\Gamma}_1(R)\otimes\Gamma_2(R)\otimes\Gamma_3(R)] \quad \text{for all } R\in G, \tag{2.4}$$

where $\otimes$ denotes tensor (or Kronecker or direct) product of matrices. If we replace R by R^{-1} in (2.4), transpose and use the unitarity of the Γ_i, i.e. $\bar{\Gamma}_i(R^{-1})^{\mathrm{T}}=\Gamma_i(R)$, we get

$$[\Gamma_1(R)\otimes\bar{\Gamma}_2(R)\otimes\bar{\Gamma}_3(R)]\mathbb{c}=\mathbb{c} \quad \text{for all } R\in G \tag{2.5}$$

(denoting by $\mathbb{c}$ the column matrix $\mathbb{r}^{\mathrm{T}}$ obtained by transposition of $\mathbb{r}$). Eq. (2.5) may be viewed as a system of matrix equations in the unknown $\mathbb{c}$ (one equation for each group element). The dimension N of the linear space of solutions is equal to the number of times the totally symmetric (trivial 1-dimensional) irrep of G occurs in $\Gamma_1\otimes\bar{\Gamma}_2\otimes\bar{\Gamma}_3$. If $N>0$ and a basis $(\mathbb{c}_1,\ldots,\mathbb{c}_N)$ for this linear space is given, *any* column $\mathbb{c}$ satisfying (2.5) may be written in the form

$$\mathbb{c}=\sum_{\beta=1}^{N}\lambda_\beta\mathbb{c}_\beta \tag{2.6}$$

with suitable complex numbers $\lambda_1,\ldots,\lambda_N$. This, in particular, is true if $\mathbb{c}$ is the column of matrix elements introduced above. So let again $\mathbb{c}$ be this particular solution to (2.5). If we then adopt the notations

$$\begin{pmatrix}\bar{\Gamma}_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \quad \text{or} \quad (\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$$

(here, the single row arrangement has been introduced for typographical convenience) for the element of $\mathbb{c}_\beta$ corresponding to the index triple $\gamma_1\gamma_2\gamma_3$ and the notation $\langle\varphi^{\Gamma_1}\|\mathcal{O}^{\Gamma_2}\|\psi^{\Gamma_3}\rangle_\beta$ for λ_β, we see that (2.6), written in coordinates, reads

$$\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle=\sum_{\beta=1}^{N}\langle\varphi^{\Gamma_1}\|\mathcal{O}^{\Gamma_2}\|\psi^{\Gamma_3}\rangle_\beta\begin{pmatrix}\bar{\Gamma}_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \quad \text{for all } \gamma_1,\gamma_2,\gamma_3. \tag{2.7}$$

This is one form of the Wigner–Eckart theorem, the difference from some conventional forms (e.g., [11, 23, 26, 28, 29] with the page references given above) being that the "group-theoretical" or "symmetry" coefficients are the numbers $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ rather than so-called coupling coefficients (Clebsch–Gordan coefficients). The latter and the former types of coefficients and their mutual relationships will be discussed in Sect. 3, and in Sect. 5.3.3 we shall give a coupling coefficient version of the Wigner–Eckart theorem. The "physical" parameters $\langle\varphi^{\Gamma_1}\|\mathcal{O}^{\Gamma_2}\|\psi^{\Gamma_3}\rangle$ are usually called *reduced matrix elements.* If $(\mathbb{c}_1,\ldots,\mathbb{c}_N)$ is an orthonormal basis, the reduced matrix elements may be recovered from (2.6) as follows:

$$\begin{aligned}\langle\varphi^{\Gamma_1}\|\mathcal{O}^{\Gamma_2}\|\psi^{\Gamma_3}\rangle_\beta &= \lambda_\beta=\langle\mathbb{c}_\beta|\mathbb{c}\rangle\\ &= \sum_{\gamma_1\gamma_2\gamma_3}\overline{\begin{pmatrix}\bar{\Gamma}_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta}\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle \quad \text{for all } \beta.\end{aligned} \tag{2.8}$$

The statement expressed by (2.6) and (2.7) is, from a mathematical point of view, not much more than a rephrasing of the definition of the coefficients $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$. However, the theorem has great practical importance because it expresses the totality of matrix elements $\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle$ by a small number of parameters (the reduced matrix elements $\langle\varphi^{\Gamma_1}|\mathcal{O}^{\Gamma_2}\|\psi^{\Gamma_3}\rangle_\beta$), which are independent of the components γ_1, γ_2, γ_3, and the symmetry coefficients $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$, which are independent of the particular operator $\mathcal{O}_{\gamma_2}$ being studied and which may (in principle) be determined once and for all for the matrix reps $\Gamma_1, \Gamma_2, \Gamma_3$. That N is a small number, at least when the Γ_i are irreducible, follows from the estimate (3.1.4) below.

Another viewpoint on the Wigner–Eckart theorem is that it serves as a *definition of the reduced matrix elements* once the symmetry coefficients have been fixed. A fixation of the latter kind is one of the main goals for the following papers in this series. It is, of course, important to specify which version of the Wigner–Eckart theorem one has used for the definition of the reduced matrix elements in a given context. The way the group G is represented on the space V, i.e. the nature of the operator rep $\mathcal{T}$, is also important for the definition of the reduced matrix elements, cf. [32].

Remarks

The notation $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ is chosen to be in accord with the conventions usually followed in the literature and dating back to Wigner's early paper on simply reducible groups [14]. It also has the advantage of giving a convenient appearance of the Wigner–Eckart theorem, since the complex conjugation appears on Γ_1 in (2.7) just as it appears on φ_{γ_1} if the matrix element $\langle\varphi_{\gamma_1}|\mathcal{O}_{\gamma_2}|\psi_{\gamma_3}\rangle$ is written as an integral $\int \bar{\varphi}_{\gamma_1}\mathcal{O}_{\gamma_2}\psi_{\gamma_3}\,d\tau$.

These remarks seem to point to (2.4) as the natural starting-point for the subsequent discussion of the coefficients $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$. We shall, however, base our treatment on (2.5), mainly for the reason that we shall be viewing the sets of such coefficients appearing in (2.4) and (2.5) as coordinate sets for certain *vectors* ("the invariant vectors in representation space" of [14], the "invariant triple products" of [8]) – and vectors are more often handled as columns than as rows when one expresses the results of linear algebra in matrix language.

Note that the use of a scalar product which is linear in the *first* variable and conjugate linear in the *second* variable, as is common in the mathematical literature, leads to placements of the complex conjugations differing from the present ones ([28], p. 276).

We note further that it has *not* been assumed in this section that the Γ_i are irreducible. This remark may, for example, be of relevance when dealing with reducible reps of point groups of the type which has been called "most reduced with a real basis" ([20], p. 223). However, in our general study below of the coefficients $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ we shall mostly have to restrict attention to the case of irreducible Γ_i.

Most proofs of the Wigner–Eckart theorem in the literature involve Schur's lemma either directly or indirectly (e.g., [11, 24, 26, 29, 31] with page references as given above; [22], Chap. 4), for example in the form of the orthogonality relations, a fact which might lead to the suspicion that (2.7) may not be established if the Γ_i are allowed to be reducible. As we have seen, the mere *separation* into symmetry coefficients and reduced matrix elements as expressed by (2.7) does not require the Γ_i to be irreducible. However, irreducibility may be a necessary condition for the coefficients $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ to have certain desired properties. See, e.g. Sect. 3.3 for the relationship with coupling coefficients and Sect. 5.3 for the properties of the coefficients of the particular type $(\bar{\Gamma}1_G\Gamma/\gamma 0\gamma')$. The latter ones correspond to totally symmetric operators, i.e., to the case of $\Gamma_2 = 1_G$ in (2.2). The particular form of the Wigner–Eckart theorem arising for the totally symmetric operators is sometimes just called Wigner's theorem (e.g. [33], Chap. 5).

A derivation of the Wigner–Eckart theorem which comes close to the above one and in which Schur's lemma is not involved is presented in Wigner's review paper [34]. The same can be said of ([28] p. 275; [35], p. 54; [36]), but these treatments involve formulae equivalent to our (3.1.5), which is also not necessary. An extremely condensed derivation (with irreducibility assumed, but not used), equivalent to the one above, is given in [37].

Note that *no assumptions regarding the properties of the group* have been used in the above derivation. However, the restriction to finite-dimensional unitary representations in general limits the applicability of the result if G is non-compact. For a discussion of Wigner–Eckart-like theorems in various different or more general set-ups than the present one, see [38–40]. As stated in Sect. 1, we shall restrict our theory to compact groups in the rest of this paper.

3. The concept of triple coefficients; general properties

3.1. Triple coefficients

The formulation of the Wigner–Eckart theorem given in Sect. 2 shows the relevance of studying sets $\mathfrak{c}$ of numbers $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ satisfying the relation

$$[\bar{\Gamma}_1(R)\otimes\bar{\Gamma}_2(R)\otimes\bar{\Gamma}_3(R)]\mathfrak{c} = \mathfrak{c} \quad \text{for all } R\in G \tag{3.1.1}$$

or, written in coordinates,

$$\sum_{\gamma_1'\gamma_2'\gamma_3'} \bar{\Gamma}_1(R)_{\gamma_1\gamma_1'}\bar{\Gamma}_2(R)_{\gamma_2\gamma_2'}\bar{\Gamma}_3(R)_{\gamma_3\gamma_3'}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1' & \gamma_2' & \gamma_3'\end{pmatrix} = \begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}$$
$$\text{for all } \gamma_1, \gamma_2, \gamma_3 \text{ and all } R\in G, \tag{3.1.2}$$

where Γ_1, Γ_2, and Γ_3 are unitary matrix reps of the group G. Eq. (3.1.1) differs from Eq. (2.5) in having $\bar{\Gamma}_1$ instead of Γ_1. In the present section we study solutions to (3.1.1), which is the most convenient form for the discussion in Sect. 3.2 of permutational properties. In Sect. 5 we discuss the subject of complex conjugation of matrix reps, describing in detail the relationship between solutions to (3.1.1) and solutions to (2.5).

Any set $\mathfrak{c}$ of numbers satisfying (3.1.1) and (3.1.2) will be called *a set of triple coefficients for the ordered matrix rep triple* $\Gamma_1\Gamma_2\Gamma_3$. We stress at once that *no conventions* as to, e.g., sign or modulus of the individual numbers $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ are implied in the definition and that the definition is concerned only with the *ordered* triple $\Gamma_1\Gamma_2\Gamma_3$.

[Note that no assumptions have at this stage been made regarding equivalence and identity of Γ_1, Γ_2, and Γ_3; thus, for example, two of them might be equivalent without being identical. For some applications where this may be useful, see, e.g., Tables 3 and 8 of [41]. However, for the subsequent developments in this paper (the concept of 3-Γ symbols), we shall have to give up this degree of freedom.]

Sets of triple coefficients for a given triple $\Gamma_1\Gamma_2\Gamma_3$ are *simultaneously fix-vectors for all the matrices*

$$\bar{\Gamma}_1(R)\otimes\bar{\Gamma}_2(R)\otimes\bar{\Gamma}_3(R), \qquad R\in G, \tag{3.1.3}$$

i.e. eigenvectors with eigenvalue 1. The set $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ of fix-vectors is a linear space, the dimension of which we shall denote $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ or just $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$, cf. Sect. A.1.1 of the appendix. With this notation, the number N of reduced matrix elements in (2.7) is $\dim \mathscr{F}(\bar{\Gamma}_1\Gamma_2\Gamma_3)$. As already indicated in Sect. 2, $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ is equal to the number of times the totally symmetric irrep of G occurs in $\bar{\Gamma}_1\otimes\bar{\Gamma}_2\otimes\bar{\Gamma}_3$. In Sect. A.1.1 we show that *if* Γ_1, Γ_2, *and* Γ_3 *are ireducible*, then

$$\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)\leq \min\{\dim\Gamma_1, \dim\Gamma_2, \dim\Gamma_3\}, \tag{3.1.4}$$

where the right-hand side denotes the smallest number among the dimensions of Γ_1, Γ_2, and Γ_3. This estimate, as pointed out in Sect. 2, shows that the number of reduced matrix elements in general is small compared to the total number of matrix elements embodied in the left-hand side of (2.7).

For irrep triples $\Gamma_1\Gamma_2\Gamma_3$, the number $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ is called the *multiplicity* of the triple. If the multiplicity is ≤ 1, the triple is said to be *multiplicity-free.* A group whose triples are all multiplicity-free is itself said to be multiplicity-free.

We note two general properties of triple coefficients:

1° Assume that G is finite of order $|G|$. Let $N=\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ and let $(\mathfrak{c}_1,\ldots,\mathfrak{c}_N)$ be an *orthonormal* basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$. We denote by $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ the elements of the fix-column $\mathfrak{c}_\beta$ for each $\beta=1,\ldots,N$. Then for all indices $\gamma_1, \gamma_2, \gamma_3, \gamma_1', \gamma_2', \gamma_3'$ the following relation holds:

$$\sum_\beta \overline{\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta} \begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1' & \gamma_2' & \gamma_3'\end{pmatrix}_\beta = \frac{1}{|G|}\sum_{R\in G}\Gamma_1(R)_{\gamma_1\gamma_1'}\Gamma_2(R)_{\gamma_2\gamma_2'}\Gamma_3(R)_{\gamma_3\gamma_3'}. \tag{3.1.5}$$

Eq. (3.1.5) and its obvious extension to compact groups are easily proven, as demonstrated in Sect. A.2, where also the literature on this identity is commented on. Note that the Γ_i do not have to be irreducible for (3.1.5) to be valid.

2° If $\mathbb{\Gamma}_1$, $\mathbb{\Gamma}_2$, and $\mathbb{\Gamma}_3$ are *irreducible* and $(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3/\gamma_1\gamma_2\gamma_3)$ are elements of a set of triple coefficients for $\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3$, the following orthogonality relation is satisfied:

$$\sum_{\gamma_1\gamma_2} \overline{\begin{pmatrix} \mathbb{\Gamma}_1 & \mathbb{\Gamma}_2 & \mathbb{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}} \begin{pmatrix} \mathbb{\Gamma}_1 & \mathbb{\Gamma}_2 & \mathbb{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3' \end{pmatrix} = a\delta(\gamma_3, \gamma_3') \quad \text{for all } \gamma_3 \text{ and } \gamma_3', \tag{3.1.6}$$

where a is a non-negative constant. Eq. (3.1.6) is proved in the appendix, Sect. A.3. There are two more orthogonality relations (with summations over γ_2, γ_3 and γ_1, γ_3) which may be obtained, as will be clear from Sect. 4, by letting the $\mathbb{\Gamma}_i$ change rôles – see (4.2) and subsequent remarks.

3.2. Permutational properties of sets of triple coefficients

Let Γ_1, Γ_2, Γ_3 be reps of a group G with matrix forms $\mathbb{\Gamma}_1$, $\mathbb{\Gamma}_2$, $\mathbb{\Gamma}_3$. We shall be concerned with two particular situations denoted (A) and (B) below.

(A) If in the triple $\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3$ the matrix reps $\mathbb{\Gamma}_1$ and $\mathbb{\Gamma}_2$ are *identical* – whereby we mean that the matrix $\mathbb{\Gamma}_1(R)$ is *identical* to the matrix $\mathbb{\Gamma}_2(R)$ for all $R \in G$ – a representation of the symmetric group S_2 on the linear space $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ of column matrices $\mathbb{c}$ satisfying (3.1.1) may be defined in the following way: a permutation $\sigma \in S_2$ acts on a column $\mathbb{c}$ with elements $(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3/\gamma_1\gamma_2\gamma_3)$ to give the column, denoted $\sigma(\mathbb{c})$, with corresponding elements $(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3/\gamma_{\sigma^{-1}(1)}\gamma_{\sigma^{-1}(2)}\gamma_3)$.

Suppose now that $\mathbb{\Gamma}_3$ is *not* identical to $\mathbb{\Gamma}_1$. If a column $\mathbb{c}$ transforms according to the totally symmetric irrep of S_2 under the above representation, i.e. if

$$\sigma(\mathbb{c}) = \mathbb{c} \text{ for all } \sigma \in S_2, \tag{3.2.1}$$

we shall say that it is *a symmetric set of triple coefficients for the triple* $\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3$ or *a symmetric fix-vector for* $\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_3$. If a column transforms according to the alternating irrep for S_2, i.e., if

$$\sigma(\mathbb{c}) = -\mathbb{c} \text{ when } \sigma \text{ is the transposition (12) in } S_2, \tag{3.2.2}$$

we shall say that it is *an antisymmetric set of triple coefficients for the triple* $\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3$ or *an antisymmetric fix-vector for* $\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_3$.

Let $\mathscr{F}_s(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ denote the set of symmetric fix-vectors for $\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_3$ and $\mathscr{F}_a(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ the set of antisymmetric fix-vectors. These sets are mutually orthogonal subspaces of $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$, and

$$\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3) = \mathscr{F}_s(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3) \oplus \mathscr{F}_a(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3). \tag{3.2.3}$$

The asserted subspace orthogonality follows from the fact that the above rep of S_2 on $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ is unitary, i.e., $\langle\sigma(\mathbb{c}')|\sigma(\mathbb{c}'')\rangle = \langle\mathbb{c}'|\mathbb{c}''\rangle$ for all $\mathbb{c}', \mathbb{c}'' \in \mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ and all $\sigma \in S_2$. Subspaces of $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ transforming as different irreps of S_2 are thus orthogonal. Eq. (3.2.3) shows that an orthonormal basis may be chosen for $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ in which each basis vector is either symmetric or antisymmetric.

For the case of the Γ_i irreducible, we show in Sect. A.1.2 that dim $\mathscr{F}_s(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ is equal to the number of times the *symmetric* part $\Gamma_1 \otimes_s \Gamma_1$ of $\Gamma_1 \otimes \Gamma_1$ contains an irrep equivalent to $\bar{\Gamma}_3$ and that dim $\mathscr{F}_a(\mathbb{\Gamma}_1\mathbb{\Gamma}_1\mathbb{\Gamma}_3)$ is equal to the number of times the *antisymmetric* part $\Gamma_1 \otimes_a \Gamma_1$ of $\Gamma_1 \otimes \Gamma_1$ contains an irrep equivalent to $\bar{\Gamma}_3$. The resolution of $\Gamma_1 \otimes_s \Gamma_1$ and $\Gamma_1 \otimes_a \Gamma_1$ as direct sums of irreps is standard information in compilations of group theoretical tables (e.g., [42, 43] and appendices in many textbooks, including some of those cited in Sect. 2).

Definitions similar to the above ones may, of course, be given in the cases where $\Gamma_1 \neq \Gamma_2 = \Gamma_3$ or $\Gamma_1 = \Gamma_3 \neq \Gamma_2$.

(B) If in the triple $\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Gamma}_3$ all three matrix reps are identical, so that the triple is of the form $\mathbf{\Gamma\Gamma\Gamma}$, a representation of the symmetric group S_3 on $\mathcal{F}(\mathbf{\Gamma\Gamma\Gamma})$ may be defined in the following way: a permutation $\sigma \in S_3$ acts on a column $\mathbb{c}$ with elements $(\mathbf{\Gamma\Gamma\Gamma}/\gamma_1\gamma_2\gamma_3)$ to give the column, denoted $\sigma(\mathbb{c})$, with corresponding elements $(\mathbf{\Gamma\Gamma\Gamma}/\gamma_{\sigma^{-1}(1)}\gamma_{\sigma^{-1}(2)}\gamma_{\sigma^{-1}(3)})$. If a column transforms according to the totally symmetric irrep of S_3 under this representation, i.e. if

$$\sigma(\mathbb{c}) = \mathbb{c} \quad \text{for all } \sigma \in S_3, \tag{3.2.4}$$

we shall say that it is *a (fully) symmetric set of triple coefficients for the triple* $\mathbf{\Gamma\Gamma\Gamma}$ or *a (fully) symmetric fix-vector for* $\bar{\mathbf{\Gamma}} \otimes \bar{\mathbf{\Gamma}} \otimes \bar{\mathbf{\Gamma}}$. If a column $\mathbb{c}$ transforms as the alternating irrep of S_3, i.e. if

$$\sigma(\mathbb{c}) = -\mathbb{c} \quad \text{for all odd permutations } \sigma \in S_3 \tag{3.2.5}$$

(and consequently $\sigma(\mathbb{c}) = \mathbb{c}$ for all even $\sigma \in S_3$), we shall say *that it is a (fully) antisymmetric set of triple coefficients for the triple* $\mathbf{\Gamma\Gamma\Gamma}$ or *a (fully) antisymmetric fix-vector for* $\bar{\mathbf{\Gamma}} \otimes \bar{\mathbf{\Gamma}} \otimes \bar{\mathbf{\Gamma}}$.

