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Phase-fixed double-group 3-Γ symbols. II. General features of double groups and their 3-Γ symbols

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Following a general exposition of the theory of 3-Γ symbols [1], we now focus on the particular features encountered when dealing with double groups of (proper as well as improper) point groups.

The paper starts with a brief outline of the definition of double groups adopted in the present work. After this, some properties of double group 3-Γ symbols are discussed which are independent of the way the 3-Γ symbols have been constructed. The main part of the paper then deals with the actual generation of 3-Γ symbols for the non-commutative double groups.

In the approach described, the 3-Γ symbols become determined in part by adaption of the standard matrix irreps to subgroup hierarchies and then completely, phases included, by the specification of *standard basis functions* (or, equivalently, *standard subduction coefficients*).

Key words: double groups for proper and improper point groups — subduction coefficients — basis functions for standard irreducible matrix representations — phase-fixation of three-gamma symbols and coupling coefficients — triple coefficients.

1. Introduction

The present paper provides the necessary link between our previous exposition of the general theory of 3-Γ symbols [1] and the following papers in the series which deal with specific double groups or families of double groups [2–5].

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The purpose of Sect. 2 is to give definitions, terminology and notation necessary for a stringent treatment of double groups in the sequel. Sect. 3 then discusses common features of 3-Γ symbols for double groups, focusing in particular on the problem of reality of 3-Γ symbols and the properties of conjugating matrices.

The main part of the paper is made up by Sect. 4 which is a description of the procedure we have followed for actually generating 3-Γ symbols for all the non-commutative double groups. The main idea is to define 3-Γ symbols by *renormalization of subgroup-adapted 3-j symbols.* The 3-Γ symbols thus obtained are completely determined, also with respect to phases, by the specification of *standard subduction coefficients* or, equivalently, *standard basis functions* for the subgroup irreps. This procedure for obtaining 3-Γ symbols is not new. Two of the present authors used the corresponding method for obtaining phase-fixed 3-Γ symbols for the point groups in 1972 [6], and since then several others have adopted the same or similar approaches for specific groups (see references in Sect. 5 and in the following papers [2–5]). The present exposition, however, attempts — as far as this is possible — to follow the philosophy of [6] in phase-fixing the 3-Γ symbols by choosing standard basis functions in a systematic way and furthermore points to several pitfalls and aspects seldomly given attention to in the literature (Sects. 4.4–4.6).

It is advantageous to have a phase-fixation which is in some respect "natural" of the 3-Γ symbols one uses, e.g. when applying the Wigner–Eckart theorem [1, Sect. 2] with the objective of standardizing parametrizations of quantum-chemical model operators (with the reduced matrix elements [1, Sect. 2] as parameters). In fact, it was the lack of standardization for parameters of semi-empirical models of the ligand field which prompted the first paper [6] on phase-fixed 3-Γ symbols. In complicated calculations based on Wigner–Racah algebra, a *consistent* choice of phases for the 3-Γ symbols is imperative, and then a "natural" or systematic phase-fixation is more safe to have than just an arbitrary phase-fixation.

2. Definition and properties of double groups of proper and improper point groups

In this section we shall review definitions and properties of double groups to the extent that we need these in the ensuing presentation of matrix irreps and 3-Γ symbols for these groups. For somewhat more elaborate treatments we refer to [7, Sect. 5.1; 8] and references therein. These references explain why double groups are a natural tool in the analysis of certain operators containing a spin-orbit coupling term, and [8] discusses the literature and gives some of the history of the double groups.

We shall start by discussing the double groups of *proper* point groups in Sect. 2.1; by the latter we mean those point groups which are subgroups of the rotation group in 3 dimensions, R_3. In Sect. 2.2 we define double groups of *improper* point groups, these latter being point groups which are subgroups of the rotation-inversion group R_{3i} but not subgroups of R_3.

2.1. Double groups of proper point groups

Double groups of proper point groups are subgroups of R_3^*, the rotation double group (cf. [1] Sect. 6 and references therein). This group is, in particular, itself the double group of R_3. The group R_3^* may, for example, be realized as unitary (2×2)-matrices with determinant $+1$, that is, it may be identified with the group $SU(2)$, or, still differently stated, it may be identified with (its own image under) the faithful matrix irrep $\mathscr{D}^{[1/2]}$. In this way, a general element of R_3^* takes the form

$$\mathscr{D}^{[1/2]}(\varphi, \theta, \psi) = \begin{pmatrix} \cos\frac{1}{2}\theta\, e^{-i(\varphi+\psi)/2} & -\sin\frac{1}{2}\theta\, e^{-i(\varphi-\psi)/2} \\ \sin\frac{1}{2}\theta\, e^{i(\varphi-\psi)/2} & \cos\frac{1}{2}\theta\, e^{i(\varphi+\psi)/2} \end{pmatrix} \tag{2.1.1}$$

with the sequence $(|\frac{1}{2}\frac{1}{2}\rangle, |\frac{1}{2}-\frac{1}{2}\rangle)$ of $|jm\rangle$ functions (*vide infra*) and with the parameters φ, θ, ψ varying in the ranges

$$0 \leq \varphi < 2\pi, \qquad 0 \leq \theta \leq \pi, \qquad 0 \leq \psi < 4\pi. \tag{2.1.2}$$

If φ and θ are numbers chosen in the ranges of (2.1.2) and ψ is a number with $0 \leq \psi < 2\pi$, then the two R_3^*-elements $\mathscr{D}^{[1/2]}(\varphi, \theta, \psi)$ and $\mathscr{D}^{[1/2]}(\varphi, \theta, \psi + 2\pi)$ – and only these two – correspond to the *rotation* (i.e. the R_3-element) with Euler angles (φ, θ, ψ). Note that the Euler angles are not uniquely defined in the literature; for example, our φ and ψ correspond to ψ and φ, respectively, of Fano and Racah [9]. See [8] for further references to the literature.