Let $\mathcal{F}_{[3]}(\mathbf{\Gamma\Gamma\Gamma})$ denote the set of fully symmetric fix-vectors and $\mathcal{F}_{[1^3]}(\mathbf{\Gamma\Gamma\Gamma})$ the set of fully antisymmetric fix-vectors. Regarding the symbols, see Sect. A.1.2. These sets are mutually orthogonal subspaces of $\mathcal{F}(\mathbf{\Gamma\Gamma\Gamma})$, and if the two-dimensional irrep of S_3 does not occur in the decomposition of the rep of S_3 on $\mathcal{F}(\mathbf{\Gamma\Gamma\Gamma})$ just described, we have

$$\mathcal{F}(\mathbf{\Gamma\Gamma\Gamma}) = \mathcal{F}_{[3]}(\mathbf{\Gamma\Gamma\Gamma}) \oplus \mathcal{F}_{[1^3]}(\mathbf{\Gamma\Gamma\Gamma}). \tag{3.2.6}$$

In this situation, an orthonormal basis may be chosen for $\mathcal{F}(\mathbf{\Gamma\Gamma\Gamma})$ in which each basis vector is either a fully symmetric fix-vector or a fully antisymmetric fix-vector.

When (3.2.6) is satisfied, the rep $\mathbf{\Gamma}$ is said to be *simple phase.* If all irreps of a finite or compact group G are simple phase, the group itself is said to be simple phase.

[The term "simple phase" was coined by van Zanten and de Vries [44] (see also [45]), but the concept was already inherent in Derome's papers [16, 46]. See the review [17] and the discussion in Sect. 4.]

For the case of Γ *irreducible and simple phase,* we show in Sect. A.1.2 that $\dim \mathcal{F}_{[3]}(\mathbf{\Gamma\Gamma\Gamma})$ is equal to the number of times the *symmetric* part $\Gamma \otimes_s \Gamma$ of $\Gamma \otimes \Gamma$ contains an irrep equivalent to $\bar{\Gamma}$ and that $\dim \mathcal{F}_{[1^3]}(\mathbf{\Gamma\Gamma\Gamma})$ is equal to the number of times the *antisymmetric* part $\Gamma \otimes_a \Gamma$ of $\Gamma \otimes \Gamma$ contains an irrep equivalent to $\bar{\Gamma}$.

3.3. The relationship between triple coefficients and coupling coefficients (Clebsch–Gordan coefficients)

We start with the following observation: if $\mathbb{\Gamma}_1$, $\mathbb{\Gamma}_2$, and $\mathbb{\Delta}$ are unitary matrix *irreps* of dimensions d_1, d_2, and d of a group G and we have a non-zero set of triple coefficients $(\bar{\Gamma}_1\bar{\Gamma}_2\Delta/\gamma_1\gamma_2\delta)$ for the ordered triple $\bar{\Gamma}_1\bar{\Gamma}_2\Delta$, the defining relation

$$\sum_{\gamma_1'\gamma_2'\delta'} \mathbb{\Gamma}_1(R)_{\gamma_1\gamma_1'}\mathbb{\Gamma}_2(R)_{\gamma_2\gamma_2'}\bar{\mathbb{\Delta}}(R)_{\delta\delta'}\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Delta\\ \gamma_1' & \gamma_2' & \delta'\end{pmatrix}=\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Delta\\ \gamma_1 & \gamma_2 & \delta\end{pmatrix}$$

for all γ_1, γ_2, δ, (3.3.1)

cf. Eq. (3.1.2), may be written, using the unitarity of $\mathbb{\Delta}$, as

$$\sum_{\gamma_1'\gamma_2'}\sum_{\delta'}[\mathbb{\Gamma}_1(R)_{\gamma_1\gamma_1'}\mathbb{\Gamma}_2(R)_{\gamma_2\gamma_2'}]\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Delta\\ \gamma_1' & \gamma_2' & \delta'\end{pmatrix}\mathbb{\Delta}(R^{-1})_{\delta'\delta}=\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Delta\\ \gamma_1 & \gamma_2 & \delta\end{pmatrix}$$

for all γ_1, γ_2, δ. (3.3.2)

Eq. (3.3.2) tells that if we form a d_1d_2 by d matrix $\mathbb{C}(\Gamma_1\Gamma_2|\Delta)$ from the numbers $(\bar{\Gamma}_1\bar{\Gamma}_2\Delta/\gamma_1\gamma_2\delta)$, using $\gamma_1\gamma_2$ as a row index and δ as a column index (with a suitable ordering), then this matrix satisfies

$$[\mathbb{\Gamma}_1(R)\otimes\mathbb{\Gamma}_2(R)]\mathbb{C}(\Gamma_1\Gamma_2|\Delta)\mathbb{\Delta}(R^{-1})=\mathbb{C}(\Gamma_1\Gamma_2|\Delta)\quad \text{for all } R\in G, \tag{3.3.3}$$

that is,

$$[\mathbb{\Gamma}_1(R)\otimes\mathbb{\Gamma}_2(R)]\mathbb{C}(\Gamma_1\Gamma_2|\Delta)=\mathbb{C}(\Gamma_1\Gamma_2|\Delta)\mathbb{\Delta}(R)\quad \text{for all } R\in G. \tag{3.3.4}$$

Property (3.3.4) motivates the choice of the particular symbol $\mathbb{C}(\Gamma_1\Gamma_2|\Delta)$. In mathematical terminology, this matrix *intertwines* the reps $\mathbb{\Gamma}_1\otimes\mathbb{\Gamma}_2$ and $\mathbb{\Delta}$.

We then turn to the situation relevant for the introduction of coupling coefficients: Assume again that $\mathbb{\Gamma}_1$ and $\mathbb{\Gamma}_2$ are unitary matrix irreps of G and let $\mathbb{\Delta}_1, \ldots, \mathbb{\Delta}_p$ be unitary matrix irreps of G such that $\mathbb{\Gamma}_1\otimes\mathbb{\Gamma}_2$ is equivalent to the direct sum of the $\mathbb{\Delta}_i$, i.e., equivalent to the rep with the diagonal block rep matrices

$$\begin{bmatrix}\mathbb{\Delta}_1(R) & & & 0\\ & \mathbb{\Delta}_2(R) & & \\ & & \ddots & \\ 0 & & & \mathbb{\Delta}_p(R)\end{bmatrix},\qquad R\in G. \tag{3.3.5}$$

Here, some of the $\mathbb{\Delta}_i$ may be equivalent irreps; if any two of the $\mathbb{\Delta}_i$ are equivalent, they are assumed to be *identical.* Let us carry out the construction of a matrix $\mathbb{C}_i=\mathbb{C}(\Gamma_1\Gamma_2|\Delta_i)$ as above for each $\mathbb{\Delta}_i$ in the following way: If a particular irrep $\mathbb{\Delta}$ occurs exactly N times in (3.3.5), the dimension of the fix-space $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\Delta)$ is also N (cf. Sect. A.1.1). We then use the columns of an N-element orthogonal basis for $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\Delta)$ for the construction of the N required matrices $\mathbb{C}(\Delta_1\Delta_2|\Delta)$. Finally, we form a d_1d_2 by d_1d_2 matrix $\mathbb{C}$ by juxtaposing the $\mathbb{C}_i$:

$$\mathbb{C}=(\mathbb{C}_1\quad \mathbb{C}_2\cdots\mathbb{C}_p). \tag{3.3.6}$$

Then from (3.3.4), we have

$$[\mathbf{\Gamma}_1(R)\otimes\mathbf{\Gamma}_2(R)]\mathbb{C}=\mathbb{C}\begin{bmatrix}\mathbf{\Delta}_1(R) & & 0\\ & \mathbf{\Delta}_2(R) & \\ & & \ddots & \\ 0 & & & \mathbf{\Delta}_p(R)\end{bmatrix}\quad \text{for all } R\in G. \tag{3.3.7}$$

We see now that we are approaching the concept of coupling coefficients. We need to know a little more about the matrix $\mathbb{C}$. In Sect. A.3, we prove, using the assumed irreducibility of the $\mathbf{\Delta}_i$, that the columns of $\mathbb{C}$ form an orthogonal set of non-zero vectors. This has the particular implication that $\mathbb{C}$ is nonsingular so that (3.3.7) may be rearranged to

$$\mathbb{C}^{-1}[\mathbf{\Gamma}_1(R)\otimes\mathbf{\Gamma}_2(R)]\mathbb{C}=\begin{bmatrix}\mathbf{\Delta}_1(R) & & 0\\ & \mathbf{\Delta}_2(R) & \\ 0 & & \mathbf{\Delta}_p(R)\end{bmatrix}\quad \text{for all } R\in G. \tag{3.3.8}$$

Actually, it is seen from the investigation of $\mathbb{C}$ in Sect. A.3 that if triple coefficients $\sqrt{\dim \mathbf{\Delta}_i}(\bar{\mathbf{\Gamma}}_1\bar{\mathbf{\Gamma}}_2\mathbf{\Delta}_i/\gamma_1\gamma_2\delta_i)$ with the $(\bar{\mathbf{\Gamma}}_1\bar{\mathbf{\Gamma}}_2\mathbf{\Delta}_i/\gamma_1\gamma_2\delta_i)$ satisfying the normalization condition

$$\sum_{\gamma_1\gamma_2\delta_i}\left|\begin{pmatrix}\bar{\mathbf{\Gamma}}_1 & \bar{\mathbf{\Gamma}}_2 & \mathbf{\Delta}_i\\ \gamma_1 & \gamma_2 & \delta_i\end{pmatrix}\right|^2=1 \tag{3.3.9}$$

are used in the construction of the matrices $\mathbb{C}_i$, the matrix $\mathbb{C}$ becomes *unitary*. In this case it would be in full accord with tradition to call the elements of $\mathbb{C}$ *coupling coefficients* (or *Clebsch–Gordan coefficients*).

[A recent author [47] has introduced a slight distinction between coupling and Clebsch–Gordan coefficients; we shall, however, in accord with tradition and [17] use the two terms interchangeably.]

If in case of repeated irreps $\mathbf{\Delta}$ in the diagonal form (3.3.5) we distinguish triple coefficients from the different sets used to construct the several matrices $\mathbb{C}_i$ with $\mathbf{\Delta}_i=\mathbf{\Delta}$ by an index β, thus writing $(\bar{\mathbf{\Gamma}}_1\bar{\mathbf{\Gamma}}_2\mathbf{\Delta}/\gamma_1\gamma_2\delta)_\beta$, we shall denote the corresponding elements of $\mathbb{C}$ as $\langle\mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2|\beta\mathbf{\Delta}\delta\rangle$, which is the traditional coupling coefficient notation, except that boldface rep symbols are used here. The two formulae

$$\sum_{\gamma_1\gamma_2\delta}\left|\begin{pmatrix}\bar{\mathbf{\Gamma}}_1 & \bar{\mathbf{\Gamma}}_2 & \mathbf{\Delta}\\ \gamma_1 & \gamma_2 & \delta\end{pmatrix}_\beta\right|^2=1 \tag{3.3.10}$$

and

$$\langle\mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2|\beta\mathbf{\Delta}\delta\rangle=\varphi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)\sqrt{\dim\mathbf{\Delta}}\begin{pmatrix}\bar{\mathbf{\Gamma}}_1 & \bar{\mathbf{\Gamma}}_2 & \mathbf{\Delta}\\ \gamma_1 & \gamma_2 & \delta\end{pmatrix}_\beta, \tag{3.3.11}$$

where $\varphi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)$ for each $\mathbf{\Delta}$ and each β is a phase factor (complex number with modulus 1), thus show how normalized triple coefficients may be used for the construction of coupling coefficients. Given the triple coefficients, the easiest choice for the phase factor is, of course, to take always $\varphi(\Gamma_1\Gamma_2\Delta\beta)=1$ (the "sensible" choice of Butler [17]); however, in Sect. 5.3 we shall suggest and justify another convention for the case of triple coefficients forming sets of 3-Γ symbols.

4. 3-Γ symbols

The preceding sections have shown that triple coefficients (Sect. 3.1) are natural group representation-theoretic quantities to require for applications of the Wigner–Eckart theorem (Sect. 2) and may also be used for the construction of coupling coefficients (Sect. 3.3). However, for practical reasons – rather than from fundamental necessity – the concept of 3-Γ symbols will now be introduced. This concept, by imposing restrictions on the relations between triple coefficients for certain different ordered irrep triples, enables a *reduction in* the *space needed for* the *tabulation* of triple coefficients and facilitates manipulations with triple coefficients. The introduction of 3-Γ symbols may also be viewed as the introduction of a natural *partial standardization* of triple coefficients since absolute values – at least for multiplicity-free triples – and certain relative phases are hereby fixed. Further standardizations will be discussed in Sect. 5 and, for specific groups, in the following papers.

The properties of 3-Γ symbols are compactly expressed in formulae (4.11) and (4.12) below; the present section is mainly concerned with a thorough treatment of the background for these formulae. Readers who have a working knowledge of 3-Γ symbols may skip this more general discussion and proceed to Sect. 5. The general literature on 3-Γ symbols is commented on at the end of the present section.

We stress that the developments of this section do not lead to the dismission of the concept of triple coefficients; see the remarks at the end of the section.

Three matrix reps $\mathbb{\Gamma}_1, \mathbb{\Gamma}_2, \mathbb{\Gamma}_3$ of a group G may give rise to up to six distinct ordered triples $\mathbb{\Gamma}_{\sigma(1)}\mathbb{\Gamma}_{\sigma(2)}\mathbb{\Gamma}_{\sigma(3)}$, where σ runs through the permutations in the symmetric group S_3. While Sect. 3.2 was concerned with permutational properties of sets of triple coefficients for *fixed* ordered matrix rep triples, we here consider possible relationships between triple coefficients for *different* ordered triples and the interplay between such relationships and the permutational properties of the individual triple coefficient sets. We may also say that in Sect. 3.2, the role of the symmetric group was *dictated* by the nature of the situation considered; here we *choose* – with the above motivation – to let the symmetric group impose further conditions on the triple coefficients.

Irrespective of possible identity of two or three of the $\mathbb{\Gamma}_i$, we may define *a family of fix-vectors for the unordered triple* $\{\mathbb{\Gamma}_1, \mathbb{\Gamma}_2, \mathbb{\Gamma}_3\}$ to be a set $\{\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} | \sigma \in S_3\}$ consisting of six column vectors $\mathbb{c}_{123}, \mathbb{c}_{231}, \mathbb{c}_{312}, \mathbb{c}_{213}, \mathbb{c}_{132}, \mathbb{c}_{321}$ with the property that

$$[\bar{\mathbb{\Gamma}}_{\sigma(1)}(R) \otimes \bar{\mathbb{\Gamma}}_{\sigma(2)}(R) \otimes \bar{\mathbb{\Gamma}}_{\sigma(3)}(R)]\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} = \mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} \quad \text{for all } R \in G \tag{4.1}$$

for each of the six $\sigma \in S_3$. Here the index triples $\sigma(1)\sigma(2)\sigma(3)$ are not to be confused with the index β of previous sections where a basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ was chosen. For a given σ, the fix-vector $\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)}$ may of course be a member of a basis for $\mathscr{F}(\Gamma_{\sigma(1)}\Gamma_{\sigma(2)}\Gamma_{\sigma(3)})$, but we are not concerned with the obtainment of such bases right now.

For any $\sigma \in S_3$, Eq. (3.1.2) is equivalent to

$$\sum_{\gamma_1'\gamma_2'\gamma_3'} \bar{\Gamma}_{\sigma(1)}(R)_{\gamma_{\sigma(1)}\gamma'_{\sigma(1)}} \bar{\Gamma}_{\sigma(2)}(R)_{\gamma_{\sigma(2)}\gamma'_{\sigma(2)}} \bar{\Gamma}_{\sigma(3)}(R)_{\gamma_{\sigma(3)}\gamma'_{\sigma(3)}} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2' & \gamma_3' \end{pmatrix} = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}$$

for all γ_1, γ_2, γ_3 and all $R \in G$. (4.2)

Here we have just permuted the factors within each term in the sum. Eq. (4.2) shows that if $\mathbb{c}_{123}$ is a fix-vector for $\Gamma_1\Gamma_2\Gamma_3$, a fix-vector $\sigma(\mathbb{c}_{123})$ for $\Gamma_{\sigma(1)}\Gamma_{\sigma(2)}\Gamma_{\sigma(3)}$ is immediately obtained by defining the $\gamma_{\sigma(1)}\gamma_{\sigma(2)}\gamma_{\sigma(3)}$-th element of $\sigma(\mathbb{c}_{123})$ to be $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$. This prescription gives a mapping σ from $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ onto $\mathscr{F}(\Gamma_{\sigma(1)}\Gamma_{\sigma(2)}\Gamma_{\sigma(3)})$. In the cases where two or three of the Γ_i are identical, this prescription agrees with the ones for mappings σ of $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ onto itself in Sect. 3.2.

Thus, an obvious way of constructing a family of fix-vectors $\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)}$ from the fix-vector $\mathbb{c}_{123}$ would be by putting

$$\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} = \sigma(\mathbb{c}_{123}) \quad \text{for every } \sigma \in S_3. \tag{4.3}$$

Since a scalar multiple of a fix-vector is a fix-vector, we could, slightly more generally, put

$$\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} = \varphi_\sigma \sigma(\mathbb{c}_{123}) \quad \text{for every } \sigma \in S_3, \tag{4.4}$$

where the φ_σ are non-zero numbers depending on σ.

It is natural to require that the φ_σ are related in such a way that if $\sigma = \rho\tau$, where $\sigma, \rho, \tau \in S_3$, we can find $\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)}$ as $\varphi_\rho\varphi_\tau\rho\tau(\mathbb{c}_{123})$. Equating these last two expressions and using (4.4), we get

$$\varphi_\sigma\sigma(\mathbb{c}_{123}) = \mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} = \varphi_\rho\varphi_\tau\sigma(\mathbb{c}_{123}), \tag{4.5}$$

which (for $\mathbb{c}_{123}$ non-zero) implies $\varphi_\sigma = \varphi_\rho\varphi_\tau$. Thus the requirement is that the numbers φ_σ with σ running through S_3 form a *representation* (necessarily one-dimensional and hence irreducible) of S_3. Now, S_3 has two one-dimensional irreps, the characters of which we shall denote $\chi_{[3]}$ (the totally symmetric irrep) and $\chi_{[1^3]}$ (the alternating irrep). Regarding this notation, see Sect. A.1.2.

We shall say that the family $\{\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} | \sigma \in S_3\}$ defined by (4.4) is *an even family of fix-vectors for* $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ if $\varphi_\sigma = \chi_{[3]}(\sigma)$ for all $\sigma \in S_3$, i.e. if

$$\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)} = \sigma(\mathbb{c}_{123}) \quad \text{for all } \sigma \in S_3. \tag{4.6}$$

We shall say that the family $\{\mathfrak{c}_{\sigma(1)\sigma(2)\sigma(3)} | \sigma \in S_3\}$ defined by (4.4) is *an odd family of fix-vectors for* $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ if $\varphi_\sigma = \chi_{[1^3]}(\sigma)$ for all $\sigma \in S_3$, i.e., if

$$\mathfrak{c}_{\sigma(1)\sigma(2)\sigma(3)} = \sigma(\mathfrak{c}_{123}) \quad \text{for all even } \sigma \in S_3$$

and (4.7)

$$\mathfrak{c}_{\sigma(1)\sigma(2)\sigma(3)} = -\sigma(\mathfrak{c}_{123}) \quad \text{for all odd } \sigma \in S_3.$$

In the following, we shall only consider even and odd families of fix-vectors, but – as noted by Griffith [1, p. 11] – this is not necessary and, in principle, might be too restrictive in some cases.

Suppose now that $\Gamma_1 = \Gamma_2 = \Gamma_3 = \Gamma$, that is, we have the situation from (B) in Sect. 3.2. A symmetric fix-vector $\mathfrak{c}_{123}$ for $\bar{\Gamma}_1 \otimes \bar{\Gamma}_2 \otimes \bar{\Gamma}_3 = \bar{\Gamma} \otimes \bar{\Gamma} \otimes \bar{\Gamma}$ according to the definition given there has the property

$$\sigma(\mathfrak{c}_{123}) = \chi_{[3]}(\sigma)\mathfrak{c}_{123} \quad \text{for all } \sigma \in S_3. \tag{4.8}$$

An antisymmetric fix-vector for $\bar{\Gamma}_1 \otimes \bar{\Gamma}_2 \otimes \bar{\Gamma}_3 = \bar{\Gamma} \otimes \bar{\Gamma} \otimes \bar{\Gamma}$ has the property

$$\sigma(\mathfrak{c}_{123}) = \chi_{[1^3]}(\sigma)\mathfrak{c}_{123} \quad \text{for all } \sigma \in S_3. \tag{4.9}$$

This means that if $\mathfrak{c}_{123}$ is either symmetric or antisymmetric, then by constructing the family $\{\mathfrak{c}_{\sigma(1)\sigma(2)\sigma(3)} | \sigma \in S_3\}$ according to (4.4) we get a set of mutually *proportional* vectors. Since there is no particular reason to have several proportional fix-vectors for a given *ordered* triple, *in casu* $\bar{\Gamma}\bar{\Gamma}\bar{\Gamma}$, we require that

$$\mathfrak{c}_{123} = \mathfrak{c}_{\sigma(1)\sigma(2)\sigma(3)} = \varphi_\sigma \sigma(\mathfrak{c}_{123}) \quad \text{for all } \sigma \in S_3. \tag{4.10}$$

Eqs. (4.4); (4.8) or (4.9), whichever is relevant; and (4.10) may all be fulfilled *if and only if* we choose $\varphi_\sigma = \chi_{[3]}(\sigma)$ for all σ if $\mathfrak{c}_{123}$ is symmetric and $\varphi_\sigma = \chi_{[1^3]}(\sigma)$ for all σ if $\mathfrak{c}_{123}$ is antisymmetric.

Similar remarks apply in cases where $\Gamma_1 = \Gamma_2 \neq \Gamma_3$, $\Gamma_1 \neq \Gamma_2 = \Gamma_3$, or $\Gamma_1 = \Gamma_3 \neq \Gamma_2$, cf. part (A) of Sect. 3.2. Here we initially only get a fixation of φ_σ when σ is the relevant transposition ($\sigma = (12)$ for $\Gamma_1 = \Gamma_2 \neq \Gamma_3$ etc.), but the restriction to even and odd families – or, equivalently, the requirement (4.5) – then fixes all φ_σ.

The preceding observations form a main part of the motivation for the following central definition:

A 3-Γ *family* (of fix-vectors) *for an unordered triple* $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ has the following properties:

(i) The family is either *even* or *odd.* If two or three of the Γ_i are identical, it is either an *even* family of *symmetric* fix-vectors or an *odd* family of *antisymmetric* fix-vectors.
(ii) Each fix-vector is a unit vector.

The totality of triple coefficients embodied in the fix-vectors of a 3-Γ family will be called *a set of 3-Γ symbols for the unordered triple* $\{\Gamma_1, \Gamma_2, \Gamma_3\}$.

From the discussion leading to the definition it is seen that if the elements of a fix-vector $\mathbb{c}_{123}$ in a 3-$\mathbb{\Gamma}$ family are denoted $(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3/\gamma_1\gamma_2\gamma_3)$, and if σ is a permutation, the symbol $(\mathbb{\Gamma}_{\sigma(1)}\mathbb{\Gamma}_{\sigma(2)}\mathbb{\Gamma}_{\sigma(3)}/\gamma_{\sigma(1)}\gamma_{s(2)}\gamma_{\sigma(3)})$ obtained by applying the permutation σ to the columns of $(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3/\gamma_1\gamma_2\gamma_3)$, may be used consistently to denote the elements of $\mathbb{c}_{\sigma(1)\sigma(2)\sigma(3)}$, which is *a priori* a fix-vector independent of $\mathbb{c}_{123}$, *as well* as the elements of $\mathbb{c}_{123}$ itself in case two or three of the $\mathbb{\Gamma}_i$ are identical.

If for a given group, *standard* unitary matrix irreps have been chosen – that is, a unitary matrix irrep is distinguished in each irrep equivalence class – and sets of 3-$\mathbb{\Gamma}$ symbols have been chosen for the various unordered standard irrep triples, the individual elements of the fix-vectors are traditionally given the simplified notation $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ – that is, no boldface symbols are used – and are called just *3-Γ symbols.* We suggest that this notation *only* be used in such well-specified situations. (In Sect. 5.3, we shall discuss 3-Γ symbols involving the complex conjugates of standard irreps.)

If a triple $\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3$ has multiplicity, (Sect. 3.1), the unordered triple may have several 3-$\mathbb{\Gamma}$ families which are independent in the sense that they correspond to linearly independent fix-vectors for any given one of the *ordered* triples. In such cases the index β, which we dropped at the beginning of this section, will be used to distinguish among the several families, giving the notation $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ for the individual elements of the fix-vectors.

For any given set of 3-Γ symbols $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$, we shall define a symbol $\pi(\Gamma_1\Gamma_2\Gamma_3\beta)$ by putting $\pi(\Gamma_1\Gamma_2\Gamma_3\beta)=+1$ if the 3-$\mathbb{\Gamma}$ family is *even* and putting $\pi(\Gamma_1\Gamma_2\Gamma_3\beta)=-1$ if it is *odd.* This phase will be called the *permutational characteristic* or the *transposition phase of* $\Gamma_1\Gamma_2\Gamma_3\beta$.

The properties (i) and (ii) may then be stated as follows:

$$\text{(i)}\ \begin{pmatrix}\Gamma_{\sigma(1)} & \Gamma_{\sigma(2)} & \Gamma_{\sigma(3)}\\ \gamma_{\sigma(1)} & \gamma_{\sigma(2)} & \gamma_{\sigma(3)}\end{pmatrix}_\beta = \pi(\Gamma_1\Gamma_2\Gamma_3\beta)\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \quad \text{for all odd } \sigma\in S_3 \tag{4.11}$$

$$\text{(ii)}\ \sum_{\gamma_1\gamma_2\gamma_3}\left|\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta\right|^2 = 1. \tag{4.12}$$

With the Γ_i irreducible, we can combine (3.1.6) with (4.12) to obtain

$$\sum_{\gamma_1\gamma_2}\overline{\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}}_\beta\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3'\end{pmatrix}_\beta = (\dim\Gamma_3)^{-1}\delta(\gamma_3,\gamma_3'). \tag{4.13}$$

Again, there are two more formulas (with summations over γ_2, γ_3 and γ_1, γ_3 respectively).

The reader will have noticed the extensive use we have made here of the words "set" and "family". This is done in order to avoid the conceptual difficulties associated with individualizing terms like "triple coefficient", "coupling coefficient", and "3-Γ symbol". Strictly speaking, it is of course meaningless to state that a single given number is, say, a triple coefficient. On the other hand, (4.11) does give some justification to expressions like "an even 3-Γ symbol" or "an odd 3-Γ symbol" and indeed to the word "symbol" itself. Because of this and in order to conform to tradition we have retained the "symbol" terminology.

From the discussion in the present section and from (B) in Sect. 3.2 it is seen that a finite (or, generally, compact) group has a complete set of 3-Γ families if and only if it is *simple phase*. The first to draw attention to this fact seems to have been Derome [15, 16, 46], who showed that SU(3) is simple phase [46] and pointed out that the symmetric group S_6 is not [16] and later showed that SU(4) is not either [48]. Van Zanten and de Vries [49] gave criteria for a group to be simple phase; see Sect. A.1.2 for one such criterion. All specific groups to be considered in the present series of papers are simple phase.

Remarks

The definition of 3-Γ symbols given above has not appeared in the present form in the literature before, but it is consistent with previous definitions [20, 50, 51]. The 3-*j* symbols of Wigner for simply reducible groups [14], in particular the rotation (double) group (cf. Sect. 6), the $\bar{V}$ coefficients of (among others) Fano and Racah [8] and Griffith [1] and the $\bar{f}$ coefficients [18, 52] of Kibler are all particular examples of 3-Γ symbols. For more information on the literature, see the reviews by Butler [17] and Kibler [18]. Unfortunately, the general 3-*j* symbols of Derome and Sharp for arbitrary compact groups [15, 46], later called 3-*jm* symbols by Butler [17, 22], are not assumed to have the property (i) above and thus, in our opinion, do not really deserve the designation "symbol".

Regarding our use of "Γ" rather than "*j*", for irreps in general, we note that it is practical for our discussion in the following papers to only use the term "3-*j* symbols" for the conventional choice of 3-Γ symbols for the rotation double group (Sect. 6).

The permutational characteristic π defined just before (4.11) is called a 3-*j* phase in [22].

Although we have now introduced the concept of 3-Γ symbols, we shall still be needing the more general concept of triple coefficients – even though all groups to be considered are simple phase. For one thing, we shall work with triple coefficients in the first part of Sect. 5, because this gives us a convenient means of discussing the problems of complex conjugation of irreps completely without implications for – or even associations to – permutational properties. Secondly, there are situations where one rather naturally gets involved with fix-vectors for irrep triples with two or three identical irreps which are neither symmetric nor antisymmetric; clearly, the concept of 3-Γ symbols is too restricted for the discussion of such cases. An example is the triple UT_2U in the group O^* (paper V).

The reader interested in alternative descriptions of the mathematics of the permutation symmetries treated in this section may refer to [53].

5. Complex conjugation of irreducible representations; conventions for triple coefficients, 3-Γ symbols, and coupling coefficients

5.1. Introduction

In Sect. 3 we discussed general properties of triple coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$. In Sect. 2 we saw that for application in the Wigner–Eckart theorem one needs coefficients of the form $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$, and in Sect. 3.3 it was demonstrated that coefficients of the form $(\bar{\Gamma}_1\bar{\Gamma}_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ are relevant for the construction of coupling coefficients. Thus, if we have a group with a complete system of standard unitary matrix irreps Γ and if we have at our disposal triple coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ for all ordered standard irrep triples $\Gamma_1\Gamma_2\Gamma_3$, we want to know how to get from $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ to triple coefficients of the forms $(\bar{\Gamma}_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ and $(\bar{\Gamma}_1\bar{\Gamma}_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$. In fact, a given triple of standard matrix irreps $\Gamma_1\Gamma_2\Gamma_3$ is associated, through complex conjugations, with 7 (not necessarily distinct) matrix irrep triples, for all of which we wish to obtain triple coefficients, if possible on the basis of coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ for the unconjugated triple. This totality of 8 triples is displayed in (5.1.1).

$$\begin{array}{ccccc} & \bar{\Gamma}_1\Gamma_2\Gamma_3 & \text{---}\,\mathbb{B}^1\,\text{---} & \Gamma_1\bar{\Gamma}_2\bar{\Gamma}_3 & \\ & \Gamma_1\bar{\Gamma}_2\Gamma_3 & \text{---}\,\mathbb{B}^2\,\text{---} & \bar{\Gamma}_1\Gamma_2\bar{\Gamma}_3 & \\ & \Gamma_1\Gamma_2\bar{\Gamma}_3 & \text{---}\,\mathbb{B}^3\,\text{---} & \bar{\Gamma}_1\bar{\Gamma}_2\Gamma_3 & \\ \Gamma_1\Gamma_2\Gamma_3 & \text{------} & \mathbb{A} & \text{------} & \bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3 \end{array} \tag{5.1.1}$$

The symbols $\mathbb{A}$, $\mathbb{B}^1$, $\mathbb{B}^2$, and $\mathbb{B}^3$ will be explained in Sect. 5.4, where further aspects of (5.1.1) are discussed.

Now, if a given standard matrix irrep Γ_i occurring in (5.1.1) is *not* equivalent to its complex conjugate, then $\bar{\Gamma}_i$ is itself among the standard irreps – assuming that the system of standard matrix irreps has been chosen in such a way that *complex conjugate irreps actually occur in complex conjugate matrix forms. This we shall always assume.* (Although of course a restriction on the generality of the Wigner–Racah algebra developed, this convention entails considerable simplifications in notation and formalism.) Thus, the interesting irreps in connection with (5.1.1) are those which are equivalent to their complex conjugate.

Observe, then, that equivalence of a unitary matrix irrep Γ and its complex conjugate $\bar{\Gamma}$ implies the existence of a unitary matrix $\mathbb{U}$ such that

$$\mathbb{U}\Gamma(R)\mathbb{U}^{-1} = \bar{\Gamma}(R) \quad \text{for all } R \in G, \tag{5.1.2}$$

cf. [54, note 11]. A unitary matrix $\mathbb{U}$ satisfying (5.1.2) will be called here *a conjugating matrix* for Γ. In mathematical terminology, the matrix $\mathbb{U}$ *intertwines* Γ and $\bar{\Gamma}$. We note at once that if $\mathbb{U}$ is a conjugating matrix for Γ, the matrices $\bar{\mathbb{U}}$ and $\mathbb{U}^{-1}$ are both conjugating matrices for $\bar{\Gamma}$.

Now, suppose $\mathbb{c}$ is a column set of triple coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)$ for $\Gamma_1\Gamma_2\Gamma_3$, and $\mathbb{U}_1$ is a conjugating matrix for Γ_1. Then the column matrix $[\mathbb{U}_1^{-1}\otimes\mathbb{1}_2\otimes\mathbb{1}_3]\mathbb{c}$, where $\mathbb{1}_2$ and $\mathbb{1}_3$ are unit matrices of dimensions $\dim\Gamma_1$ and $\dim\Gamma_3$, respectively, will be a fix-vector for $\Gamma_1 \otimes \bar{\Gamma}_2 \otimes \bar{\Gamma}_3$, so that its elements may be used as triple coefficients $(\bar{\Gamma}_1 \Gamma_2 \Gamma_3 / \gamma_1 \gamma_2 \gamma_3)$. This is seen from the following calculation:

$$\begin{aligned}
&[\Gamma_1(R) \otimes \bar{\Gamma}_2(R) \otimes \bar{\Gamma}_3(R)][\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3]\mathbb{c} \\
&\quad = [(\mathbb{U}_1^{-1}\mathbb{U}_1 \Gamma_1(R) \mathbb{U}_1^{-1}) \otimes \bar{\Gamma}_2(R) \otimes \bar{\Gamma}_3(R)]\mathbb{c} \\
&\quad = [\mathbb{U}_1^{-1} \bar{\Gamma}_1(R) \otimes \bar{\Gamma}_2(R) \otimes \bar{\Gamma}_3(R)]\mathbb{c} \\
&\quad = [\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3][\bar{\Gamma}_1(R) \otimes \bar{\Gamma}_2(R) \otimes \bar{\Gamma}_3(R)]\mathbb{c} \\
&\quad = [\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3]\mathbb{c} \quad \text{for all } R \in G.
\end{aligned} \tag{5.1.3}$$

If we denote the elements of $\mathbb{U}_1$ as $u_1(\gamma_1, \gamma_1')$ and those of $\mathbb{U}_1^{-1}$ as $\check{u}_1(\gamma_1, \gamma_1')$ and *if we agree* to use the elements of $[\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3]\mathbb{c}$ as triple coefficients of the form $(\bar{\Gamma}_1 \Gamma_2 \Gamma_3 / \gamma_1 \gamma_2 \gamma_3)$, we get the following formula:

$$\begin{aligned}
\begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} &= \sum_{\gamma_1'} \check{u}_1(\gamma_1, \gamma_1') \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2 & \gamma_3 \end{pmatrix} \\
&= \sum_{\gamma_1'} \overline{u_1(\gamma_1', \gamma_1)} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2 & \gamma_3 \end{pmatrix},
\end{aligned} \tag{5.1.4}$$

using the unitarity of $\mathbb{U}_1$. similarly, if $\mathbb{U}_1$ and $\mathbb{U}_2$ are conjugating matrices for Γ_1 and Γ_2, respectively, and $\mathbb{c} \in \mathscr{F}(\Gamma_1 \Gamma_2 \Gamma_3)$, we get $[\mathbb{U}_1^{-1} \otimes \mathbb{U}_2^{-1} \otimes \mathbb{1}_3]\mathbb{c} \in \mathscr{F}(\bar{\Gamma}_1 \bar{\Gamma}_2 \Gamma_3)$ and thus the formula

$$\begin{aligned}
\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} &= \sum_{\gamma_1' \gamma_2'} \check{u}_1(\gamma_1, \gamma_1') \check{u}_2(\gamma_2, \gamma_2') \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2' & \gamma_3 \end{pmatrix} \\
&= \sum_{\gamma_1' \gamma_2'} \overline{u_1(\gamma_1', \gamma_1)}\, \overline{u_2(\gamma_2', \gamma_2)} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2' & \gamma_3 \end{pmatrix}.
\end{aligned} \tag{5.1.5}$$

We stress that (5.1.4) and (5.1.5), when the conjugating matrices are given, are *definitions* which we adopt for the triple coefficients on the left-hand sides; the reasons for adopting exactly *these* definitions will become apparent in the following.

If we have fixed a conjugating matrix $\mathbb{U}$ for a *standard* unitary matrix irrep Γ, we shall make use of the above observation and take $\mathbb{U}^{-1}$ as our conjugating matrix for the complex conjugate matrix irrep $\bar{\Gamma}$. This convention ensures that we can operate consistently with *double conjugations* by just removing them, *e.g.*, we obtain formulae like

$$\begin{pmatrix} \bar{\bar{\Gamma}}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \tag{5.1.6}$$

(to see this, refer to calculation (5.1.3) and note that $\mathbb{c} = [\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3]\mathbb{c} = [(\mathbb{U}^{-1})^{-1}\mathbb{U}^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3]\mathbb{c}$).

Formulae (5.1.4) and (5.1.5) show that we have enough information for the purpose mentioned at the beginning of this section if we have studied conjugating matrices for the individual standard matrix irreps, and this is what we shall do in the subsequent section. Note that the restriction to *irreducible* $\mathbb{\Gamma}_i$ is essential for the following developments.

5.2. Conjugating matrices for unitary irreducible matrix representations: The Frobenius–Schur classification

If $\mathbb{U}$ is a square matrix with elements $u_{\gamma\gamma'}$, we shall in the following associate with $\mathbb{U}$ a *column matrix* $\mathbb{u}$, formed by listing the elements $u_{\gamma\gamma'}$ lexicographically according to the index pairs $\gamma\gamma'$.

Now assume that $\mathbb{\Gamma}$ is a unitary matrix irrep of a group G, and that $\mathbb{\Gamma}$ is equivalent to $\bar{\mathbb{\Gamma}}$.