[The particular form of the $j = 1/2$ matrix representative chosen in (2.1.1) will be discussed in Sect. 4 in connection with the description of the action of rotation operators on angular momentum eigenfunctions $|jm\rangle$.

For a mathematical description of the correspondence between R_3^* and R_3, there is a *homomorphism* of R_3^* *onto* R_3 mapping the elements $\mathscr{D}^{[1/2]}(\varphi, \theta, \psi)$ and $\mathscr{D}^{[1/2]}(\varphi, \theta, \psi + 2\pi)$ of R_3^* onto the same element of R_3, namely, the rotation with Euler angles (φ, θ, ψ). (We are assuming here a coordinate system chosen once and for all, so that all R_3-rotations may be described with a set of Euler angles with φ and θ restricted by (2.1.2) and $0 \leq \psi < 2\pi$).]

Given an ordinary rotation $\boldsymbol{R}$ with Euler angles (φ, θ, ψ), we wish to have a short notation for the two elements of R_3^* which correspond to $\boldsymbol{R}$ in the above-described manner – a notation which reminds one of their relation to $\boldsymbol{R}$ and which, preferably, is more descriptive than specifying φ, θ, ψ themselves. We shall employ the convention in this and the subsequent papers that $\boldsymbol{R}^*$ means the double group element with parameter triple (φ, θ, ψ); the element of R_3^* with parameter triple $(\varphi, \theta, \psi + 2\pi)$ is then $-\boldsymbol{R}^*$ when regarded as a matrix in the above way. We shall thus meet with expressions like $\boldsymbol{C}_4^{Y*}$, $-\boldsymbol{C}_3^*$ etc. This notation convention is discussed in [8].

We shall particularly often encounter the R_3^*-elements $\boldsymbol{C}_{2\pi/\alpha}^{Z*}$, $\boldsymbol{C}_2^{X*}$, and $\boldsymbol{C}_2^{Y*}$ defined by

$$\boldsymbol{C}_{2\pi/\alpha}^{Z*} = \mathscr{D}^{[1/2]}(\alpha, 0, 0) = \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} \tag{2.1.3}$$

$$C_2^{X*} = \mathscr{D}^{[1/2]}(\pi, \pi, 0) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \tag{2.1.4}$$

$$C_2^{Y*} = \mathscr{D}^{[1/2]}(0, \pi, 0) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{2.1.5}$$

Note that one has to be careful with relations which may seem obvious from the relations existing between the corresponding R_3-elements; for example,

$$C_2^{Y*} = C_2^{X*} C_2^{Z*},$$

but

$$C_2^{Y*} = -C_2^{Z*} C_2^{X*},$$

as one may ascertain from (2.1.3)–(2.1.5).

If G is a proper point group, its double group G^* is defined to be the set of corresponding elements in R_3^*. Thus, $G^* = \{\boldsymbol{R}^* | \boldsymbol{R} \in G\} \cup \{-\boldsymbol{R}^* | \boldsymbol{R} \in G\}$.

The irreps of such a double group G^* always fall in two distinct non-empty classes: (1) the irreps which assign the same matrix to the elements $\boldsymbol{R}^*$ and $-\boldsymbol{R}^*$ for all $\boldsymbol{R}$ in G and which may, therefore, also be regarded as irreps of G; and (2) the irreps which distinguish $\boldsymbol{R}^*$ and $-\boldsymbol{R}^*$ for all $\boldsymbol{R}$ in G. *All* irreps of G arise from irreps of G^* of the first of these types. The irreps in class (1) are sometimes called the *vector* irreps or the *tensor* irreps of G^*, while those in class (2) are called *spin* or *spinor* irreps. Unfortunately, the literature does not agree completely on these terms. We shall use "vector" and "spin" as defined here. For R_3^* itself, the irreps $\mathscr{D}^{[j]}$ with $j = 0, 1, 2, \ldots$ are of vector type, while those with $j = 1/2$, 3,/2, 5/2, ... are of spin type. For all the non-commutative double groups, irreps of the first Frobenius–Schur kind ([1], Sect. 5.2) are vector irreps and irreps of the second F–S kind are spin irreps, while irreps of the third F–S kind may be either of vector or of spin type. (This is not true for the cyclic double groups C_n^*. For example, the non-trivial irrep of C_1^* is obviously of the first kind, but also a spin irrep.)

If Γ_1, Γ_2, Γ_3 are irreps of a double group G^* and $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3) > 0$ (i.e., the triple has non-zero triple coefficients), then necessarily an *even* number of the three irreps is of spin type (i.e., either two of them or none of them are spin irreps). This is easily proven:

Let $\boldsymbol{\Gamma}_1$, $\boldsymbol{\Gamma}_2$, $\boldsymbol{\Gamma}_3$ be matrix forms of Γ_1, Γ_2, Γ_3. Let $\boldsymbol{E} \in G$ be the identity operation (the neutral element in G). The elements in G^* corresponding to $\boldsymbol{E}$ are

$$\boldsymbol{E}^*, \text{or} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{and} \quad -\boldsymbol{E}^*, \text{or} \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For a vector irrep Γ of G^* we have $\boldsymbol{\Gamma}(-\boldsymbol{E}^*) = \boldsymbol{\Gamma}(\boldsymbol{E}^*) = +\mathbb{1}$, while for a spin irrep Γ we have $\boldsymbol{\Gamma}(-\boldsymbol{E}^*) = -\boldsymbol{\Gamma}(\boldsymbol{E}^*) = -\mathbb{1}$. Thus if an odd number of $\boldsymbol{\Gamma}_1$, $\boldsymbol{\Gamma}_2$, and $\boldsymbol{\Gamma}_3$ is of spin type and $\mathbb{c} \in \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$, we have

$$\mathbb{c} = [\bar{\Gamma}_1(-\boldsymbol{E}^*)\otimes\bar{\Gamma}_2(-\boldsymbol{E}^*)\otimes\bar{\Gamma}_3(-\boldsymbol{E}^*)]\mathbb{c} \qquad \text{(fix-vector property)}$$
$$= -\mathbb{c}$$

and thus $\mathbb{c}$ is necessarily zero.

2.2. *Double groups of improper point groups*

Let G be an improper point group. Since G is not a subgroup of R_3, we do not immediately have a definition of a double group of G. However, considerations to be found in ([7], Sect. 5.1) and discussed in detail in [8] show that the following prescriptions give a natural definition for this situation. We distinguish two cases:

(i) If G contains the inversion $\boldsymbol{I} = S_2$, it is the direct product of its intersection G_0 with R_3 (the subgroup of G consisting of proper rotations) and the inversion group $S_2 = \{\boldsymbol{E}, \boldsymbol{I}\} = C_i$, i.e. $G = G_0 \times S_2$. In this case, the double group G^* is defined to be $G_0^* \times S_2$.

(ii) If G does *not* contain the inversion $\boldsymbol{I}$, the set containing all the proper rotations in G *and* all the improper ones *multiplied by* $\boldsymbol{I}$ will be a subgroup G' of R_3 isomorphic to G. The double group G^* is then defined to be $(G')^*$.

Examples of case (i) are $G = O_h$ and $G = D_{4h}$, and examples of case (ii) are $G = T_d$ and $G = D_{3h}$, for which we get $G' = O$ and $G' = D_6$, respectively. For a full tabulation of the consequences of definitions (i) and (ii), see [8].

3. General considerations regarding 3-Γ symbols for double groups

3.1. *Introduction*

All double groups are simple phase and thus allow complete collections of 3-Γ symbols to be constructed ([1] Sect. 4). In Sect. 4 of the present paper we shall explain how we actually generate 3-Γ symbols for the double groups. In the present section we have collected some general considerations which do not depend on the particular way in which the 3-Γ symbols are generated and to some extent do not even depend on the group in question being a double group.

The general theme is that of simplifying the 3-Γ symbols as much as possible by suitably adjusting the matrix irreps. The first parts of this section discuss the possibilities of obtaining real 3-Γ symbols and convenient forms of conjugating matrices ([1] Sect. 5). Sect. 3.5 then gives examples of relations satisfied in certain cases by 3-Γ symbols as a direct consequence of their fix-vector property. The last part, 3.6, is concerned with the definition of 3-Γ symbols for double groups of improper point groups.

One remark is in place here. From Sect. 2.1 it is seen that if we construct 3-Γ symbols for the double group G^* of a proper point group G, we get, in particular, a full set of 3-Γ symbols for G (because we get, in particular, 3-Γ symbols for all irrep triples consisting of three *vector* reps). It might seem, then, that the present work makes that of [6] superfluous. However, in [6] all irreps were chosen to have certain real matrix forms (only the ambivalent point groups were considered). In the present work irreps of the first kind are in an interplay with irreps of the second and third kinds, and those real matrix forms of the first-kind irreps are usually not suitable if the various requirements listed below in this section are to be fulfilled. Thus the 3-Γ symbols of the subsequent papers generally correspond to other standard matrix forms of the irreps than those of [6]. They are thus generally incomparable, but both kinds may be useful, depending on the application to be made.

3.2. Reality of 3-Γ symbols

We shall meet with three general situations where a choice of a complete set of *real* 3-Γ symbols is possible:

(i) *Group generators with symmetric irrep matrices*
Suppose a given simple phase group is generated by elements R_1, $R_2, \ldots$ If we can establish the situation that for every standard matrix irrep Γ of the group, the matrices $\Gamma(R_1)$, $\Gamma(R_2), \ldots$ are all *symmetric* matrices, then the family of standard matrix irreps selected allows real 3-Γ symbols to be chosen. This fact is proved in the appendix.

(ii) *Group generators with real triple tensor products of irrep matrices*
Suppose, as in (i), that a group is generated by elements R_1, $R_2, \ldots$ If we can establish the situation that for every triple $\Gamma_1\Gamma_2\Gamma_3$ of standard matrix irreps of the group having non-zero triple coefficients, the matrices

$$\Gamma_1(R_1)\otimes\Gamma_2(R_1)\otimes\Gamma_3(R_1), \qquad \Gamma_1(R_2)\otimes\Gamma_2(R_2)\otimes\Gamma_3(R_2), \ldots$$

are all *real* matrices, then the family of standard matrix irreps selected allows real 3-Γ symbols to be chosen. This is also proved in the appendix. The condition is evidently satisfied when all standard irreps are real matrix reps (as was the case in [6]). In the present work we may sometimes have the condition satisfied by having the situation that for all *vector*-type standard matrix irreps Γ of a given double group, the matrices $\Gamma(R_1)$, $\Gamma(R_2), \ldots,$ are all *real*, and for all *spin*-type standard matrix irreps Γ the generator irrep matrices $\Gamma(R_1)$, $\Gamma(R_2), \ldots$ are all *purely imaginary* (to see that the condition is then satisfied, use the remark from Sect. 2.1 that for all irrep triples with non-zero triple coefficients, an even number of the irreps is of spin type).

(iii) *Irrep conjugation by the irrep matrices of a fixed group element*
This is the situation described in ([1] Sect. 5.5), to which we refer for a detailed discussion.

3.3. General remarks on conjugating matrices

In ([1], Sect. 5.3) we showed how 3-Γ symbols of the form $(\Gamma 1_G \Gamma/\gamma 0 \gamma')$ are used, in the present formalism, for conjugating individual irreps Γ in the 3-Γ symbols. The formulas there were kept at a rather general level; here we indicate how they may, in the cases to be treated below, be somewhat simplified.