We need the following observation: a square matrix $\mathbb{U}$ of dimension dim $\mathbb{\Gamma}$ satisfies

$$\mathbb{U}\mathbb{\Gamma}(R)=\bar{\mathbb{\Gamma}}(R)\mathbb{U} \quad \text{for all } R\in G \tag{5.2.1}$$

if and only if the associated column matrix $\mathbb{u}$ satisfies

$$[\bar{\mathbb{\Gamma}}(R)\otimes\bar{\mathbb{\Gamma}}(R)]\mathbb{u}=\mathbb{u} \quad \text{for all } R\in G. \tag{5.2.2}$$

Here it is understood that the elements $\bar{\mathbb{\Gamma}}(R)_{\gamma\delta}\bar{\mathbb{\Gamma}}(R)_{\gamma'\delta'}$ of the product matrices $\bar{\mathbb{\Gamma}}(R)\otimes\bar{\mathbb{\Gamma}}(R)$ are also ordered lexicographically (rows according to the index pairs $\gamma\gamma'$, columns according to the index pairs $\delta\delta'$). The équivalence of (5.2.1) and (5.2.2) is immediately verified by writing each of them in coordinates.

Eq. (5.2.2) may evidently also be written

$$[\bar{\mathbb{\Gamma}}(R)\otimes\bar{1}_G\otimes\bar{\mathbb{\Gamma}}(R)]\mathbb{u}=\mathbb{u} \quad \text{for all } R\in G. \tag{5.2.3}$$

Thus, the elements $u_{\gamma\gamma'}$ of $\mathbb{u}$ are triple coefficients of the type $(\mathbb{\Gamma}1_G\mathbb{\Gamma}/\gamma0\gamma')$.

[In (5.2.3), the irrep 1_G could of course equally well have been placed as the first or the third factor in the tensor product. The choice here of the middle position is a matter of convention, and its consequences in connection with 3-Γ symbols will become clear in Sect. 5.3, in paper II, and in paper V.]

We now apply the above considerations to the subject of conjugating matrices. If $\mathbb{U}$ is a conjugating matrix for $\mathbb{\Gamma}$, then $\mathbb{U}$ is in particular a non-zero matrix satisfying (5.21) and $\mathbb{u}$ thus a non-zero column matrix satisfying (5.2.3). Suppose, conversely, that $\mathbb{u}$ is a non-zero solution to (5.2.3). Then, from (3.1.6), there is a non-negative real number a such that

$$\sum_{\gamma}\overline{u_{\gamma\gamma'}}u_{\gamma\gamma''}=a\delta(\gamma',\gamma'') \quad \text{for all } \gamma',\gamma''. \tag{5.2.4}$$

Since $\mathbb{u}$ is non-zero, a must in fact be positive. Thus the columns of $\mathbb{U}$ are non-zero and form an orthogonal system, implying that $\mathbb{U}$ is non-singular. In fact, $\mathbb{U}$ is proportional to a conjugating matrix for $\mathbb{\Gamma}$. This follows by rewriting (5.2.4) as

$$\sum_{\gamma}\overline{(a^{-1/2}u_{\gamma\gamma'})}(a^{-1/2}u_{\gamma\gamma''})=\delta(\gamma',\gamma''). \tag{5.2.5}$$

Since $\mathbb{\Gamma}$ is irreducible, we conclude from (3.1.4) that $\dim \mathscr{F}(\Gamma 1_G \Gamma) = \dim 1_G = 1$. Combining this with the discussion in Sect. 3.2 of symmetric and antisymmetric fix-vectors, we see that if $\mathbb{U}$ is a conjugating matrix for $\mathbb{\Gamma}$, then the column $\mathbb{u}$ is either a symmetric or an antisymmetric fix-vector for $\bar{\mathbb{\Gamma}} \otimes \bar{1}_G \otimes \bar{\mathbb{\Gamma}}$. Translating back to $\mathbb{U}$, we conclude that the matrix *is either symmetric or antisymmetric. Any* conjugating matrix for $\mathbb{\Gamma}$ gives an associated column matrix which is in the space $\mathscr{F}(\Gamma 1_G \Gamma)$ and is thus proportional to $\mathbb{u}$; therefore, all conjugating matrices of $\mathbb{\Gamma}$ have same symmetry. This gives rise to the *Frobenius–Schur classification*:

A unitary matrix irrep $\mathbb{\Gamma}$ is of the *first kind* if its conjugating matrices are *symmetric*. It is of the *second kind* if its conjugating matrices are *antisymmetric*. It is of the *third kind* if $\dim \mathscr{F}(\Gamma 1_G \Gamma) = 0$, i.e. if $\mathbb{\Gamma}$ is not equivalent to $\bar{\mathbb{\Gamma}}$.

This classification was first set up in a slightly different formulation by Frobenius and Schur [55] (for not necessarily unitary matrix irreps). In their paper, the criterion for an irrep to be of the first kind was the existence of a *real* matrix form, a criterion which we shall also use in the following. Its equivalence to the above criterion follows from results stated in [56] which essentially tell that conjugation matrices can be prescribed arbitrarily within the symmetry/antisymmetry-restriction stated above. Except for these remarks and obvious consequences of them, we shall not need further information on the *F–S* classification here; see [56] and the literature cited therein.

We do observe, though, that the classification of an irrep is independent of its actual matrix form. To see this, note for example that if $\mathbb{U}$ is a conjugating matrix for $\mathbb{\Gamma}$ and $\mathbb{Q}$ is any unitary matrix, then we have

$$[\overline{\mathbb{Q}\Gamma(R)\mathbb{Q}^{-1}} \otimes \overline{\mathbb{Q}\Gamma(R)\mathbb{Q}^{-1}}][\bar{\mathbb{Q}} \otimes \bar{\mathbb{Q}}]\mathbb{u} = [\bar{\mathbb{Q}} \otimes \bar{\mathbb{Q}}]\mathbb{u} \quad \text{for all } R \in G. \tag{5.2.6}$$

Thus, the irrep $\mathbb{Q}\Gamma\mathbb{Q}^{-1}$ has conjugating matrices with associated columns proportional to $[\bar{\mathbb{Q}} \otimes \bar{\mathbb{Q}}]\mathbb{u}$ cf. (5.2.). Obviously, $[\bar{\mathbb{Q}} \otimes \bar{\mathbb{Q}}]\mathbb{u}$ is non-zero, symmetric, or antisymmetric, if and only if $\mathbb{u}$ has the same properties, respectively. Therefore, *equivalent unitary matrix irreps are of the same Frobenius–Schur kind.*

The column matrix $[\bar{\mathbb{Q}} \otimes \bar{\mathbb{Q}}]\mathbb{u}$ is the associated column form of the square matrix

$$\tilde{\mathbb{U}} = \bar{\mathbb{Q}}\mathbb{U}\mathbb{Q}^{-1}. \tag{5.2.7}$$

[From the form of (5.2.7), one might suspect that $\tilde{\mathbb{U}}$ is only equivalent to $\mathbb{U}$ when $\mathbb{Q}$ is real, as is asserted by Fano and Racah [8, appendix C]. This is not correct, a fact which is demonstrated by the following example:

Let

$$\mathbb{U} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

(then $\mathbb{\Gamma}$ might be the $j = 1/2$ irrep of the rotation group, cf. Sect. 6) and let

$$\mathbb{Q} = \begin{pmatrix} \omega & 0 \\ 0 & \bar{\omega} \end{pmatrix},$$

where ω is any complex number with modulus 1. Then one may check that $\bar{\mathbb{Q}}\mathbb{U}\mathbb{Q}^{-1}=\mathbb{U}$ which is certainly equivalent to $\mathbb{U}$.]

If $\mathbb{\Gamma}$ is an irrep which is equivalent to its complex conjugate, we shall put $\pi(\mathbb{\Gamma}1_G\mathbb{\Gamma})=1$ if $\mathbb{\Gamma}$ is of the first kind and $\pi(\mathbb{\Gamma}1_G\mathbb{\Gamma})=-1$ if $\mathbb{\Gamma}$ is of the second kind. This is a natural extension of the notation introduced in Sect. 4 in connection with 3-Γ symbols, since 3-Γ symbols $(\Gamma 1_G\Gamma/\gamma 0\gamma')$ will necessarily be even $(\pi(\Gamma 1_G\Gamma)=1)$ if Γ is of the first kind and odd $(\pi(\Gamma 1_G\Gamma)=-1)$ if γ is of the second kind.

5.3. Conjugation formulae for triple coefficients, 3-Γ symbols, and coupling coefficients

Having studied conjugating matrices in Sect. 5.2, we shall now fix our conventions regarding triple coefficients, 3-Γ symbols, and coupling coefficients with a complex conjugation on one or more of the involved representations.

5.3.1. Triple coefficients

We shall start by considering the following rather general situation: A system of standard unitary matrix irreps $\mathbb{\Gamma}$ of a group G is given, and for each ordered standard irrep triple $\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3$ with $\dim \mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3)>0$ triple coefficients $(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3/\gamma_1\gamma_2\gamma_3)_\beta$ have been established. We shall assume that for any standard irrep $\mathbb{\Gamma}$ of the first or second kind the normalization condition (5.3.1) is fulfilled.

$$\sum_{\gamma\gamma'}\left|\begin{pmatrix}\mathbb{\Gamma} & 1_G & \mathbb{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix}\right|^2=1. \tag{5.3.1}$$

This condition is introduced in order to avoid dragging the left-hand side of (5.3.1) along as a normalization constant into all the formulas to follow; it is a trivial (but probably uninteresting) matter to drop this requirement.

We shall base the conventions to be developed on those already set up in Sects. 5.1 and 5.2. Following the discussion there, we shall *define* the conjugating matrix $\mathbb{U}$ for a given standard irrep $\mathbb{\Gamma}$ of the first or second kind by the following formula for its elements:

$$u_{\gamma\gamma'}=b\begin{pmatrix}\mathbb{\Gamma} & 1_G & \mathbb{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix}\quad \text{for all } \gamma,\gamma', \tag{5.3.2}$$

where b is a positive number to be chosen so that $\mathbb{U}$ is unitary. Inserting (5.3.2) in the unitarity condition, (5.2.4) with $a=1$, and using (5.3.1) gives $b=\sqrt{\dim \mathbb{\Gamma}}$ Thus our definition reads:

$$u_{\gamma\gamma'}=\sqrt{\dim \mathbb{\Gamma}}\begin{pmatrix}\mathbb{\Gamma} & 1_G & \mathbb{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix}\quad \text{for all } \gamma,\gamma'. \tag{5.3.3}$$

With this definition, formulae (5.1.4) and (5.1.5) become:

$$\begin{pmatrix}\bar{\mathbb{\Gamma}}_1 & \mathbb{\Gamma}_2 & \mathbb{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}=\sum_{\gamma_1'}\sqrt{\dim \mathbb{\Gamma}_1}\,\overline{\begin{pmatrix}\mathbb{\Gamma}_1 & 1_G & \mathbb{\Gamma}_1\\ \gamma_1' & 0 & \gamma_1\end{pmatrix}}\begin{pmatrix}\mathbb{\Gamma}_1 & \mathbb{\Gamma}_2 & \mathbb{\Gamma}_3\\ \gamma_1' & \gamma_2 & \gamma_3\end{pmatrix} \tag{5.3.4}$$

and

$$\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix} = \sum_{\gamma_1',\gamma_2'} \sqrt{\dim \Gamma_1}\sqrt{\dim \Gamma_2}\,\overline{\begin{pmatrix}\Gamma_1 & 1_G & \Gamma_2\\ \gamma_1' & 0 & \gamma_1\end{pmatrix}}\,\overline{\begin{pmatrix}\Gamma_2 & 1_G & \Gamma_2\\ \gamma_2' & 0 & \gamma_2\end{pmatrix}}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1' & \gamma_2' & \gamma_3\end{pmatrix} \tag{5.3.5}$$

and we of course obtain a series of analogous formulae for still different distributions of one or more conjugation bars on standard irreps of the first or second kind.

We note immediately some consequences of formula (5.3.4) and one of its analogues: Suppose Γ is a *standard* irrep of the first or second kind. Then for the triple coefficients of the particular type $(\bar{\Gamma}1_G\Gamma/\gamma 0\gamma')$ we see that

$$\begin{aligned}\begin{pmatrix}\bar{\Gamma} & 1_G & \Gamma\\ \gamma & 0 & \gamma'\end{pmatrix} &= \sum_{\gamma''}\sqrt{\dim \Gamma}\,\overline{\begin{pmatrix}\Gamma & 1_G & \Gamma\\ \gamma'' & 0 & \gamma\end{pmatrix}}\begin{pmatrix}\Gamma & 1_G & \Gamma\\ \gamma'' & 0 & \gamma'\end{pmatrix}\\ &= (\dim \Gamma)^{-1/2}\sum_{\gamma''}\overline{u_{\gamma''\gamma}}u_{\gamma''\gamma'}\\ &= \delta(\gamma,\gamma')(\dim \Gamma)^{-1/2}\end{aligned} \tag{5.3.6}$$

while for those of the particular type $(\Gamma 1_G\bar{\Gamma}/\gamma 0\gamma')$ we get

$$\begin{aligned}\begin{pmatrix}\Gamma & 1_G & \bar{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix} &= \sum_{\gamma''}\sqrt{\dim \Gamma}\,\overline{\begin{pmatrix}\Gamma & 1_G & \Gamma\\ \gamma'' & 0 & \gamma'\end{pmatrix}}\begin{pmatrix}\Gamma & 1_G & \Gamma\\ \gamma & 0 & \gamma''\end{pmatrix}\\ &= (\dim \Gamma)^{-1/2}\sum_{\gamma''}\overline{u_{\gamma''\gamma'}}u_{\gamma\gamma''}\\ &= (\dim \Gamma)^{-1/2}\sum_{\gamma''}\overline{u_{\gamma''\gamma'}}(\pm u_{\gamma''\gamma})\\ &= \pm\delta(\gamma,\gamma')(\dim \Gamma)^{-1/2}\end{aligned} \tag{5.3.7}$$

where "+" applies when Γ is of the first kind and "−" applies when Γ is of the second kind (symmetric and antisymmetric conjugation matrices, respectively).

Remarks

1° Note that the above formulae involving coefficients of the types $(\Gamma 1_G\Gamma/\gamma 0\gamma')$, $(\Gamma 1_G\bar{\Gamma}/\gamma 0\gamma')$, and $(\bar{\Gamma}1_G\Gamma/\gamma 0\gamma')$ are stated only for standard irreps Γ of the first or second kind. If Γ is of the third kind, $\dim \mathscr{F}(\Gamma 1_G\Gamma)=0$ (Sect. 5.2) so that triple coefficients of the first type necessarily vanish. The formulae given here involving this type of coefficient would generally be wrong if applied to third-kind irreps Γ. On the other hand, for *any* irrep Γ, we have $\dim \mathscr{F}(\bar{\Gamma}1_G\Gamma)=1=\dim \mathscr{F}(\Gamma 1_G\bar{\Gamma})$; in fact it is an easy exercise, using the unitarity of Γ, to check that for any phases $\omega(\bar{\Gamma},\Gamma)$ and $\omega(\Gamma,\bar{\Gamma})$, the formulas

$$\begin{pmatrix}\bar{\Gamma} & 1_G & \Gamma\\ \gamma & 0 & \gamma'\end{pmatrix} = \omega(\bar{\Gamma},\Gamma)(\dim \Gamma)^{-1/2}\delta(\gamma,\gamma') \tag{5.3.8}$$

and

$$\begin{pmatrix} \Gamma & 1_G & \bar{\Gamma} \\ \gamma & 0 & \gamma' \end{pmatrix} = \omega(\Gamma, \bar{\Gamma})(\dim \Gamma)^{-1/2}\delta(\gamma, \gamma') \tag{5.3.9}$$

define triple coefficients for the triples $\bar{\Gamma}1_G\Gamma$ and $\Gamma 1_G\bar{\Gamma}$, respectively. For irreps Γ of the first or second kind, $\omega(\bar{\Gamma}, \Gamma)$ and $\omega(\Gamma, \bar{\Gamma})$ are fixed by our conventions to be

$$\omega(\bar{\Gamma}, \Gamma) = +1 \qquad \text{(formula (5.3.6))}$$

and

$$\omega(\Gamma, \bar{\Gamma}) = \begin{Bmatrix} +1 & \text{for } \Gamma \text{ first-kind} \\ -1 & \text{for } \Gamma \text{ second-kind} \end{Bmatrix} = \pi(\Gamma 1_G \Gamma) \qquad \text{(formula (5.3.7))},$$

but for Γ of the third kind these phases can be chosen freely. In paper II we shall discuss how we fix them also for third-kind irreps for the double groups treated there.

2° From a comparison of formulae (5.3.6) and (5.3.7) it is clear that for irreps of the first and second kind it is very important to distinguish between the *standard* irreps themselves and their complex conjugates. *This is generally true for the Wigner–Racah algebra we are developing here.*

For further discussion of complex conjugation in triple coefficients, relating to display (5.1.1), see Sect. 5.4.

3° Triple coefficients of the form $(\Gamma 1_G \Gamma / \gamma 0 \gamma')$ satisfying (5.3.1) correspond to Wigner's 1-*j* symbols [14]. In the later literature, there has been quite some diversity in terminology and definitions of the same or like concepts. We shall not introduce any new terminology in this connection

5.3.2. 3-Γ symbols

We shall of course carry over all the formulae implied in Sect. 5.3.1 to the special case where the triple coefficients involved form sets of 3-Γ symbols (Sect. 4). For example, formula (5.3.4) in the notation for 3-Γ symbols becomes

$$\begin{pmatrix} \bar{\Gamma} & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta = \sum_{\gamma_1'} \sqrt{\dim \Gamma_1} \begin{pmatrix} \Gamma_1 & 1_G & \Gamma_1 \\ \gamma_1' & 0 & \gamma_1 \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2 & \gamma_3 \end{pmatrix}_\beta . \tag{5.3.10}$$

A collection of formulas thus obtained for 3-Γ symbols will be available in [21] and in off-print from the authors.

We note two consequences for 3-Γ symbols of the formalism introduced:

1° If *real* 3-Γ symbols are given for all triples of *standard* irreps, then all 3-Γ symbols involving complex conjugates of standard irreps are also real (in a formula like (5.3.10), the right-hand side by the assumption only involves real numbers, and thus the left-hand side also becomes a real number).

2° The *permutational characteristic* (oddness/eveness) of 3-Γ symbols is preserved when standard irreps of the first or second kind are conjugated; thus, for example,

$$\begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta = \pi(\Gamma_1\Gamma_2\Gamma_3\beta)\begin{pmatrix} \Gamma_2 & \bar{\Gamma}_1 & \Gamma_3 \\ \gamma_2 & \gamma_1 & \gamma_3 \end{pmatrix}_\beta \tag{5.3.11}$$

if Γ_1 is of either the first or the second kind. This is easily checked by using (5.3.10) as it stands as well as for the triple $\Gamma_2\Gamma_1\Gamma_3$.

Considering *2°*, it is natural to extend – and this we do now – the definition of $\pi(\Gamma_1\Gamma_2\Gamma_3\beta)$ to allow the Γ_i to be standard irreps *or* complex conjugates of standard irreps of the first or second kind, by simply removing the conjugations in the latter case; thus with reference to (5.3.11), we have

$$\pi(\bar{\Gamma}_1\Gamma_2\Gamma_3\beta) = \pi(\Gamma_1\Gamma_2\Gamma_3\beta). \tag{5.3.12}$$

As a special case, we get with this extended definition:

$$\pi(\Gamma 1_G\bar{\Gamma}) = \pi(\bar{\Gamma} 1_G\Gamma) = \pi(\bar{\Gamma} 1_G\bar{\Gamma}) = \pi(\Gamma 1_G\Gamma) = \begin{cases} +1 \text{ if } \Gamma \text{ is of the first kind} \\ -1 \text{ if } \Gamma \text{ is of the second kind.} \end{cases} \tag{5.3.13}$$

Butler in [22] calls this phase the *2-j* phase. Note that $\pi(\Gamma 1_G\bar{\Gamma}) = \pi(\bar{\Gamma} 1_G\Gamma)$, trivially, also if Γ is of the third kind, but that $\pi(\Gamma 1_G\Gamma)$ and $\pi(\bar{\Gamma} 1_G\bar{\Gamma})$ are not defined in this case (since $\dim \mathscr{F}(\Gamma 1_G\Gamma) = 0 = \dim \mathscr{F}(\bar{\Gamma} 1_G\bar{\Gamma})$ when Γ is of the third kind). See paper II regarding our convention for $\pi(\Gamma 1_G\bar{\Gamma})$ for third-kind irreps of the non-commutative double groups.