It has turned out to be in all cases compatible with our other requirements to have 3-Γ symbols $(\Gamma 1_G \Gamma/\gamma 0 \gamma')$ of the simple form

$$\begin{pmatrix} \Gamma & 1_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix} = (\dim \Gamma)^{-1/2} \varphi_\Gamma(\gamma) \delta(\gamma, \sigma_\Gamma(\gamma')), \tag{3.3.1}$$

where φ_Γ is a function with $\varphi_\Gamma(\gamma) = \pm 1$ for all γ and σ_Γ is a permutation of the components. Thus the conjugating matrix for Γ defined by ([1] (5.3.3)) has the form of a permutation matrix, possibly with varying signs on the non-zero elements. ("Permutation matrix" means a matrix obtained by some permutation of the rows (or of the columns) of a unit matrix.) This turns, e.g. formula (5.3.4) of [1], applied to 3-Γ symbols, into

$$\begin{aligned} \begin{pmatrix} \bar{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta &= \sum_{\gamma_1'} \varphi_{\Gamma_1}(\gamma_1') \delta(\gamma_1', \sigma_{\Gamma_1}(\gamma_1)) \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \\ &= \varphi_{\Gamma_1}(\sigma_{\Gamma_1}(\gamma_1)) \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \sigma_{\Gamma_1}(\gamma_1) & \gamma_2 & \gamma_3 \end{pmatrix}_\beta, \end{aligned} \tag{3.3.2}$$

and for the conjugation of all three irreps we get

$$\begin{aligned} \begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta &= \varphi_{\Gamma_1}(\sigma_{\Gamma_1}(\gamma_1)) \varphi_{\Gamma_2}(\sigma_{\Gamma_2}(\gamma_2)) \varphi_{\Gamma_3}(\sigma_{\Gamma_3}(\gamma_3)) \\ &\quad \times \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \sigma_{\Gamma_1}(\gamma_1) & \sigma_{\Gamma_2}(\gamma_2) & \sigma_{\Gamma_3}(\gamma_3) \end{pmatrix}_\beta. \end{aligned} \tag{3.3.3}$$

Formulas like (3.3.2) and (3.3.3) are easy to use; given a table of the 3-Γ symbols (3.3.1), one immediately reads off what $\sigma_\Gamma(\gamma)$ and $\varphi_\Gamma(\sigma_\Gamma(\gamma))$ are for each component γ of Γ. This is made even easier than one might think at first sight because of the fact that σ_Γ actually necessarily is a product of disjoint *transpositions* (permutations of just two components). This may be seen by recalling that conjugating matrices are either symmetric or antisymmetric ([1] Sect. 5.2). As an example, we see in ([2] Table 5 (i), concerned with the group D_3^*) that

$$(\mathrm{E}_{1/2}\mathrm{A}_1\mathrm{E}_{1/2}/\tfrac{1}{2}\,0\,-\tfrac{1}{2}) = -\sqrt{\tfrac{1}{2}}.$$

Since also $\pi(\mathrm{E}_{1/2}\mathrm{A}_1\mathrm{E}_{1/2}) = -1$ (see definition in [1, Sect. 4]), we have further

$$(\mathrm{E}_{1/2}\mathrm{A}_1\mathrm{E}_{1/2}/-\tfrac{1}{2}\,0\,\tfrac{1}{2}) = +\sqrt{\tfrac{1}{2}}.$$

Thus $\sigma_{\mathrm{E}_{1/2}}(\frac{1}{2}) = -\frac{1}{2}$ (and therefore $\sigma_{\mathrm{E}_{1/2}}(-\frac{1}{2}) = \frac{1}{2}$), and $\varphi_{\mathrm{E}_{1/2}}(\frac{1}{2}) = -1$ and $\varphi_{\mathrm{E}_{1/2}}(-\frac{1}{2}) = +1$. This means that we get the general conjugation formulae

$$\begin{pmatrix} \cdots & \bar{\mathrm{E}}_{1/2} & \cdots \\ & 1/2 & \end{pmatrix} = \begin{pmatrix} \cdots & \mathrm{E}_{1/2} & \cdots \\ & -1/2 & \end{pmatrix}$$

and

$$\begin{pmatrix} \cdots & \bar{\mathrm{E}}_{1/2} & \cdots \\ & -1/2 & \end{pmatrix} = -\begin{pmatrix} \cdots & \mathrm{E}_{1/2} & \cdots \\ & 1/2 & \end{pmatrix}.$$

In some cases further facilitation arises because the 3-Γ symbols of (3.3.1) may be given by a convenient *explicit* formula. The prime example of this is the rotation double group with the traditional standards ([1] formula (6.2)). In our treatment of the hierarchy $I^* \supset C_5^*$, a completely analogous formula is established ([5], (3.2.1)).

3.4. Subgroup adaption and component designations

All double-group 3-Γ symbols to be presented below correspond to standard matrix irreps which have been adapted to group-subgroup hierarchies of the form $G \supset G_1 \supset G_2 \supset \cdots \supset C_n^*$, that is, hierarchies terminating with a cyclic double group. The presence of this terminal group implies that we have distinguished an element $\boldsymbol{C}_n^* \in G$ and have arranged that for all standard matrix irreps $\mathbb{\Gamma}$, the matrix $\mathbb{\Gamma}(\boldsymbol{C}_n^*)$ is diagonal.

For a given irrep $\mathbb{\Gamma}$ of G, the adaption to the subgroup hierarchy furnishes us with a sequence of subgroup irreps which may be used for labeling the components of $\mathbb{\Gamma}$. In particular, these strings of irrep symbols terminate with a symbol for an irrep of the group C_n^*, or, equivalently, for an eigenvalue of the diagonal matrix $\mathbb{\Gamma}(\boldsymbol{C}_n^*)$. We shall here adopt the general convention that a component designation γ with respect to C_n^* means an eigenvalue $\exp(-i\gamma 2\pi/n)$ of $\mathbb{\Gamma}(\boldsymbol{C}_n^*)$.

We shall make one kind of exception to this convention, however. In most of the cases where we have irreps of the third Frobenius–Schur kind ([1] Sect. 5.2), adoption of the convention would be in opposition to a fundamental requirement of the formalism developed in [1], namely that a standard matrix irrep and its complex conjugate have the same component designations for corresponding components. Thus, to avoid any confusion, we have given the third-kind irreps component designations which are letters, not numbers (the combination of an irrep and a component may then be translated into a number which relates to a $\mathbb{\Gamma}(\boldsymbol{C}_n^*)$ diagonal entry, as above). For examples of this, see the cases of the groups D_n^* with n odd [2] and the group T^* [3].

3.5. Simplifying relations satisfied by 3-Γ symbols

Given three irreps $\mathbb{\Gamma}_1$, $\mathbb{\Gamma}_2$, $\mathbb{\Gamma}_3$ of a group G and a set of 3-Γ symbols for $\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3$, the fundamental equation, ([1] (3.1.2)), of course imposes some restrictions on the set of 3-Γ symbols. In some cases, these restrictions are expressible as explicit formulas and thus become useful for reduction of tables and when manipulating the 3-Γ symbols. We give here a couple of examples of this.

(i) The adaptation to a cyclic double group C_n^* described in Sect. 3.4 implies for the 3-Γ symbols a relation of the form

$$\sum_{\gamma_1'\gamma_2'\gamma_3'} \delta(\gamma_1, \gamma_1')\, \overline{e^{-i\gamma_1 2\pi/n}}\, \delta(\gamma_2, \gamma_2')\, \overline{e^{-i\gamma_2 2\pi/n}}\, \delta(\gamma_3, \gamma_3')\, \overline{e^{-i\gamma_3 2\pi/n}} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1' & \gamma_2' & \gamma_3' \end{pmatrix}_\beta$$

$$= \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta$$

or

$$e^{i(\gamma_1+\gamma_2+\gamma_3)2\pi/n}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta=\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \tag{3.5.1}$$

which gives the "selection rule"

$$\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta \neq 0 \Rightarrow \gamma_1+\gamma_2+\gamma_3\equiv 0 \pmod n. \tag{3.5.2}$$

This rule and the derivation of it of course have only meaning when the γ_i are numerical component designations. Thus, as explained in Sect. 3.4, for irreps of the third kind it will be necessary to translate – in the obvious way – components which we for other reasons name with letters into numbers to be able to apply the selection rule.

An extreme case of this kind of rule (resulting from adaption to C_n^* for *all* $n=1, 2, 3, \ldots$ simultaneously) is the rule

$$\begin{pmatrix}j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix}\neq 0 \Rightarrow m_1+m_2+m_3=0 \tag{3.5.3}$$

satisfied by the 3-j symbols of R_3^* [1, Sect. 6] and the corresponding rule for the $D_\infty^* \supset C_\infty^*$ 3-Γ symbols [2, Sect. 2].

(ii) In many of the examples to be treated below, there is a group element S (in fact, always $C_2^{Y^*}$) with the property that for every standard matrix irrep Γ the matrix $\Gamma(S)$ is a permutation matrix, possibly with varying phases added on the non-zero entries. This makes for useful relations between different 3-Γ symbols. Examples include ([1], formula (6.6)), the hierarchy $D_\infty^* \supset C_\infty^*$ ([2], formula (2.4)) and the hierarchy $I^* \supset C_5^*$ [5] for the latter of which the 3-Γ symbols satisfy the relation

$$\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ -\gamma_1 & -\gamma_2 & -\gamma_3\end{pmatrix}_\beta=(-1)^{j(\Gamma_1)+j(\Gamma_2)+j(\Gamma_3)-\gamma_1-\gamma_2-\gamma_3}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_\beta$$
$$\text{for all } \gamma_1, \gamma_2, \gamma_3 \tag{3.54}$$

with the numbers $j(\Gamma_i)$ suitably defined.

3.6. 3-Γ *symbols for double groups of improper point groups*

Given 3-Γ symbols for the double groups of the proper point groups and the definitions in Sect. 2.2 of double groups of improper point groups, there is a natural way to define 3-Γ symbols for the lattter groups. We distinguish the same two cases as in Sect. 2.2:

(i) Suppose G is a point group containing the inversion. Then G^* is of the form $G_0^* \times S_2$, where G_0 is a proper point group. The irreps of G^* are thus all of the form Γ_g or Γ_u, where Γ is an irrep of G_0^* and Γ_g is its direct product with the totally symmetric (*gerade*) irrep A_g of S_2 and Γ_u its direct product with the *ungerade* irrep A_u of S_2. We then take as 3-Γ symbols for G^* those of G_0^* with parity added in the obvious way, i.e.

$$\underset{G^*}{\begin{pmatrix} \Gamma_{1p_1} & \Gamma_{2p_2} & \Gamma_{3p_3} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} = \underset{G_0^*}{\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta} \tag{3.6.1}$$

if an *even* number of the parity labels p_1, p_2, p_3 are *ungerade* and

$$\begin{pmatrix} \Gamma_{1p_1} & \Gamma_{2p_2} & \Gamma_{3p_3} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} = 0 \tag{3.6.2}$$

otherwise.

(ii) If G is an improper group which does *not* contain the inversion, its double group is of the form $(G')^*$ where G' is a proper point group, and so we directly have the 3-Γ symbols for G^* by having those for $(G')^*$.

Thus the rest of the present paper and the following papers in the series [2, 3, 4, 5] will concentrate on 3-Γ symbols for double groups which are subgroups of R_3^*.

4. The actual generation of phase-fixed 3-Γ symbols for the double groups

4.1. Introduction

Having discussed the general theory of 3-Γ symbols in [1] and the specific features which are common to all or several of the double groups in the preceding sections of the present paper, we now address the practical problem of actually obtaining complete sets of 3-Γ symbols for these concrete groups.