5.3.3. Coupling coefficients; the Wigner–Eckart theorem with coupling coefficients

We now define coupling coefficients by the 3-Γ symbol version of (3.3.11):

$$\langle\Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\Gamma_3\gamma_3\rangle = \varphi(\Gamma_1\Gamma_2\Gamma_3\beta)\sqrt{\dim\Gamma_3}\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta. \tag{5.3.14}$$

We still have to decide which phase factor $\varphi(\Gamma_1\Gamma_2\Gamma_3\beta)$ to use in this formula. Also, we want to allow the Γ_i in the coupling coefficient (5.3.14) to be complex conjugates of standard irreps, so that we can obtain, e.g., coupling coefficients of the type $\langle\Gamma_1\gamma_1\bar{\Gamma}_2\gamma_2|\beta\Gamma_3\gamma_3\rangle$, where Γ_2 is of the first or second kind. Regarding the latter problem, note that as a consequence of the convention introduced at the end of Sect. 5.1, we may in such cases remove any double conjugations $\bar{\bar{\Gamma}}$ initially arising on the right-hand side of (5.3.14) by $\bar{\bar{\Gamma}} \to \Gamma$ before using the formula.

As for the phase, we have demonstrated in Sect. A.4 that the requirement of the so-called associativity of the invariant triple product leads in a natural way to the choice

$$\varphi(\Gamma_1\Gamma_2\Gamma_3\beta) = \pi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)\pi(\Gamma_1 1_G\bar{\Gamma}_1)\,\mathrm{sign}\,(\bar{\Gamma}_3 1_G\Gamma_3) \tag{5.3.15}$$

of the phase factor. Here sign $(\bar{\Gamma}_3 1_G\Gamma_3)$ is the common sign of the 3-Γ symbols $(\bar{\Gamma}_3 1_G\Gamma_3/\gamma 0\gamma')$, cf. Sect. 5.3.1. To illustrate the use of (5.3.14) and (5.3.15) in connection with the above convention on doubly conjugated standard irreps, we note that

$$\langle \Gamma_1 \gamma_1 \bar{\Gamma}_2 \gamma_2 | \beta \Gamma_3 \gamma_3 \rangle = \pi(\Gamma_1 \bar{\Gamma}_2 \bar{\Gamma}_3 \beta) \pi(\Gamma_1 1_G \bar{\Gamma}_1) \operatorname{sign}(\bar{\Gamma}_3 1_G \Gamma_3) \sqrt{\dim \Gamma_3} \begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta . \tag{5.3.16}$$

The coupling coefficients defined by these conventions have permutational properties that may easily be derived; e.g., from (5.3.14) and (5.3.15) one deduces that

$$\langle \Gamma_1 \gamma_1 \Gamma_2 \gamma_2 | \beta \Gamma_3 \gamma_3 \rangle = \pi(\Gamma_1 1_G \bar{\Gamma}_1) \pi(\Gamma_2 1_G \bar{\Gamma}_2) \pi(\bar{\Gamma}_1 \bar{\Gamma}_2 \Gamma_3 \beta) \langle \Gamma_2 \gamma_2 \Gamma_1 \gamma_1 | \beta \Gamma_3 \gamma_3 \rangle . \tag{5.3.17}$$

Comparing the 3-Γ symbol appearing on the right side of (5.3.16) with (2.7), we see that the *Wigner–Eckart theorem* may be formulated within the present formalism as

$$\langle \varphi^{\Gamma_1}_{\gamma_1} | \mathcal{O}^{\Gamma_2}_{\gamma_2} | \psi^{\Gamma_3}_{\gamma_3} \rangle = \sum_{\beta=1}^{N} \langle \varphi^{\Gamma_1} \| \mathcal{O}^{\Gamma_2} \| \psi^{\Gamma_3} \rangle_\beta \langle \Gamma_1 \gamma_1 \bar{\Gamma}_2 \gamma_2 | \beta \Gamma_3 \gamma_3 \rangle \tag{5.3.18}$$

or, permuting the Γ_i cyclically in the 3-Γ symbol before converting to coupling coefficients, as

$$\langle \varphi^{\Gamma_1}_{\gamma_1} | \mathcal{O}^{\Gamma_2}_{\gamma_2} | \psi^{\Gamma_3}_{\gamma_3} \rangle = \sum_{\beta=1}^{N} \langle \varphi^{\Gamma_1} \| \mathcal{O}^{\Gamma_2} \| \psi^{\Gamma_3} \rangle_\beta \langle \bar{\Gamma}_3 \gamma_3 \Gamma_1 \gamma_1 | \beta \Gamma_2 \gamma_2 \rangle . \tag{5.3.19}$$

Note that *the reduced matrix elements* of (5.3.18) and (5.3.19) *differ* from those of (2.7) by factors $\sqrt{\dim \Gamma}$ and sign factors.

Remark

We see from (5.3.14) and (5.3.15) that if real 3-Γ symbols are given for a group, then all coupling coefficients by the present conventions will be real numbers, too. (Cf. 1° in Sect. 5.3.2.)

Concluding remarks on Sect. 5.3

The formalism developed here has been constructed so as to be everywhere consistent with that of Wigner's 1940 paper on simply reducible groups [14]. For explicit examples in the particular case of the rotation double group, see Sect. 6.

As we have seen, there is a reason – which one may find important or not – for choosing the particular phase factor (5.3.15) in the relation between coupling coefficients and 3-Γ symbols rather than the admittedly more obvious "sensible" [17] choice of $\varphi(\Gamma_1 \Gamma_2 \Gamma_3 \beta) = 1$. Butler [e.g. 22, 17, 57] consistently suppresses this aspect, claiming that the phase factor, in its particular form for the group R_3^* (Sect. 6 of the present paper), only exists for "historical reasons".

5.4. Derome–Sharp matrices and related matters

Suppose $\Gamma_1, \Gamma_2, \Gamma_3$ to be standard unitary irreducible matrix irreps. Let $(\mathfrak{c}_1, \ldots, \mathfrak{c}_N)$ be an orthonormal basis for the fix-vector space $\mathcal{F}(\Gamma_1 \Gamma_2 \Gamma_3)$ consisting of columns

$\mathbb{c}_\beta$ of triple coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$. Further, let $(\tilde{\mathbb{c}}_1, \ldots, \tilde{\mathbb{c}}_N)$ be a basis for the fix-vector space $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3)$, chosen in accord with the conventions in Sect. 5.3.1 if any of the Γ_i are of the first or the second kind. Since the fix-vector property

$$[\bar{\Gamma}_1(R)\otimes\bar{\Gamma}_2(R)\otimes\bar{\Gamma}_3(R)]\tilde{\mathbb{c}}_\beta = \tilde{\mathbb{c}}_\beta \quad \text{for all } R \in G \tag{5.4.1}$$

is, trivially, equivalent to

$$[\Gamma_1(R)\otimes\Gamma_2(R)\otimes\Gamma_3(R)]\bar{\tilde{\mathbb{c}}}_\beta = \bar{\tilde{\mathbb{c}}}_\beta \quad \text{for all } R \in G, \tag{5.4.2}$$

the orthonormal set $(\bar{\tilde{\mathbb{c}}}_1, \ldots, \bar{\tilde{\mathbb{c}}}_N)$, consisting of the complex conjugate columns $\bar{\tilde{\mathbb{c}}}_\beta$, is also an orthonormal basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$. Thus, there must be a unitary matrix $\mathbb{A} = \mathbb{A}(\Gamma_1\Gamma_2\Gamma_3)$ relating the two bases:

$$(\bar{\tilde{\mathbb{c}}}_1 \cdots \bar{\tilde{\mathbb{c}}}_N) = (\mathbb{c}_1 \cdots \mathbb{c}_N)\mathbb{A} \tag{5.4.3}$$

Indeed, the elements $\mathbb{A}_{\alpha\beta}$ of $\mathbb{A}$ are given by

$$\mathbb{A}_{\alpha\beta} = \langle \mathbb{c}_\alpha | \bar{\tilde{\mathbb{c}}}_\beta \rangle = \sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\alpha} \, \overline{\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} . \tag{5.4.4}$$

There are corresponding matrices $\mathbb{B}^i = \mathbb{B}^i(\Gamma_1\Gamma_2\Gamma_3)$ relating triples with one conjugation to triples with two conjugations, defined by

$$\mathbb{B}^1_{\alpha\beta} = \sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\alpha} \, \overline{\begin{pmatrix} \Gamma_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} \tag{5.4.5}$$

$$\mathbb{B}^2_{\alpha\beta} = \sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix} \Gamma_1 & \bar{\Gamma}_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\alpha} \, \overline{\begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} \tag{5.4.6}$$

$$\mathbb{B}^3_{\alpha\beta} = \sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix} \Gamma_1 & \Gamma_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\alpha} \, \overline{\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} \tag{5.4.7}$$

The introduction of the matrices $\mathbb{A}(\Gamma_1\Gamma_2\Gamma_3)$, $\mathbb{B}^1(\Gamma_1\Gamma_2\Gamma_3)$, $\mathbb{B}^2(\Gamma_1\Gamma_2\Gamma_3)$, and $\mathbb{B}^3(\Gamma_1\Gamma_2\Gamma_3)$ for a triple $\Gamma_1\Gamma_2\Gamma_3$ of standard unitary matrix irreps was anticipated already in display (5.1.1). We see that if we have these four matrices at our disposal, we have reduced the problem of dealing with triple coefficients for the eight triples in (5.1.1) to that of dealing with the four triples in the left half of the figure.

We shall call the matrix $\mathbb{A}(\Gamma_1\Gamma_2\Gamma_3)$ the *Derome–Sharp* matrix of the triple $\Gamma_1\Gamma_2\Gamma_3$ with the chosen triple coefficients, since this kind of matrix was first studied in a general context in [15].

This far we can get in the general case. If the Γ_i are of the first or second kind, further reduction may be achieved by the use of conjugating matrices. Formula (5.3.4) and (5.3.5) thus show how to get to the triples $\bar{\Gamma}_1\Gamma_2\Gamma_3$ and $\bar{\Gamma}_1\bar{\Gamma}_2\Gamma_3$ from the unconjugated triple $\Gamma_1\Gamma_2\Gamma_3$. Note that such *formulae involving conjugating matrices apply irrespective of the Frobenius–Schur kind of those irreps which are unaffected by the conjugations.*

If Γ_1, Γ_2, Γ_3 have conjugating matrices $\mathbb{U}_i$, the conventions of Sect. 5.3.1 lead to the following formulae for the elements of the $\mathbb{A}$ and $\mathbb{B}$ matrices:

$$\mathbb{A}_{\alpha\beta} = \langle \mathbb{c}_\alpha | \bar{\bar{\mathbb{c}}}_\beta \rangle = \langle \mathbb{c}_\alpha | \overline{[\mathbb{U}_1^{-1} \otimes \mathbb{U}_2^{-1} \otimes \mathbb{U}_3^{-1}] \mathbb{c}_\beta} \rangle \tag{5.4.8}$$

$$\mathbb{B}^1_{\alpha\beta} = \langle [\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{1}_3] \mathbb{c}_\alpha | \overline{[\mathbb{1}_1 \otimes \mathbb{U}_2^{-1} \otimes \mathbb{U}_3^{-1}] \mathbb{c}_\beta} \rangle = \pi(\Gamma_1 1_G \Gamma_1) \mathbb{A}_{\alpha\beta} \tag{5.4.9}$$

$$\mathbb{B}^2_{\alpha\beta} = \langle [\mathbb{1}_1 \otimes \mathbb{U}_2^{-1} \otimes \mathbb{1}_3] \mathbb{c}_\alpha | \overline{[\mathbb{U}_1^{-1} \otimes \mathbb{1}_2 \otimes \mathbb{U}_3^{-1}] \mathbb{c}_\beta} \rangle = \pi(\Gamma_2 1_G \Gamma_2) \mathbb{A}_{\alpha\beta} \tag{5.4.10}$$

$$\mathbb{B}^3_{\alpha\beta} = \langle [\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{U}_3^{-1}] \mathbb{c}_\alpha | \overline{[\mathbb{U}_1^{-1} \otimes \mathbb{U}_2^{-1} \otimes \mathbb{1}_3] \mathbb{c}_\beta} \rangle = \pi(\Gamma_3 1_G \Gamma_3) \mathbb{A}_{\alpha\beta}. \tag{5.4.11}$$

Thus, these matrices may be calculated from the triple coefficients for the unconjugated triple and the conjugating matrices. In the general case, they have to be calculated from the relevant triple coefficients by the defining formulae (5.4.4)–(5.4.7). For the particularly convenient type of Wigner–Racah algebra described in Sect. 5.5, simple general formulae may be given for the $\mathbb{A}$ and $\mathbb{B}^i$ matrices (see Eqs. (5.5.4)–(5.5.7) below).

Remarks

If the matrix $\mathbb{A}$ is symmetric for a *given single* triple $\Gamma_1\Gamma_2\Gamma_3$ with a certain choice of bases for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ and $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3)$, one may choose new bases for these spaces such that the new matrix is the *unit* matrix; this is proved in Sect. A.5. The possibility of establishing a Wigner–Racah algebra with $\mathbb{A} = \mathbb{1}$ consistently for *all* triples was discussed by Wigner [14] for *simply reducible groups* (multiplicity-free groups with no irreps of the third kind) and has been investigated more generally by Butler [17], some prerequisite results being derived in [45]. A particular case where $\mathbb{A}$ matrices are necessarily *symmetric* is that of multiplicity-free groups (because for these, all $\mathbb{A}$ matrices are 1×1); another one is made up by the ambivalent groups (groups with no third-kind irreps) with a representation algebra "regular with respect to the Frobenius–Schur classification" (see [54] and Eq. (5.5.1) below). In the latter case, $\mathbb{A}$ matrices are given by Eq. (5.4.8) and are always symmetric because an *even* number of the $\mathbb{U}_i$ appearing there are antisymmetric. The simply reducible groups [14] belong to this class. So do the groups we discuss in Sect. 5.5, for which the assumptions stated there have as one consequence that *all* $\mathbb{A}$ matrices are *automatically* unit matrices. In other cases requirements which we have taken as more fundamental may prevent us from having unit $\mathbb{A}$ matrices for all triples (for examples, see the general discussion of triples $\bar{\Gamma} 1_G \Gamma$ in the double groups, where Γ is of the third kind, in paper II; the triple EEE in D_3^* (paper III); and the triple TTT in T^*, discussed in paper IV).

5.5. Complex conjugation by the irreducible representation matrices of a fixed group element

We now restrict the scope to study the particularly convenient Wigner–Racah algebra which may be established for a certain class of groups to which belong the rotation groups R_3 and R_3^*, the octahedral and icosahedral double groups O^* and I^*, the dihedral double groups D_n^* with n even, and D_∞^*, and those finite (or compact) groups – point groups or not – which have only irreps of the first kind. The group property on which we focus is the following one:

(#) *There exists an element R_0 in G and a choice of standard unitary matrix irreps of G, such that for every standard irrep $\mathbb{\Gamma}$, $\mathbb{\Gamma}(R_0)$ is a conjugating matrix for $\mathbb{\Gamma}$.*

Evidently, a group with this property has no irreps of the third kind, that is, it is *ambivalent.* In Sect. IV of [54] we deduced a necessary and sufficient condition for a group to have the property (#); from this it follows that the above-mentioned groups, in particular, have it. For explicit demonstrations, see Sect. 6 of this paper (the rotation double group), paper III (the dihedral double groups), [50] and paper V (the octahedral double group), and paper VI (the icosahedral double group).

We write down some important consequences of having the above situation. Suppose G is a group enjoying the property (#) and that we have fixed an element R_0 in G accordingly. Then:

1° Whatever choice of standard matrix irreps $\mathbb{\Gamma}$ is made in accordance with (#), the matrices $\mathbb{\Gamma}(R_0)$ will always be *real.* This is seen by putting $\mathbb{U} = \mathbb{\Gamma}(R_0)$ and $R = R_0$ in (5.1.2). Moreover, by a suitable choice of standard irreps $\mathbb{\Gamma}$, one may have $\mathbb{\Gamma}(R_0)$ to be a conjugating matrix for $\mathbb{\Gamma}$ for each $\mathbb{\Gamma}$ and *at the same time* prescribe the form of $\mathbb{\Gamma}(R_0)$ almost arbitrarily. Indeed,
(i) For an irrep of the *first* kind, any *symmetric real orthogonal matrix* with its trace equal to the character of the irrep at R_0 may be obtained as $\mathbb{\Gamma}(R_0)$.
(ii) For an irrep of the *second* kind, any *antisymmetric real orthogonal matrix* may be obtained as $\mathbb{\Gamma}(R_0)$.

2° If a choice of standard matrix irreps $\mathbb{\Gamma}$ has been made such that $\mathbb{\Gamma}(R_0)$ is a conjugating matrix for $\mathbb{\Gamma}$ for all standard $\mathbb{\Gamma}$, then *real triple coefficients may be chosen* for each standard irrep triple. That is, given standard irreps $\mathbb{\Gamma}_1$, $\mathbb{\Gamma}_2$, $\mathbb{\Gamma}_3$ there exists an orthonormal basis $(\mathfrak{c}_1, \ldots, \mathfrak{c}_N)$ for the linear space $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ such that all the $\mathfrak{c}_\beta$ are *real* column matrices.

3° For all irrep triples $\Gamma_1\Gamma_2\Gamma_3$ having non-zero fix-vectors, the phases $\pi(\Gamma_i 1_G \Gamma_i)$ defined in Sect. 5.2 satisfy

$$\pi(\Gamma_1 1_G \Gamma_1)\pi(\Gamma_2 1_G \Gamma_2)\pi(\Gamma_3 1_G \Gamma_3) = 1. \tag{5.5.1}$$

The assertions *1°* and *2°* have been proved in [54] and [56], while *3°* has been proved and discussed in ([54], Sect. V.). Ambivalent groups having property *3°* were said there to have a "representation algebra" which was "regular with respect to the Frobenius–Schur classification". Differently stated, (5.5.1) expresses the fact that the tensor product of two irreps of the *same* Frobenius–Schur kind only contains irreps of the *first* kind.

If $\Gamma(R_0)$ is our choice of a conjugating matrix for Γ for all standard Γ, we must – to be consistent with (5.3.3) – define triple coefficients of the type $(\Gamma 1_G \Gamma/\gamma 0 \gamma')$ by

$$\begin{pmatrix} \Gamma & 1_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix} = (\dim \Gamma)^{-1/2} \Gamma(R_0)_{\gamma\gamma'}. \tag{5.5.2}$$

Making use of the double rôle of the $\Gamma(R_0)$ as irrep matrices and as conjugating matrices, one may derive formulae concerning the addition of or removal of complex conjugations in triple coefficients, as we shall now see.