In general, given a simple phase group ([1] Sect. 4), it is a non-trivial problem just to find any collection of matrix irreps and corresponding 3-Γ symbols. For the point groups and their double groups, the group structure and representation algebra are so well understood that this problem has already been solved in various ways. (Due credit will be given, below and in the following papers of this series [2–5], to earlier work in the field). Thus, what we believe to be original in the present contribution is the presentation of 3-Γ symbols which obey the general formulas described above, which are *real*, and which are *phase-fixed* in the sense to be discussed in Sect. 4.4.

4.2. The standard matrix irreps of the rotation double group R_3^*

In ([1], Sect. 6) we briefly discussed the conventional choice of standard matrix irreps $\mathcal{D}^{[j]}$, $j = 1/2, 1, 3/2, 2, \ldots$, for R_3^* and the 3-j symbols which are a choice of real 3-Γ symbols corresponding to the irreps $\mathcal{D}^{[j]}$. Some key references to the abundant literature on R_3^* were given there. We add here that the irreps $\mathcal{D}^{[j]}$ are often thought of as being generated by the action on *function bases* $\{|jm\rangle\}$ of operators $\hat{\mathcal{P}}(R)$ representing the group elements R, as expressed in the following equation:

$$\hat{\mathcal{P}}(R)|jm\rangle = \sum_{m'=-j}^{j} \mathcal{D}^{[j]}(R)_{m'm}|jm'\rangle. \tag{4.2.1}$$

Several concrete realizations of such function bases and corresponding operator representations $\hat{\mathscr{P}}$ of R_3^* are described in the literature [10, 11]; however, once the matrix irreps $\mathscr{D}^{[j]}$ are given (an explicit formula exists – see [9, App. D]) it is sufficient for our present purpose to take the symbols $\hat{\mathscr{P}}(R)$ and $|jm\rangle$ to be *defined* by (4.2.1). Discussions of some of the differing conventions present in the literature regarding basis functions and standard matrix irreps of R_3^* may be found in [12, 13].

4.3. Subgroup 3-Γ symbols by transformation and renormalization of 3-j symbols

Given an irrep $\mathscr{D}^{[j]}$ of R_3^* (see Sect. 4.2) and a proper subgroup $G\subset R_3^*$, the representation obtained by restricting $\mathscr{D}^{[j]}$ to G will, in general, be reducible, and one may find unitary matrices $\mathbb{S}$ with the property that the representation $R\to\mathbb{S}\mathscr{D}^{[j]}(R)\mathbb{S}^\dagger$, $R\in G$, is a matrix direct sum of matrix irreps $\mathbb{\Gamma}$ of the subgroup. For a given such $\mathbb{\Gamma}$ we may focus on submatrices $\mathbb{S}^{ja\mathbf{\Gamma}}$ of $\mathbb{S}$ which specifically produce $\mathbb{\Gamma}$ from $\mathscr{D}^{[j]}$ in the sense that

$$\mathbb{S}^{ja\mathbf{\Gamma}}\mathscr{D}^{[j]}(R)=\mathbb{\Gamma}(R)\mathbb{S}^{ja\mathbf{\Gamma}}\quad\text{for all } R\in G. \tag{4.3.1}$$

The branching multiplicity index (or repetition index of the first kind [14]), a, allows for the possible existence of several linearly independent submatrices $\mathbb{S}^{ja\mathbf{\Gamma}}$ with property (4.3.1). The elements $s(jm,ja\Gamma\gamma)$ of the adjoint (transpose and complex conjugate) matrix $(\mathbb{S}^{ja\mathbf{\Gamma}})^\dagger$ may be viewed as coefficients defining new *basis functions*

$$|ja\Gamma\gamma\rangle\equiv\sum_{m=-j}^{j}s(jm,ja\Gamma\gamma)|jm\rangle \tag{4.3.2}$$

which under the operators $\hat{\mathscr{P}}(R)$ transform as $\mathbb{\Gamma}$:

$$\hat{\mathscr{P}}(R)|ja\Gamma\gamma\rangle=\sum_{\gamma'}\mathbb{\Gamma}(R)_{\gamma'\gamma}|ja\Gamma\gamma'\rangle \tag{4.3.3}$$

(cf. Eq. (4.2.1.)). We shall call the coefficients $s(jm,ja\Gamma\gamma)$ *subduction coefficients.* (This term has been used before in the literature [15], and several alternative terms exist: decomposition coefficients [14], expansion coefficients [16], and just transformation coefficients [17, 18]). Subduction coefficients may be used for the construction of triple coefficients for G from 3-j symbols ([1], Sect. 6). If $\mathbb{c}$ is a column of triple coefficients ([1], Sect. 3) for an ordered R_3^*-irrep triple $\mathscr{D}^{[j_1]}\mathscr{D}^{[j_2]}\mathscr{D}^{[j_3]}$ and $\mathbb{S}^{j_ia_i\mathbf{\Gamma}_i}$ subduces $\mathscr{D}^{[j_i]}$ to the irrep Γ_i of G, $i=1,2,3$, the complex conjugate of the column $[\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}\otimes\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}\otimes\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}]\bar{\mathbb{c}}$ is a column of triple coefficients for $\Gamma_1\Gamma_2\Gamma_3$:

$$\begin{aligned}
&[\bar{\mathbb{\Gamma}}_1(R)\otimes\bar{\mathbb{\Gamma}}_2(R)\otimes\bar{\mathbb{\Gamma}}_3(R)][\overline{\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}}\otimes\overline{\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}}\otimes\overline{\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}}]\mathbb{c}\\
&\quad=[\bar{\mathbb{\Gamma}}_1(R)\overline{\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}}\otimes\bar{\mathbb{\Gamma}}_2(R)\overline{\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}}\otimes\bar{\mathbb{\Gamma}}_3(R)\overline{\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}}]\mathbb{c}\\
&\quad=[\overline{\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}\mathscr{D}^{[j_1]}(R)}\otimes\overline{\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}\mathscr{D}^{[j_2]}(R)}\otimes\overline{\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}\mathscr{D}^{[j_3]}(R)}]\mathbb{c}\\
&\quad=[\overline{\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}}\otimes\overline{\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}}\otimes\overline{\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}}][\overline{\mathscr{D}^{[j_1]}(R)}\otimes\overline{\mathscr{D}^{[j_2]}(R)}\otimes\overline{\mathscr{D}^{[j_3]}(R)}]\mathbb{c}\\
&\quad=[\overline{\mathbb{S}^{j_1a_1\mathbf{\Gamma}_1}}\otimes\overline{\mathbb{S}^{j_2a_2\mathbf{\Gamma}_2}}\otimes\overline{\mathbb{S}^{j_3a_3\mathbf{\Gamma}_3}}]\mathbb{c}\quad\text{for all } R\in G.
\end{aligned} \tag{4.3.4}$$

If the R_3^*-triple coefficients are 3-j symbols, we may write the G-triple coefficients thus obtained as

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a_3\Gamma_3\gamma_3 \end{pmatrix}$$
$$= \sum_{m_1m_2m_3} s(j_1m_1, j_1a_1\Gamma_1\gamma_1)s(j_2m_2, j_2a_2\Gamma_2\gamma_2)s[(j_3m_3, j_3a_3\Gamma_3\gamma_3)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{4.3.5}$$

When the matrix forms of the Γ_i can be taken as given, we shall often just write Γ_i in this kind of formula. The basic idea is then to attempt a definition of a set of 3-Γ symbols for the (unordered) triple $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ ([1], Sect. 4) by putting

$$\begin{pmatrix} \Gamma_{\pi(1)} & \Gamma_{\pi(2)} & \Gamma_{\pi(3)} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{\beta=j_1a_1j_2a_2j_3a_3}$$
$$= \left[\sum_{\gamma_1'\gamma_2'\gamma_3'} \left|\begin{pmatrix} j_1 & j_2 & j_3 \\ a_1\Gamma_1\gamma_1' & a_2\Gamma_2\gamma_2' & a_3\Gamma_3\gamma_3' \end{pmatrix}\right|^2\right]^{-1/2}$$
$$\times \begin{pmatrix} j_{\pi(1)} & j_{\pi(2)} & j_{\pi(3)} \\ a_{\pi(1)}\Gamma_{\pi(1)}\gamma_1 & a_{\pi(2)}\Gamma_{\pi(2)}\gamma_2 & a_{\pi(3)}\Gamma_{\pi(3)}\gamma_3 \end{pmatrix} \tag{4.3.6}$$

for all permutations π of $\{1, 2, 3\}$ necessary to produce the six, three or just single distinct permuted forms of $\Gamma_1\Gamma_2\Gamma_3$. The square root factor ensures proper normalization ([1], Eq. (4.12)). There are, however, some reservations to be taken before one can be sure that this definition works.

Firstly, the G-triple coefficients obtained by (4.3.5) must form a non-zero set. To see that even this condition may fail, consider, e.g., the transformed 3-j symbols

$$\begin{pmatrix} 1 & 1 & 1 \\ \mathrm{E}_1\gamma_1 & \mathrm{E}_1\gamma_2 & \mathrm{E}_1\gamma_3 \end{pmatrix}$$

referring to the subgroup $D_3^* \subset R_3^*$ [2].

If they do form a non-zero set, (4.3.6) will always work if the three irreps Γ_i are distinct, and the *permutational characteristic* or *transposition phase* ([1], Sect. 4) will become

$$\pi(\Gamma_1\Gamma_2\Gamma_3\beta)|_{\beta=j_1a_1j_2a_2j_3a_3} = (-1)^{j_1+j_2+j_3}. \tag{4.3.7}$$

From the point of view of the group G, this fixation of the permutational characteristic for $\Gamma_1\Gamma_2\Gamma_3\beta$ is completely arbitrary.

If two or three of the Γ_i are identical, but the corresponding pairs j_ia_i are different, Eq. (4.3.6) may not be consistent. Consider, e.g. the octahedral double group O^* and the example $j_1 = 3/2$, $j_2 = 2$, $j_3 = 5/2$, $\Gamma_1 = \mathrm{U}$, $\Gamma_3 = \mathrm{U}$, $\Gamma_2 = \mathrm{T}_2$ (cf. [4], Sect. 3). The transformed 3-j symbols

$$\begin{pmatrix} 3/2 & 2 & 5/2 \\ U\gamma_1 & T_2\gamma_2 & U\gamma_3 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 5/2 & 2 & 3/2 \\ U\gamma_1 & T_2\gamma_2 & U\gamma_3 \end{pmatrix}$$

are *not* generally equal and therefore they cannot be used for the construction of 3-Γ symbols of the type

$$\begin{pmatrix} U & T_2 & U \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta$$

by the definition (4.3.6). Even fixing, say, 3/2 to be always in the first position – thereby deviating from the prescription of (4.3.6) – will not help, because the UT_2U-fix-vector thus derived is neither symmetric nor antisymmetric).

Another, milder case is that of the icosahedral double group [5] and the example $j_1=3$, $j_2=4$, $j_3=1$ and $\Gamma_1=U$, $\Gamma_2=U$, $\Gamma_3=T_1$. For transformed 3-j symbols it turns out that

$$\begin{pmatrix} 4 & 3 & 1 \\ U\gamma_1 & U\gamma_2 & T_1\gamma_3 \end{pmatrix} = -\begin{pmatrix} 3 & 4 & 1 \\ U\gamma_1 & U\gamma_2 & T_1\gamma_3 \end{pmatrix}$$

for all γ_1, γ_2, γ_3. This means that it would be of importance to remember whether the 3-Γ symbols $(UUT_1/\gamma_1\gamma_2\gamma_3)$ were defined from $j_1j_2j_3$ equal to 341 or 431 (and correspondingly for the UT_1U and T_1UU 3-Γ symbols), which is clearly inconvenient.

Thus, in the cases to be considered in [2, 3, 4, 5], we must always check that our use of (4.3.6) is consistent and workable. When (4.3.6) *is* used consistently, the phase formula (4.3.7) will also hold for cases with identical Γ_i.