First, suppose that $(\mathbb{c}_1, \ldots, \mathbb{c}_N)$ is a basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$. By using the fix-vector property (3.1.1) for the group element R_0^{-1} and the fact that the $\Gamma_i(R_0)$ are *real* matrices (see *1°* above), we get

$$\begin{aligned} \mathbb{c}_\beta &= [\bar{\Gamma}_1(R_0^{-1}) \otimes \bar{\Gamma}_2(R_0^{-1}) \otimes \bar{\Gamma}_3(R_0^{-1})]\mathbb{c}_\beta \\ &= [\Gamma_1(R_0)^{-1} \otimes \Gamma_2(R_0)^{-1} \otimes \Gamma_3(R_0)^{-1}]\mathbb{c}_\beta \quad \text{for all } \beta, \end{aligned} \tag{5.5.3}$$

which when written in coordinates, according to the definitions in Sect. 5.1 for the use of conjugating matrices, reads

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta = \begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \quad \text{for all } \beta \text{ and } \gamma_1, \gamma_2, \gamma_3. \tag{5.5.4}$$

Eq. (5.5.4) shows that for all triples $\Gamma_1\Gamma_2\Gamma_3$, the Derome–Sharp matrix $\mathbb{A} = \mathbb{A}(\Gamma_1\Gamma_2\Gamma_3)$ defined in Sect. 5.4 is the *unit matrix*, provided we choose *real* triple coefficients (cf. *2°* above); to see this, combine Eqs. (5.4.4) and (5.5.4).

Using analogous arguments, one may show that the $\mathbb{B}$ matrices defined in Sect. 5.4 are given by the following formulae, when real triple coefficients have been chosen:

$$\mathbb{B}^1_{\alpha\beta} = \mathbb{B}^1(\Gamma_1\Gamma_2\Gamma_3)_{\alpha\beta} = \pi(\Gamma_1 1_G \Gamma_1)\delta(\alpha, \beta) \tag{5.5.5}$$

$$\mathbb{B}^2_{\alpha\beta} = \mathbb{B}^2(\Gamma_1\Gamma_2\Gamma_3)_{\alpha\beta} = \pi(\Gamma_2 1_G \Gamma_2)\delta(\alpha, \beta) \tag{5.5.6}$$

$$\mathbb{B}^3_{\alpha\beta} = \mathbb{B}^3(\Gamma_1\Gamma_2\Gamma_3)_{\alpha\beta} = \pi(\Gamma_3 1_G \Gamma_3)\delta(\alpha, \beta) \tag{5.5.7}$$

[*Note of warning.* The requirement (5.5.2) may, in some cases, have a slightly surprising consequence. Suppose Γ is a *real* matrix irrep, i.e. $\Gamma(R)$ is a real matrix for all $R \in G$. Suppose further that R_0 is an element such that $\Gamma(R_0)$ is not the unit matrix $\mathbb{1}$; in this case it is necessarily $-\mathbb{1}$, since this is the only real multiple of $\mathbb{1}$ (all conjugating matrices for Γ are proportional, Sect. 5.2). Using the conjugating matrix defined by (5.5.2) according to, say, (5.3.4), will then produce a sign change even though Γ itself is not changed by complex conjugation; i.e. generally we will have

$$\begin{pmatrix} \cdots & \bar{\Gamma} & \cdots \\ & \gamma & \end{pmatrix} = -\begin{pmatrix} \cdots & \Gamma & \cdots \\ & \gamma & \end{pmatrix}.$$

An example is the irrep A_2 in the octahedral double group which has $A_2(R_0) = -1$ for some of the cases studied in paper V.]

Suppose that 3-Γ symbols $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ have been chosen for a group with the property (#) and in accordance with (5.5.2). Then these 3-Γ symbols will of course also satisfy relations corresponding to (5.5.4)–(5.5.7).

Suppose furthermore that we wish to construct coupling coefficients from these 3-Γ symbols according to our conventions from Sect. 5.3. We look first at the expression (5.3.15) for the connecting phase factor. This expression here becomes

$$\varphi(\Gamma_1\Gamma_2\Gamma_3\beta)=\pi(\Gamma_1\Gamma_2\Gamma_3\beta)\pi(\Gamma_1 1_G\Gamma_1), \tag{5.5.8}$$

because all the Γ_i are of the first or second kind and because sign $(\bar{\Gamma}_3 1_G\Gamma_3)=+1$ (see (5.3.6)). Formula (5.3.14) thus becomes

$$\langle\Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\Gamma_3\gamma_3\rangle=\pi(\Gamma_1\Gamma_2\Gamma_3\beta)\pi(\Gamma_1 1_G\Gamma_1)\sqrt{\dim\Gamma_3}\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta. \tag{5.5.9}$$

By the use of (5.5.1) and (5.5.7) we may rewrite (5.5.9) to give a formula involving only one complex conjugation:

$$\langle\Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\Gamma_3\gamma_3\rangle=\pi(\Gamma_1\Gamma_2\Gamma_3\beta)\pi(\Gamma_2 1_G\Gamma_2)\sqrt{\dim\Gamma_3}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \bar{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta. \tag{5.5.10}$$

6. Example: The particular case of the rotation double group, R_3^*

To illustrate the developments in the preceding sections, we now display some formulae for the particular case of the group R_3^*. Classical references on this case are [7, 8, 9, 23]; Sect. 2 of [50] gives some of the essentials. The mathematics of the rotation group is further dealt with extensively in [10, 12, 13] and other sources, partly referred to in [58], but too numerous to be cited here. Being a double group, R_3^* is also among the groups we are concerned with in paper II.

For R_3^* there is a conventional choice of standard matrix forms $\mathscr{D}^{[j]}$ (actually called the "contrastandard" by Fano and Racah [8]) of the irreps D_j, $j=0$, 1/2, 1, 3/2, 2, ..., with the property that for every j the irrep matrix $\mathscr{D}^{[j]}(C_2^{Y*})$ is a conjugating matrix for $\mathscr{D}^{[j]}$. Here C_2^{Y*} is a double-group element corresponding to the two-fold rotation about the Y axis, cf. Sect. 2.1 of Paper II. The matrices $\mathscr{D}^{[j]}(C_2^{Y*})$ are explicitly given by

$$\mathscr{D}^{[j]}(C_2^{Y*})_{mm'}=(-1)^{j+m}\delta(-m,m') \tag{6.1}$$

where m and m' take on the values $j, j-1, \ldots, -j+1, -j$. Explicit formulae for the elements of an arbitrary standard irrep matrix $\mathscr{D}^{[j]}(R)$, $R\in R_3^*$, may be found in, e.g. ([8], App. D). It is seen that the matrices (6.1) are symmetric for $j=0$, 1, 2, 3, ... and antisymmetric for $j=1/2$, 3/2, 5/2, ..., corresponding to the fact that the irreps $\mathscr{D}^{[j]}$ are of the first kind for j equal to an integer and of the second kind for j equal to half an odd integer.

Thus, R_3^* fits into the framework of Sect. 5.5. Furthermore, R_3^* is multiplicity-free and therefore simple phase. In all, real 3-Γ symbols may be chosen for R_3^* corresponding to the $\mathscr{D}^{[j]}$. The well-known 3-j symbols $(j_1j_2j_3/m_1m_2m_3)$ make up the conventional choice of such 3-Γ symbols; for clarity, we shall denote them sometimes as

$$\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

in the present section. Note that no "β" is needed here because R_3^* is multiplicity-free. An explicit formula for $(j_1 j_2 j_3 / m_1 m_2 m_3)$ exists (e.g. [9, Eq. (1.5)]).

The 3-j symbols conform to the convention of (5.5.2) with $R_0 = C_2^{Y^*}$, that is, using (6.1),

$$\begin{pmatrix} j & 0 & j \\ m & 0 & m' \end{pmatrix} = \begin{pmatrix} \mathscr{D}^{[j]} & \mathscr{D}^{[0]} & \mathscr{D}^{[j]} \\ m & 0 & m' \end{pmatrix} = (2j+1)^{-1/2}(-1)^{j+m}\delta(-m, m'). \tag{6.2}$$

As an example of the use of these conjugating matrices, Eq. (5.3.4) here reads

$$\begin{aligned} &\begin{pmatrix} \overline{\mathscr{D}^{[j_1]}} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ m_1 & m_2 & m_3 \end{pmatrix} \\ &= \sum_{m_1'} \sqrt{2_{j_1}+1}\,(2_{j_1}+1)^{-1/2}(-1)^{j_1+m_1'}\delta(-m_1', m_1)\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ m_1' & m_2 & m_3 \end{pmatrix} \\ &= (-1)^{j_1-m_1}\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ -m_1 & m_2 & m_3 \end{pmatrix} \end{aligned} \tag{6.3}$$

and (5.3.5) correspondingly becomes

$$\begin{pmatrix} \overline{\mathscr{D}^{[j_1]}} & \overline{\mathscr{D}^{[j_2]}} & \mathscr{D}^{[j_3]} \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-m_1}(-1)^{j_2-m_2}\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ -m_1 & -m_2 & +m_3 \end{pmatrix} \tag{6.4}$$

which are the conventional formulae for complex conjugation in 3-j symbols (e.g., [7], p. 293). Note the convenience arising from the especially simple form (6.1) of the conjugating matrices. The general existence of conjugating matrices with simple forms is ensured by statement *1°* of Sect. 5.5. With (6.3) established, the Wigner–Eckart theorem, (2.7), for R_3^* takes the form

$$\langle \varphi^{j_1}_{m_1} | \mathcal{O}^{j_2}_{m_2} | \psi^{j_3}_{m_3} \rangle = \langle \varphi^{j_1} \| \mathcal{O}^{j_2} \| \psi^{j_3} \rangle (-1)^{j_1-m_1}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_2 & m_3 \end{pmatrix}, \tag{6.5}$$

which is the conventional one; see the references given in Sect. 2 or ([9], p. 6).

The unit $\mathbb{A}$ matrix property (5.5.4), cf. Sect. 5.4, becomes

$$\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-m_1}(-1)^{j_2-m_2}(-1)^{j_3-m_3}\begin{pmatrix} \mathscr{D}^{[j_1]} & \mathscr{D}^{[j_2]} & \mathscr{D}^{[j_3]} \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \tag{6.6}$$

which, after a change of notation and after noting the (well-known) property, proved also in paper II, of the 3-j symbols that they vanish unless $m_1+m_2+m_3=0$, gives the formula

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \tag{6.7}$$

From the above-noted distribution of first- and second-kind $\mathscr{D}^{[j]}$ on integer and half-integer j, we have the rule

$$\pi(\mathscr{D}^{[j]}\mathscr{D}^{[0]}\mathscr{D}^{[j]}) = (-1)^{2j}. \tag{6.8}$$

In fact, the general permutational property of the 3-j symbols is

$$\pi(\mathscr{D}^{[j_1]}\mathscr{D}^{[j_2]}\mathscr{D}^{[j_3]}) = (-1)^{j_1+j_2+j_3}. \tag{6.9}$$

The $\mathbb{B}^i$ matrix formulae (5.5.5)–(5.5.7) thus here take the form

$$\mathbb{B}^i(j_1 j_2 j_3) = (-1)^{2j_i}. \tag{6.10}$$

The definition (5.5.10) for coupling coefficients gives

$$\begin{aligned}\langle j_1 m_1 j_2 m_2 | j_3 m_3\rangle &= (-1)^{j_1+j_2+j_3}(-1)^{2j_2}\sqrt{2_{j_3}+1}\,(-1)^{j_3-m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3\end{pmatrix} \\ &= (-1)^{j_2-j_1-m_3}\sqrt{2j_3+1}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3\end{pmatrix},\end{aligned} \tag{6.11}$$

where we used (5.5.1) and (6.8) to see that we could multiply by $(-1)^{-2j_1}(-1)^{-2j_2}(-1)^{-2j_3} = (-1)^{2j_1}(-1)^{2j_2}(-1)^{2j_3} = 1$. Hence (5.5.10) leads to the conventional relationship ([8], p. 50; [9], p. 1) between 3-j symbols and coupling coefficients for R_3^* (Wigner coefficients).

These latter coefficients further, from (5.3.17) have the permutational property

$$\begin{aligned}\langle j_1 m_1 j_2 m_2 | j_3 m_3\rangle &= (-1)^{2j_1}(-1)^{2j_2}(-1)^{j_1+j_2+j_3}\langle j_2 m_2 j_1 m_1 | j_3 m_3\rangle \\ &= (-1)^{j_1+j_2-j_3}\langle j_2 m_2 j_1 m_1 | j_3 m_3\rangle\end{aligned} \tag{6.12}$$

where we used (5.5.1) to see that $(-1)^{2j_1}(-1)^{2j_2} = (-1)^{2j_3}$ and further used that $(-1)^{4j_3} = +1$.

If one restricts attention to the D_j with integer j, or, equivalently, studies just the rotation group R_3, one may establish a Wigner–Racah algebra based on standard orthogonal, i.e. *real* unitary, matrix irreps. This is described in [2].

7. Conclusion

This paper has developed the theory of the basic constructs in Wigner–Racah algebra, in our terminology *triple coefficients, coupling coefficients,* and *3-Γ symbols.* A transparent treatment of permutational symmetry in these coefficient types has been achieved by starting from triple coefficients rather than coupling coefficients. A thorough discussion of the Wigner–Eckart theorem has connected them to one of their immediate areas of application. Future work will demonstrate how the remaining Wigner–Racah algebra (recoupling formalism, 6-Γ and 9-Γ symbols) is built up from 3-Γ symbols [21, 59].

The results obtained for triple coefficients and coupling coefficients are generally valid for compact groups, whereas the formalism pertaining to 3-Γ symbols of course only is interesting for simple phase groups (or at least simple phase irreducible representations). A consequent focusing on *matrix* representations whenever relevant and the use of a separate notation for such representations (in contradistinction to the equivalence classes they generate) has, in our opinion, enabled a much clearer discussion of the consequences of complex conjugation than that hitherto present in the literature. By imposing the very mild restriction of having complex conjugate representations actually occur in complex matrix forms, considerable simplifications is introduced into the formalism.

Since 1940 there has been interest in generalizations of the Wigner–Racah algebra of the rotation (double) group. Wigner [14] chose to focus on the simply reducible groups. It is apparent from our exposition that the restrictive condition of being multiplicity-free is not crucial. A generalized rotation-group-like algebra has been established in Sect. 5.5 for a class of ambivalent groups having an algebra of irreducible representations which is "regular with respect to the Frobenius–Schur classification": real 3-Γ symbols may be chosen (if the group is simple phase), all Derome–Sharp matrices are unit matrices, and the "associativity of the invariant triple product" may be established by choosing a suitable connecting phase between coupling coefficients and triple coefficients.

Readers familiar with the Derome–Sharp–Butler formulation of Wigner–Racah algebra [15, 16, 17, 19, 22, 57] will see that there are many differences in *notation*, *terminology*, and *conventions*, as already indicated in connection with complex conjugation. Further, we put much more emphasis on 3-Γ symbols, which is natural because the groups we are interested in in papers II–VI are all simple phase.

We reserve for paper II our comments on the different approaches to the actual construction of Wigner–Racah algebras for the double groups.

Appendix

In this appendix we have collected some material of a mathematical nature which naturally belongs to the exposition of the present paper but which could be left out of the main text without inconvenience.

A.1. Remarks on tensor products of irreps

Let G be a compact group (cf. remark in Sect. 1) and let $\Gamma_1, \Gamma_2, \Gamma_3$ be three irreps of G of dimensions d_1, d_2, d_3. For any finite-dimensional rep Γ of G, let χ_Γ denote the character of Γ.

A.1.1. Multiplicities

Suppose Γ is any finite-dimensional rep of G and Γ' is an irrep of G. We define – just for the purpose of the present discussion – the symbol $\mathcal{M}(\Gamma'|\Gamma)$ to mean the *multiplicity* (or *frequency*) of Γ' in Γ, that is, the number of times Γ, when decomposed into a direct sum of irreps, contains an irrep equivalent to Γ'.

In case G is finite of order $|G|$, this number, as is known from character theory, may be computed by

$$\mathcal{M}(\Gamma'|\Gamma) = \frac{1}{|G|} \sum_{R \in G} \overline{\chi_{\Gamma'}(R)} \chi_\Gamma(R) \tag{A.1.1}$$

(and in general it may be found by the analogous formula involving an integral over G).

For matrix forms $\mathbb{\Gamma}_1, \mathbb{\Gamma}_2, \mathbb{\Gamma}_3$ of $\Gamma_1, \Gamma_2, \Gamma_3$ we have defined in Sect. 3.1 the linear space $\mathcal{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3)$ of fix-vectors for the tensor product rep $\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_2 \otimes \bar{\mathbb{\Gamma}}_3$. As noted there, the dimension of this space is equal to the multiplicity of the totally symmetric irrep 1_G of G in $\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_2 \otimes \bar{\mathbb{\Gamma}}_3$; thus,

$$\begin{aligned} \dim \mathcal{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3) &= \mathcal{M}(1_G|\bar{\mathbb{\Gamma}}_1 \otimes \bar{\mathbb{\Gamma}}_2 \otimes \bar{\mathbb{\Gamma}}_3) \\ &= \mathcal{M}(1_G|\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3), \end{aligned} \tag{A.1.2}$$

where the last equality comes from complex conjugation of the whole formula ($\dim \mathcal{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3)$ is, of course, a real number). Note that this number is independent of the particular matrix forms chosen for $\Gamma_1, \Gamma_2, \Gamma_3$; we shall thus often just write $\dim \mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$, even though we do not define the symbol $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ itself.

If σ is a permutation of the symbols 1, 2, 3, we have

$$\begin{aligned} \dim \mathcal{F}(\Gamma_{\sigma(1)}\Gamma_{\sigma(2)}\Gamma_{\sigma(3)}) &= \mathcal{M}(1_G|\Gamma_{\sigma(1)} \otimes \Gamma_{\sigma(2)} \otimes \Gamma_{\sigma(3)}) \\ &= \mathcal{M}(1_G|\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3) = \dim \mathcal{F}(\Gamma_1\Gamma_2\Gamma_3), \end{aligned} \tag{A.1.3}$$

where the second identity follows from (A.1.1), using the fact that

$$\chi_{\Gamma_{\sigma(1)}}\chi_{\Gamma_{\sigma(2)}}\chi_{\Gamma_{\sigma(3)}} = \chi_{\Gamma_1}\chi_{\Gamma_2}\chi_{\Gamma_3}. \tag{A.1.4}$$

From (A.1.1), one may furthermore show that

$$\mathcal{M}(1_G|\Gamma \otimes \Gamma') = \mathcal{M}(\bar{\Gamma}|\Gamma')$$

and thus, in particular, that

$$\mathcal{M}(1_G|\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3) = \mathcal{M}(\bar{\Gamma}_{\sigma(1)}|\Gamma_{\sigma(2)} \otimes \Gamma_{\sigma(3)}) \tag{A.1.5}$$

for any permutation σ. We may use this to prove the estimate (3.1.4). Choose σ so that the dimensions satisfy $d_{\sigma(1)} \geq d_{\sigma(2)} \geq d_{\sigma(3)}$. Let $\mathbb{\Gamma}_1, \mathbb{\Gamma}_2, \mathbb{\Gamma}_3$ be any matrix forms of $\Gamma_1, \Gamma_2, \Gamma_3$. Since the matrices in the rep $\mathbb{\Gamma}_{\sigma(2)} \otimes \mathbb{\Gamma}_{\sigma(3)}$ are of size $d_{\sigma(2)}d_{\sigma(3)} \times d_{\sigma(2)}d_{\sigma(3)}$ and the matrices in the irrep $\bar{\mathbb{\Gamma}}_{\sigma(1)}$ are of size $d_{\sigma(1)} \times d_{\sigma(1)}$, the latter irrep can obviously occur at the most $d_{\sigma(2)}d_{\sigma(3)}/d_{\sigma(1)}$ times as a subrepresentation of the former, i.e.

$$\begin{aligned} \mathcal{M}(\bar{\Gamma}_{\sigma(1)}|\Gamma_{\sigma(2)} \otimes \Gamma_{\sigma(3)}) &\leq d_{\sigma(2)}d_{\sigma(3)}/d_{\sigma(1)} \\ &= d_{\sigma(3)} \times (d_{\sigma(2)}/d_{\sigma(1)}) \leq d_{\sigma(3)} = \min\{d_1, d_2, d_3\}. \end{aligned} \tag{A.1.6}$$

Combining (A.1.6) with (A.1.5) and (A.1.2) gives the estimate (3.1.4). Note that we used the assumed irreducibility of the Γ_i in interpreting the number on the right side of (A.1.5) as the multiplicity of $\bar{\Gamma}_{\sigma(1)}$ in $\Gamma_{\sigma(2)} \otimes \Gamma_{\sigma(3)}$.

A.1.2. Permutational properties

The purpose of this section is to establish the connection between the permutational properties of sets of triple coefficients discussed in Sect. 3.2 and the information which is usually readily available in compilations of character and related tables, namely the resolution of tensor squares of irreps into symmetric and antisymmetric parts.

If V is a finite-dimensional vector space and n an integer (we shall actually only be interested in the cases $n=2$ and $n=3$), we can form the n-fold tensor product space $V^{\otimes n} = V \otimes \cdots \otimes V$ (n factors). It may now easily be verified that the prescription

$$\Pi_n(\sigma)(v_1 \otimes \cdots \otimes v_n) = v_{\sigma^{-1}(1)} \otimes \cdots \otimes v_{\sigma^{-1}(n)} \tag{A.1.7}$$

for all $v_1, \ldots, v_n \in V$ and all permutations σ of the symbols $1, \ldots, n$ defines an (operator) rep Π_n of the symmetric group S_n on $V^{\otimes n}$. The space $V^{\otimes n}$ can then be written as a direct sum

$$V^{\otimes n} = \bigoplus_{\substack{\text{irreps} \\ \Phi \text{ of } S_n}} (V^{\otimes n})_\Phi \tag{A.1.8}$$

where for each irrep Φ of S_n we denote by $(V^{\otimes n})_\Phi$ or $(V \otimes \cdots \otimes V)_\Phi$ *the* subspace of $V^{\otimes n}$ transforming under Π_n as Φ. (By this we mean that $(V^{\otimes n})_\Phi$ is the sum of all subspaces of $V^{\otimes n}$ which are invariant and irreducible under Π_n and transform as Φ.)

If $\mathcal{T}$ is an (operator) rep of G on V and Φ is an irrep of S_n, it can easily be shown that $(V^{\otimes n})_\Phi$ is invariant under the n-fold tensor product $\mathcal{T}^{\otimes n}$ of $\mathcal{T}$ (which is a rep on $V^{\otimes n}$); we shall denote the rep of G on $(V^{\otimes n})_\Phi$ formed by restriction of all the operators $\mathcal{T}^{\otimes n}(R)$, $R \in G$, to this subspace as $(\mathcal{T}^{\otimes n})_\Phi$.

To proceed from here, we recall the basic facts about irreps of S_2 and S_3 by giving their character tables:

	S_2	$\{e\}$	$\{(12)\}$	
irreps	s or $[2]$	1	1	(totally *s*ymmetric irrep)
	a or $[1^2]$	1	−1	(*a*lternating irrep)

(A.1.9)

	S_3	$\{e\}$	$\{(123), (123)^{-1}\}$	$\{(12), (23), 31)\}$
		conjugacy classes		
irreps	$[3]$	1	1	1
	$[2, 1]$	2	−1	0
	$[1^3]$	1	1	−1

(A.1.10)

The symbols [2], $[1^2]$ etc. for the irreps derive from the theory of Young diagrams (e.g. [60, 61]).

Suppose now that $\mathcal{T}$ from before is equivalent to some irrep Γ of G. For $n=2$, we obtain the reps $(\mathcal{T}\otimes\mathcal{T})_{[2]}$ and $(\mathcal{T}\otimes\mathcal{T})_{[1^2]}$ from the above considerations; we shall use the symbols

$$(\Gamma\otimes\Gamma)_{[2]} \quad \text{or} \quad \Gamma\otimes_s\Gamma$$

and (A.1.11)

$$(\Gamma\otimes\Gamma)_{[1^2]} \quad \text{or} \quad \Gamma\otimes_a\Gamma$$

for the equivalence classes of these reps. For $n=3$, we get in a similar manner the three reps $(\Gamma\otimes\Gamma\otimes\Gamma)_{[3]}$, $(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]}$ and $(\Gamma\otimes\Gamma\otimes\Gamma)_{[1^3]}$. It turns out that the following general formulas giving the connection between the character χ_Γ of Γ and the characters of the S_n-adapted parts of its second and third powers may be derived (e.g., [53]; [61], II, p. 73):

$$\chi_{\Gamma\otimes_s\Gamma}(R)=\tfrac{1}{2}\chi_\Gamma(R)^2+\tfrac{1}{2}\chi_\Gamma(R^2);$$
$$\chi_{\Gamma\otimes_a\Gamma}(R)=\tfrac{1}{2}\chi_\Gamma(R)^2-\tfrac{1}{2}\chi_\Gamma(R^2);$$
$$\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[3]}}(R)=\tfrac{1}{6}\chi_\Gamma(R)^3+\tfrac{1}{2}\chi_\Gamma(R)\chi_\Gamma(R^2)+\tfrac{1}{3}\chi_\Gamma(R^3);$$
$$\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]}}(R)=\tfrac{2}{3}\chi_\Gamma(R)^3-\tfrac{2}{3}\chi_\Gamma(R^3);$$
$$\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[1^3]}}(R)=\tfrac{1}{6}\chi_\Gamma(R)^3-\tfrac{1}{2}\chi_\Gamma(R)\chi_\Gamma(R^2)+\tfrac{1}{3}\chi_\Gamma(R^3); \quad \text{for all } R\in G. \tag{A.1.12}$$

Note that (of course) $\chi_{\Gamma\otimes_s\Gamma}+\chi_{\Gamma\otimes_a\Gamma}=\chi_\Gamma^2$ and $\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[3]}}+\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]}}+\chi_{(\Gamma\otimes\Gamma\otimes\Gamma)_{[1^3]}}=\chi_\Gamma^3$.

We may now turn to the situations considered in Sect. 3.2. In part (A) of that section the relevant information is the frequency of the totally symmetric irrep in $(\Gamma_1\otimes_s\Gamma_1)\otimes\Gamma_3$ and $(\Gamma_1\otimes_a\Gamma_1)\otimes\Gamma_3$, since obviously

$$\dim \mathscr{F}_s(\Gamma_1\Gamma_1\Gamma_3)=\mathscr{M}(1_G|(\Gamma_1\otimes_s\Gamma_1)\otimes\Gamma_3)$$

and (A.1.13)

$$\dim \mathscr{F}_a(\Gamma_1\Gamma_1\Gamma_3)=\mathscr{M}(1_G|(\Gamma_1\otimes_a\Gamma_1)\otimes\Gamma_3).$$

But by the equation preceding (A.1.5), we have

$$\mathscr{M}(1_G|(\Gamma_1\otimes_s\Gamma_1)\otimes\Gamma_3)=\mathscr{M}(\bar{\Gamma}_3|\Gamma_1\otimes_s\Gamma_1)$$

and (A.1.14)

$$\mathscr{M}(1_G|(\Gamma_1\otimes_a\Gamma_1)\otimes\Gamma_3)=\mathscr{M}(\bar{\Gamma}_3|\Gamma_1\otimes_a\Gamma_1).$$

Formulae (A.1.14) are important in that they show that $\dim \mathscr{F}_s(\Gamma_1\Gamma_1\Gamma_3)$ and $\dim \mathscr{F}_a(\Gamma_1\Gamma_1\Gamma_3)$ can be found directly from the information available in many tables of irrep tensor products (e.g. [42, 43]), namely the separate resolution of $\Gamma\otimes_s\Gamma$ and $\Gamma\otimes_a\Gamma$ into irreps.

Turning to the situation in part (B) of Sect. 3.2, we see that the information we seek there is

$$\dim \mathscr{F}_{[3]}(\Gamma\Gamma\Gamma) = \mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[3]})$$

and (A.1.15)

$$\dim \mathscr{F}_{[1^3]}(\Gamma\Gamma\Gamma) = \mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[1^3]}).$$

Eqs. (A.1.1), (A.1.12), and (A.1.15) in principle enable us to calculate these dimensions. However, one could again ask whether the standard information, $\mathscr{M}(\bar{\Gamma}|\Gamma\otimes_s\Gamma)$ and $\mathscr{M}(\bar{\Gamma}|\Gamma\otimes_a\Gamma)$, is of any relevance. If one calculates these quantities as well as those on the right sides of Eqs. (A.1.15) by using (A.1.1) and (A.1.12), one gets the result that

$$\mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[3]}) = \mathscr{M}(\bar{\Gamma}|\Gamma\otimes_s\Gamma) - \tfrac{1}{2}\mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]})$$

and (A.1.16)

$$\mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[1^3]} = \mathscr{M}(\bar{\Gamma}|\Gamma\otimes_a\Gamma) - \tfrac{1}{2}\mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]}),$$

that is, $\dim \mathscr{F}_{[3]}(\Gamma\Gamma\Gamma)$ may be computed as $\mathscr{M}(\bar{\Gamma}|\Gamma\otimes_s\Gamma)$ and $\dim \mathscr{F}_{[1^3]}(\Gamma\Gamma\Gamma)$ as $\mathscr{M}(\bar{\Gamma}|\Gamma\otimes_a\Gamma)$ *if and only if* $\mathscr{M}(1_G|(\Gamma\otimes\Gamma\otimes\Gamma)_{[2,1]})=0$, a condition which is (cf. Sect. 3.2) equivalent to Γ being a *simple phase* irrep. Note from (A.1.12) that Γ is simple phase if and only if

$$\frac{1}{|G|}\sum_{R\in G}\frac{2}{3}[\chi_\Gamma(R)^3 - \chi_\Gamma(R^3)] = 0$$

or (A.1.17)

$$\sum_{R\in G}\chi_\Gamma(R)^3 = \sum_{R\in G}\chi_\Gamma(R^3)$$

(for G finite).

Proceeding from triples of irreps to quadruples etc., one finds that the property analogous to the simple phase property (i.e. occurrence of only the totally symmetric and the alternating irrep of the symmetric group) is not even possessed by a simply reducible group like SU(2) [62].

A.2. Discussion of Eq. (3.1.5)

If $(\mathbb{c}_1, \ldots, \mathbb{c}_N)$ is an orthonormal basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$, i.e.

$$\mathbb{c}_\beta^\dagger \mathbb{c}_{\beta'} = \delta(\beta, \beta') \quad \text{for all } \beta, \beta', \tag{A.2.1}$$

then it may easily be shown that the matrix

$$\mathbb{P} = \sum_{\beta=1}^{N} \mathbb{c}_\beta \mathbb{c}_\beta^\dagger \tag{A.2.2}$$

has the properties $\mathbb{P}^\dagger = \mathbb{P}$; $\mathbb{P}^2 = \mathbb{P}$; $\mathbb{P}\mathbb{c}_\beta = \mathbb{c}_\beta$ for all $\beta = 1, \ldots, N$. Further, for a column matrix $\mathbb{x}$, $\langle\mathbb{x}|\mathbb{c}_\beta\rangle = 0$ for all β implies $\mathbb{P}\mathbb{x} = \mathbb{0}$. Thus $\mathbb{P}$ is the matrix for the orthogonal projection onto $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$.

In Sect. II of [54] we dsicussed the fact that

$$\mathbb{\Gamma} = |G|^{-1} \sum_{R \in G} \bar{\mathbb{\Gamma}}_1(R) \otimes \bar{\mathbb{\Gamma}}_2(R) \otimes \bar{\mathbb{\Gamma}}_3(R) \tag{A.2.3}$$

is also the matrix of the orthogonal projection onto $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$. Writing out the equation $\mathbb{P} = \mathbb{\Gamma}$ in coordinates and taking the complex conjugate on both sides gives Eq. (3.1.5).

Thus this equation is of a rather general nature and does not for its verification require the "long manipulation" mentioned in ([52], p. 102). Note that it has not been necessary to assume the $\mathbb{\Gamma}_i$ irreducible. A proof of an analogue of Eq. (3.1.5) for coupling coefficients using also the projection operator idea is given in [36]. A proof of Eq. (3.1.5) in a context completely different from the present one appears in [35].

In the special case of the rotation group, which is multiplicity-free, the sum on the left-hand side of Eq. (3.1.5) has only one term. In [7] Wigner used the analogue in Eq. (3.1.5) for coupling coefficients in his derivation of coupling coefficients for the rotation group (Sect. 6). Further elaborations on this kind of formula for the rotation group may be found in [63].

A.3. Investigation of the matrix $\mathbb{C}$ defined in Eq. (3.3.6)

Suppose $\mathbb{\Delta}_i$ and $\mathbb{\Delta}_j$ are two of the irreps appearing in (3.3.5). We form the matrix

$$\mathbb{C}_{ij} = \mathbb{C}_i^\dagger \mathbb{C}_j. \tag{A.3.1}$$

From (3.3.4), applied to $\mathbb{\Delta}_i$ and $\mathbb{\Delta}_j$, and the unitarity of the considered matrix reps, we then have

$$\begin{aligned}
\mathbb{C}_{ij}\mathbb{\Delta}_j(R) \\
&= \mathbb{C}_i^\dagger(\mathbb{C}_j\mathbb{\Delta}_j(R)) = \mathbb{C}_i^\dagger([\mathbb{\Gamma}_1(R)\otimes\mathbb{\Gamma}_2(R)]\mathbb{C}_j) \\
&= ([\mathbb{\Gamma}_1(R)\otimes\mathbb{\Gamma}_2(R)]^\dagger\mathbb{C}_i)^\dagger\mathbb{C}_j = ([\mathbb{\Gamma}_1(R^{-1})\otimes\mathbb{\Gamma}_2(R^{-1})]\mathbb{C}_i)^\dagger\mathbb{C}_j \\
&= (\mathbb{C}_i\mathbb{\Delta}_i(R^{-1}))^\dagger\mathbb{C}_j = \mathbb{\Delta}_i(R^{-1})^\dagger\mathbb{C}_i^\dagger\mathbb{C}_j \\
&= \mathbb{\Delta}_i(R)\mathbb{C}_{ij} \quad \text{for all } R \in G.
\end{aligned} \tag{A.3.2}$$

By Schur's lemma and the assumption that *equivalent* irreps occurring in (3.3.5) are chosen *identical* we conclude that

$$\mathbb{C}_i^\dagger\mathbb{C}_j = \mathbb{C}_{ij} = \mathbb{0} \quad \text{if } \mathbb{\Delta}_i \neq \mathbb{\Delta}_j \tag{A.3.3}$$

and

$$\mathbb{C}_i^\dagger\mathbb{C}_j = \mathbb{C}_{ij} = \lambda_{ij}\mathbb{1} \tag{A.3.4}$$

for some suitable number λ_{ij} if $\mathbb{\Delta}_i = \mathbb{\Delta}_j$. We stress that $\mathbb{\Delta}_i = \mathbb{\Delta}_j$ here means $\mathbb{\Delta}_i(R) = \mathbb{\Delta}_j(R)$ for all $R \in G$.

If $i \neq j$ in (A.3.4), the matrices $\mathbb{C}_i$ and $\mathbb{C}_j$ have been constructed from mutually orthogonal sets of triple coefficients denoted by, say,

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_i} \quad \text{and} \quad \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_j}$$

(we write $\Delta = \Delta_i = \Delta_j$). Letting $d = \dim \Delta$ and denoting by Tr the trace of a matrix, we then have

$$d\lambda_{ij} = \mathrm{Tr}\,(\lambda_{ij}\mathbb{1}) = \mathrm{Tr}\,(\mathbb{C}_i^\dagger \mathbb{C}_j)$$

$$= \sum_\delta \sum_{\gamma_1\gamma_2} \overline{\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_i}} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_j} = 0 \tag{A.3.5}$$

that is,

$$\mathbb{C}_i^\dagger \mathbb{C}_j = \lambda_{ij}\mathbb{1} = \mathbb{0}. \tag{A.3.6}$$

In conclusion, there are numbers $\lambda_1, \ldots, \lambda_p$ such that

$$\mathbb{C}_i^\dagger \mathbb{C}_j = \delta_{ij}\lambda_i \quad \text{for } i, j = 1, \ldots, p. \tag{A.3.7}$$

Suppose, given an index i, that $\mathbb{C}_i$ was constructed from a set of triple coefficients

$$\sqrt{\dim \Delta_i} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta_i \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_i}.$$

Putting $d_i = \dim \Delta_i$, we get by the same type of calculation as in (A.3.5) that

$$d_i\lambda_i = \sum_{\gamma_1\gamma_2\delta} d_i \left| \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Delta_i \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_{\beta_i} \right|^2 > 0 \tag{A.3.8}$$

so that $\lambda_i > 0$. We see from (A.3.7) and (A.3.8) that $\mathbb{C}$ defined in (3.3.6) is non-singular. If triple coefficients normalized according to (3.3.10) have been used we see from (A.3.8) that all $\lambda_i = 1$; eq. (A.3.7) then gives

$$\mathbb{C}^\dagger \mathbb{C} = \begin{pmatrix} \mathbb{C}_1^\dagger \\ \mathbb{C}_2^\dagger \\ \vdots \\ \mathbb{C}_p^\dagger \end{pmatrix} (\mathbb{C}_1 \mathbb{C}_2 \cdots \mathbb{C}_p) = \mathbb{1} \tag{A.3.9}$$

i.e. $\mathbb{C}$ is unitary.

Note that Eq. (3.1.6) follows by writing (A.3.4) in coordinates in the case $i = j$; the argument of (A.3.8) shows that $a \geq 0$ in (3.1.6).

A.4. Associativity of invariant triple products

In this section we shall consider the following situation: A finite or compact simple phase (cf. Sect. 3.2) group G is given. A system of standard unitary matrix irreps of G and a corresponding complete system of sets of 3-Γ symbols are also assumed to be given. Suppose that three (finite-dimensional) Hilbert spaces V_1, V_2, V_3 and unitary operator reps $\mathcal{T}_1$, $\mathcal{T}_2$, $\mathcal{T}_3$ of G on V_1, V_2, and V_3, respectively, are given, and that for each $i=1, 2, 3$ an orthonormal basis consisting of vectors $\varphi^{\Gamma_i}_{\gamma_i}=|\Gamma_i\gamma_i\rangle$ may be chosen in V_i transforming under $\mathscr{T}_i$ as the standard form $\mathbf{\Gamma}_i$ of a certain irrep Γ_i of G (that is, satisfying

$$\mathscr{T}_i(R)|\Gamma_i\gamma_i\rangle=\sum_{\gamma_i'}\Gamma_i(R)_{\gamma_i'\gamma_i}|\Gamma_i\gamma_i'\rangle \quad \text{for all } R\in G). \tag{A.4.1}$$

We are interested in fix-vectors for the triple tensor product rep $\mathscr{T}_1\otimes\mathscr{T}_2\otimes\mathscr{T}_3$ in the tensor product space $V_1\otimes V_2\otimes V_3$ spanned by the products $\varphi^{\Gamma_1}_{\gamma_1}\otimes\varphi^{\Gamma_2}_{\gamma_2}\otimes\varphi^{\Gamma_3}_{\gamma_3}=|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle$. Such fix-vectors have been called *invariant triple products* [8]. By the definition of 3-Γ symbols, a vector of the form

$$\sum_{\gamma_1\gamma_2\gamma_3}\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{\beta}|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle \tag{A.4.2}$$

is such a fix-vector (where β as usual allows for possible multiplicity in the triple $\Gamma_1\Gamma_2\Gamma_3$). However, fix-vectors may also be formed by coupling (tensoring) together the $|\Gamma_i\gamma_i\rangle$ two at a time using coupling coefficients derived by Eq. (5.3.14) from the given 3-Γ symbols. Our aim here is to show how a suitable choice of the phase $\varphi(\Gamma_1\Gamma_2\Gamma_3\beta)$ in (5.3.14) – for groups satisfying a certain technical condition on their "representation algebra" (Eq. (A.4.12) below) – may ensure that the two fix-vectors arrived at by the *coupling schemes*

$$\begin{aligned}&\text{(i) } \Gamma_1\otimes\Gamma_2\to\bar{\Gamma}_3,\ \bar{\Gamma}_3\otimes\Gamma_3\to 1_G\\ &\text{(ii) } \Gamma_2\otimes\Gamma_3\to\bar{\Gamma}_1,\ \Gamma_1\otimes\bar{\Gamma}_1\to 1_G\end{aligned} \tag{A.4.3}$$

are identical and how the *same* choice of the phase may ensure that, in the case of G ambivalent (no irreps of the third Frobenius–Schur kind (Sect. 5.2)), one arrives *also* at identical fix-vectors using either of the coupling schemes

$$\begin{aligned}&\text{(i) } \Gamma_1\otimes\Gamma_2\to\Gamma_3,\ \Gamma_3\otimes\Gamma_3\to 1_G\\ &\text{(ii) } \Gamma_2\otimes\Gamma_3\to\Gamma_1,\ \Gamma_1\otimes\Gamma_1\to 1_G\end{aligned} \tag{A.4.4}$$

(the meaning of these coupling schemes is explained below). The property alluded to has been called the "associative property" of the invariant triple product [8].

Since a complete set of 3-Γ symbols for G is supposed to be given we have in particular for each irrep Γ the 3-Γ symbols

$$\begin{pmatrix}\bar{\Gamma} & 1_G & \Gamma\\ \gamma & 0 & \gamma'\end{pmatrix} \quad\text{and}\quad \begin{pmatrix}\Gamma & 1_G & \bar{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix}$$

(since, as remarked in Sect. 5.3, $\dim\mathscr{F}(\bar{\Gamma}1_G\Gamma)=1=\dim\mathscr{F}(\Gamma1_G\bar{\Gamma})$ for any irrep Γ). By the discussion in Sect. 5.3, these 3-Γ symbols always satisfy

$$\begin{aligned}\operatorname{sign}(\Gamma1_G\bar{\Gamma})\delta(\gamma,\gamma')(\dim\Gamma)^{-1/2}&=\begin{pmatrix}\Gamma & 1_G & \bar{\Gamma}\\ \gamma & 0 & \gamma'\end{pmatrix}\\ &=\pi(\bar{\Gamma}1_G\Gamma)\begin{pmatrix}\bar{\Gamma} & 1_G & \Gamma\\ \gamma' & 0 & \gamma\end{pmatrix}\\ &=\pi(\bar{\Gamma}1_G\Gamma)\operatorname{sign}(\bar{\Gamma}1_G\Gamma)\delta(\gamma,\gamma')(\dim\Gamma)^{-1/2}\end{aligned} \tag{A.4.5}$$

where sign $(\bar{\Gamma}1_G\Gamma)$ and sign $(\Gamma 1_G\bar{\Gamma})$ are phase factors satisfying sign $(\bar{\Gamma}1_G\Gamma)=\pi(\Gamma 1_G\bar{\Gamma})$ sign $(\Gamma 1_G\bar{\Gamma})$ for all Γ and sign $(\bar{\Gamma}1_G\Gamma)=+1$ for all standard Γ of the first or second kind.

We now study the first coupling scheme, (i), in (A.4.3).

We assume a fixed but arbitrary value of the multiplicity index β. By "coupling Γ_1 and Γ_2 to get $\bar{\Gamma}_3$" we mean forming the vectors

$$|\beta\bar{\Gamma}_3\gamma_3\rangle_{V_1\otimes V_2}=\sum_{\gamma_1\gamma_2}\langle\Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\bar{\Gamma}_3\gamma_3\rangle|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle \tag{A.4.6}$$

in $V_1\otimes V_2$ (these make up a set transforming as $\bar{\Gamma}_3$ under $\mathscr{T}_1\otimes\mathscr{T}_2$). The subsequent coupling of $\bar{\Gamma}_3$ with Γ_3 to get the totally symmetric irrep 1_G consists in forming the vector

$$\begin{aligned}|\beta 1_G 0\rangle^{(i)}_{V_1\otimes V_2\otimes V_3}&=\sum_{\gamma_3\gamma_3'}\langle\bar{\Gamma}_3\gamma_3'\Gamma_3\gamma_3|1_G0\rangle|\beta\bar{\Gamma}_3\gamma_3'\rangle_{V_1\otimes V_2}|\Gamma_3\gamma_3\rangle\\&=\sum_{\gamma_1\gamma_2\gamma_3\gamma_3'}\langle\bar{\Gamma}_3\gamma_3'\Gamma_3\gamma_3|1_G0\rangle\langle\Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\bar{\Gamma}_3\gamma_3'\rangle|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle\end{aligned} \tag{A.4.7}$$

in $V_1\otimes V_2\otimes V_3$; this vector is, by construction, a fix-vector for $\mathscr{T}_1\otimes\mathscr{T}_2\otimes\mathscr{T}_3$, that is, an invariant triple product.

The coupling scheme (ii) in (A.4.3) leads by a completely analogous two-step construction, with a chosen multiplicity index β', to the fix-vector

$$\begin{aligned}&|\beta' 1_G 0\rangle^{(ii)}_{V_1\otimes V_2\otimes V_3}\\&=\sum_{\gamma_1'\gamma_1\gamma_2\gamma_3}\langle\Gamma_1\gamma_1\bar{\Gamma}_1\gamma_1'|1_G0\rangle\langle\Gamma_2\gamma_2\Gamma_3\gamma_3|\beta'\bar{\Gamma}_1\gamma_1'\rangle|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle.\end{aligned} \tag{A.4.8}$$

We now express the coupling coefficients appearing in the expansions of $|\beta 1_G 0\rangle^{(i)}_{V_1\otimes V_2\otimes V_3}$ and $|\beta' 1_G 0\rangle^{(ii)}_{V_1\otimes V_2\otimes V_3}$ as linear combinations of the $|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle$, by 3-$\Gamma$ symbols, using (5.3.14). This gives, remembering (A.4.5),

$$\begin{aligned}&|\beta 1_G 0\rangle^{(i)}_{V_1\otimes V_2\otimes V_3}\\&=\sum_{\gamma_1\gamma_2\gamma_3\gamma_3'}\varphi(\bar{\Gamma}_3\Gamma_3 1G)\begin{pmatrix}\Gamma_3 & \bar{\Gamma}_3 & 1_G\\ \gamma_3' & \gamma_3 & 0\end{pmatrix}\varphi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)\sqrt{\dim\Gamma_3}\\&\quad\times\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3'\end{pmatrix}_\beta|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle\\&=\sum_{\gamma_1\gamma_2\gamma_3}\varphi(\bar{\Gamma}_3\Gamma_3 1_G)\,\text{sign}\,(\bar{\Gamma}_3 1_G\Gamma_3)\varphi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta\\&\quad\times|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle\end{aligned} \tag{A.4.9}$$

and

$$|\beta' 1_G 0\rangle^{(\mathrm{ii})}_{V_1\otimes V_2\otimes V_3}$$

$$= \sum_{\gamma_1\gamma_1'\gamma_2\gamma_3} \varphi(\Gamma_1\bar{\Gamma}_1 1_G)\begin{pmatrix}\bar{\Gamma}_1 & \Gamma_1 & 1_G\\ \gamma_1 & \gamma_1' & 0\end{pmatrix}\varphi(\Gamma_2\Gamma_3\bar{\Gamma}_1\beta')\sqrt{\dim\Gamma_1}\begin{pmatrix}\bar{\Gamma}_2 & \bar{\Gamma}_3 & \bar{\Gamma}_1\\ \gamma_2 & \gamma_3 & \gamma_1'\end{pmatrix}_{\beta'}$$

$$\times|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle$$

$$= \sum_{\gamma_1\gamma_2\gamma_3} \varphi(\Gamma_1\bar{\Gamma}_1 1_G)\pi(\bar{\Gamma}_1 1_G\Gamma_1)\ \mathrm{sign}\,(\bar{\Gamma}_1 1_G\Gamma_1)\varphi(\bar{\Gamma}_1\Gamma_2\Gamma_3\beta')\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{\beta'}$$

$$\times|\Gamma_1\gamma_1\rangle|\Gamma_2\gamma_2\rangle|\Gamma_3\gamma_3\rangle. \quad \text{(A.4.10)}$$

(The reader should notice that we have here used (5.3.14) in the way described in Sect. 5.3, that is, we allow conjugated standard irreps in the coupling coefficient on the left-hand side of the formula but then agree that entities of the type "$\bar{\bar{\Gamma}}$" appearing in this situation on the right-hand side are immediately rewritten using $\bar{\bar{\Gamma}}=\Gamma$ before further use is made of the right-hand side.)

We see now, firstly, that there is no chance of having $|\beta 1_G 0\rangle^{(\mathrm{i})}_{V_1\otimes V_2\otimes V_3} = |\beta' 1_G 0\rangle^{(\mathrm{ii})}_{V_1\otimes V_2\otimes V_3}$ unless $\beta=\beta'$ and, secondly, that if the equality is to hold for all standard irrep triples $\Gamma_1\Gamma_2\Gamma_3$ and all β, the phase function $\varphi(\Gamma_1\Gamma_2\Gamma_3\beta)$ must satisfy

$$\varphi(\bar{\Gamma}_3\Gamma_3 1_G)\ \mathrm{sign}\,(\bar{\Gamma}_3 1_G\Gamma_3)\varphi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)$$

$$= \varphi(\Gamma_1\bar{\Gamma}_1 1_G)\pi(\bar{\Gamma}_1 1_G\Gamma_1)\ \mathrm{sign}\,(\bar{\Gamma}_1 1_G\Gamma_1)\varphi(\bar{\Gamma}_1\Gamma_2\Gamma_3\beta) \quad \text{(A.4.11)}$$

for all standard irrep triples $\Gamma_1\Gamma_2\Gamma_3$ and all β. Although this condition looks a little involved it turns out to be relatively easy to spot a solution if one assumes the 3-Γ symbols chosen for G to have the property that

$$\pi(\Gamma_1 1_G\bar{\Gamma}_1)\pi(\Gamma_2 1_G\bar{\Gamma}_2)\pi(\Gamma_3 1_G\bar{\Gamma}_3) = 1 \quad \text{(A.4.12)}$$

whenever $\dim\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3) > 0$.

This condition is always fulfilled for the 3-Γ symbols for the non-commutative double groups generated by the procedure of paper II (see Sect. 4.4 there). For ambivalent groups G the condition reduces to a "group-theoretic" one (the "regularity" of the "representation algebra" of G discussed in Ref. [54]). For the particularly nice ambivalent groups studied in Sect. 5.5 the condition is always fulfilled (see Eq. (5.5.1)). Butler has investigated to what further extent the condition may be fulfilled for various groups [45, 17].

Under this assumption the reader may easily verify that the phase function defined by

$$\varphi(\Gamma_1\Gamma_2\Gamma_3\beta) = \pi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)\pi(\Gamma_1 1_G\bar{\Gamma}_1)\ \mathrm{sign}\,(\bar{\Gamma}_3 1_G\Gamma_3) \quad \text{(A.4.13)}$$

(for all irreps $\Gamma_1\Gamma_2\Gamma_3$ which are either standard irreps or conjugates of first- or second-kind standard irreps) solves the problem. We believe that (A.4.13) is the simplest formula leading to a phase fulfilling the stated requirement, and even though we have not proved in a strict sense that this is the case, we shall adopt (A.4.13) as our definition of $\varphi(\Gamma_1\Gamma_2\Gamma_3\beta)$.

An appealing feature of this choice is, as anticipated above, that formula (A.4.13) also ensures the associativity of the invariant triple products arrived at by the schemes (i) and (ii), respectively, in (A.4.4), in the special case of ambivalent groups satisfying (A.4.12). We leave it to the reader to check this in detail. (The two schemes in (A.4.4) do *not in general* lead to non-zero triple fix-vectors since coupling coefficients of the type $\langle \Gamma\gamma\Gamma\gamma'|1_G 0\rangle$ are zero when Γ is of the third kind). In the even more special case of the rotation group, formula (A.4.13) leads to exactly the conventional phase relation between coupling coefficients and 3-j symbols (see Eq. (6.11)).

For further discussion of associativity and its connection with *recoupling* coefficients, see [21, 59].

Summarizing, the requirement that "invariant triple products" should have the "associativity property" has led us to fix the relationship between 3-Γ symbols and coupling coefficients by the formula

$$\langle \Gamma_1\gamma_1\Gamma_2\gamma_2|\beta\Gamma_3\gamma_3\rangle$$

$$= \pi(\Gamma_1\Gamma_2\bar{\Gamma}_3\beta)\pi(\Gamma_1 1_G\bar{\Gamma}_1)\,\mathrm{sign}\,(\bar{\Gamma}_3 1_G\Gamma_3)\sqrt{\dim \Gamma_3}\begin{pmatrix}\bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \qquad (A.4.14)$$

for all Γ_1, Γ_2, Γ_3 which are standard irreps or complex conjugates of first- or second-kind standard irreps.

In [50] the reverse line of argument was followed: by an analysis of invariant triple products the phase required to produce 3-Γ symbols from coupling coefficients for the octahedral double group was determined.

A.5. On the existence of unit Derome–Sharp $\mathbb{A}$ matrices

With reference to the remarks in Sect. 5.4, assume $\Gamma_1, \Gamma_2, \Gamma_3$ to be standard unitary matrix irreps and suppose $(\mathfrak{c}_1, \ldots, \mathfrak{c}_N)$ and $(\tilde{\mathfrak{c}}_1, \ldots, \tilde{\mathfrak{c}}_N)$ to be orthonormal bases in the fix-spaces $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ and $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3)$, respectively, chosen according to the conjugation conventions of Sect. 5.3.1 to the extent that these are relevant. Assume further that the $\mathbb{A}$ matrix with elements $\mathbb{A}_{\alpha\beta} = \langle \mathfrak{c}_\alpha|\bar{\tilde{\mathfrak{c}}}_\beta\rangle$ is a symmetric matrix. We shall prove now that in this situation we may choose new fix-vector bases generating a unit $\mathbb{A}$ matrix. We have to distinguish several cases:

(i) If all three irreps are of the third kind, there are no ties between our basis choices in $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ and $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3)$, and the argument may run as follows: Since $\mathbb{A}$ is symmetric and unitary, it may be written $\mathbb{A} = \mathbb{Q}\bar{\mathbb{Q}}^{-1}$ with a suitably chosen unitary matrix $\mathbb{Q}$ (e.g. [8] Appendix C; [64] pp. 57–58). Choose $(\mathfrak{c}'_1, \ldots, \mathfrak{c}'_N)$ defined by

$$(\mathfrak{c}'_1 \cdots \mathfrak{c}'_N) = (\mathfrak{c}_1 \cdots \mathfrak{c}_N)\mathbb{Q} \qquad (A.5.1)$$

as the new orthonormal basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ and

$$(\tilde{\mathfrak{c}}'_1 \cdots \tilde{\mathfrak{c}}'_N) = (\tilde{\mathfrak{c}}_1 \cdots \tilde{\mathfrak{c}}_N)\mathbb{Q} \qquad (A.5.2)$$

as the new basis for $\mathscr{F}(\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3)$. We then have

$$(\overline{\tilde{c}'_1} \cdots \overline{\tilde{c}'_N}) = (\bar{\tilde{c}}_1 \cdots \bar{\tilde{c}}_N)\bar{\mathbb{Q}} = (c_1 \cdots c_N)\mathbb{A}\bar{\mathbb{Q}}$$
$$= (c_1 \cdots c_N)\mathbb{Q} = (c'_1 \cdots c'_N), \tag{A.5.3}$$

showing that the new $\mathbb{A}$ matrix for $\Gamma_1\Gamma_2\Gamma_3$ is the unit matrix. Note that the new $\mathbb{A}$ matrix for $\bar{\Gamma}_1\bar{\Gamma}_2\bar{\Gamma}_3$ simultaneously becomes also the unit matrix; thus, in this case, our argument takes care of *two standard* irrep triples.

(ii) Suppose, to go to the opposite extreme, that all three Γ_i have conjugating matrices $\mathbb{U}_i$. In this case, we are dealing with only *one standard* irrep triple, but our conventions lead to formula (5.4.8) for the $\mathbb{A}$ matrix for any choice of an orthonormal basis in $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$. We proceed initially as in (i), choosing $\mathbb{Q}$ and defining $(c'_1, \ldots, c'_N)$ as in (A.5.1), but then must define $(\tilde{c}'_1, \ldots, \tilde{c}'_N)$ by

$$\tilde{c}'_\beta = \mathbb{U}c'_\beta \quad \text{for all } \beta = 1, \ldots, N, \tag{A.5.4}$$

where $\mathbb{U} = \mathbb{U}_1^{-1} \otimes \mathbb{U}_2^{-1} \otimes \mathbb{U}_3^{-1}$. We then get

$$(\overline{\tilde{c}'_1} \cdots \overline{\tilde{c}'_N}) = (\overline{\mathbb{U}c'_1} \cdots \overline{\mathbb{U}c'_N})$$
$$= (\bar{\mathbb{U}}\bar{c}_1 \cdots \bar{\mathbb{U}}\bar{c}_N)\mathbb{Q} = (c_1 \cdots c_N)\mathbb{A}\bar{\mathbb{Q}}$$
$$= (c_1 \cdots c_N)\mathbb{Q} = (c'_1 \cdots c'_N) \tag{A.5.5}$$

so that the new $\mathbb{A}$ matrix is a unit matrix.

(iii) In the cases where precisely one of the Γ_i or precisely two of the Γ_i are of the third kind, proofs may be constructed along similar lines. In all these cases there are again *two standard* irrep triples involved, and our conventions give a *partial* tie between our basis choices in the relevant fix-spaces. Note, however, that this time we may not be sure to be able to produce *simultaneously* unit $\mathbb{A}$ matrices for the two triples involved. In fact, from our definitions, one may easily derive formulae like e.g.

$$\mathbb{A}(\Gamma_1\bar{\Gamma}_2\bar{\Gamma}_3) = \pi(\Gamma_1 1_G \Gamma_1)\mathbb{A}(\Gamma_1\Gamma_2\Gamma_3) \tag{A.5.6}$$

and

$$\mathbb{A}(\Gamma_1\Gamma_2\bar{\Gamma}_3) = \pi(\Gamma_1 1_G \Gamma_1)\pi(\Gamma_2 1_G \Gamma_2)\mathbb{A}(\Gamma_1\Gamma_2\Gamma_3) \tag{A.5.7}$$

for the cases with precisely two third-kind irreps and precisely one third-kind irrep, respectively. These formulae are a consequence of our conjugation conventions for first- and second-kind irreps. We see that if, for example, Γ_1 in (A.5.6) is of the second kind, we *necessarily* have

$$\mathbb{A}(\Gamma_1\bar{\Gamma}_2\bar{\Gamma}_3) = -\mathbb{A}(\Gamma_1\Gamma_2\Gamma_3).$$

An example to illustrate (A.5.7) could be the triple $E_1E_{1/2}R_1$ in D_3^* (see paper III).

[As noted in Sect. 5.4, Butler has also discussed the possibilities of obtaining unit $\mathbb{A}$ matrices. Essentially the same proof as ours in (i) and (ii) above is featured in ([17], Sect. 8), but due to – apparently – other conventions for conjugating first- and second-kind irreps, the discussion cannot be carried over into our present Wigner–Racah algebra.]

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