We have not seen an explicit discussion of these reservations for using (4.3.6) in the literature.

4.4. The choice of standard basis functions

Proceeding from the considerations of Sect. 4.3, we see that given a subgroup $G \subset R_3^*$, what we need in order to obtain a complete collection of 3-Γ symbols for G by the method represented by (4.3.6) is

(a) A choice of standard matrix forms $\mathbb{\Gamma}$ of the irreps Γ of G.
(b) A choice of j-triplets for all Γ-triples, sufficiently many to supply the required number of linearly independent sets of 3-Γ symbols for triples $\Gamma_1\Gamma_2\Gamma_3$ with multiplicity (i.e. with dim $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3) > 1$ ([1], Sect. 4)).
(c) A choice of standard subduction coefficients for all corresponding $\mathbb{\Gamma}$ and j selected in (a) and (b).

In practice, items (a) and (c) are intimately connected, (c) in fact implying (a), but (a) may also be influenced by conditions expressible without talking about subduction coefficients – in our treatment of the double groups, chiefly the adaption to a cyclic subgroup C_n^* and sometimes intermediate groups in a hierarchy $G \supset \cdots \supset C_n^*$. We shall speak of (a)–(c) as the process of choosing *standard basis* functions for the irreps of G.

In [6], collections of 3-Γ symbols for the crystallographic point groups were given which were *phase-fixed* in the non-trivial sense that they were generated by a minimal number of standard basis functions, the phases of which were fixed by a few very simple rules. In the present work on the double groups, the choices of standard basis functions we have made can – in retrospect – be described by the rules given below. Since the rules are so elaborate and not even completely explicitly expressed, we admit that the term "phase-fixed" looses some of its significance here; however, the 3-Γ symbols generated are still, undeniably, phase-fixed in the sense that their phases are dictated by the standard basis functions instead of being arbitrarily chosen. See further remarks on phase-fixation in Sect. 5.

As for the choice of function bases for individual subgroup irreps, the rules we have followed are:

(1) Lowest possible j values are chosen, except that when more than one basis set is needed for a given irrep, each new basis is chosen from a new j set. The lowest j-value assigned to an irrep of G is called its *primary* j-value.
(2) Only irreps of the first kind may have such supplementary bases.
(3) The basis functions chosen within each of the j sets selected by (1) and (2) are fixed so far as to ensure that the matrix irreps they generate are adapted to the subgroup hierarchy $G \supset G_1 \supset G_2 \supset \cdots \supset C_n^*$ in question.
(4) The primary basis functions for all irreps are further adjusted so as to make the 3-Γ symbols

$$\begin{pmatrix} \Gamma & 1_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix}$$

real; in situations of the type described in ([1], Sect. 5.5), the relationship

$$\begin{pmatrix} \Gamma & 1_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix} = (\dim \Gamma)^{-1/2} \Gamma(R_0)_{\gamma\gamma'} \tag{4.4.1}$$

should further be satisfied.

At this stage, a first check is made on the 3-Γ symbols generated by the preliminary basis functions found by the application of (1)–(4). If not all 3-Γ symbols are real, further restrictions are placed on the basis functions to ensure a maximum number of real 3-Γ symbols. If not all 3-Γ symbols can be made real, it is attempted to have at least those for triples of three vector irreps (cf. Sect. 2) real.

After this, there will generally be one or several free phases still to be decided upon within each basis set. These remaining phases are fixed by application of the following hierarchial set of rules (5)–(8), starting for each irrep Γ with the primary basis set and proceeding with increasing j values if there are supplementary bases:

(5) A maximal number of subduction coefficients $s(jm, ja\Gamma\gamma)$ should be real.
(6) A maximum number of the real subduction coefficients should be positive.
(7) A maximum number of real coefficients $s(jm, ja\Gamma\gamma)$ with $m > 0$ should be positive.
(8) A maximum number of real coefficients of the particular type $s(jj, ja\Gamma\gamma)$ should be positive.

Once all the standard basis functions have been chosen, they are applied using the following further rules hierarchially:

(9) If two of the irreps in a triple are equivalent and neither one is equivalent to the third irrep, it is the latter one which shall have supplementary bases in order to produce the sufficient number of linearly independent sets of 3-Γ symbols.
(10) Triples $j_1 j_2 j_3$ of j values corresponding to $\Gamma_1\Gamma_2\Gamma_3$ are chosen so that $j_1 + j_2 + j_3$ is minimal.

These rules warrant several further comments:

If the subgroup hierarchy alluded to in (3) is *canonical*, i.e. with no branching multiplicities at any place in the hierarchy, the basis functions corresponding to the various irrep components, regarded individually, will be fixed up to a phase factor. However, since focusing on canonical hierarchies may prevent one from having other desirable properties of the matrix irreps or the 3-Γ symbols, we shall also consider non-canonical hierarchies (see [3] for $T^* \supset C_2^*$).

Rule (4) is only concerned with primary bases because these empirically are sufficient to generate the 3-Γ symbols $(\Gamma 1_G \Gamma / \gamma 0 \gamma')$. (This would not be the case if we were studying the cyclic double groups.) In all the cases where we have established (4.4.1), we have $R_0 = C_2^{Y*}$ (cf. Sect. 2.1).

Note that if *all* subduction coefficients are real, all 3-Γ symbols will also be real (this is a trivial, but useful, consequence of (4.3.6)).

The above rules have the particular consequence that the totally symmetric irrep 1_G is always assigned the standard basis function $|jm\rangle = |0\,0\rangle$. This again implies that $(1_G 1_G 1_G/000) = +1$ so that in all formulas involving the conjugated symbol $\bar{1}_G$, the bar may be removed without consequences.

A straightforward calculation then further shows that if Γ is of the first or second kind, we shall have $\mathbb{A}(\Gamma 1_G \Gamma) = (+1)$ for the Derome–Sharp $\mathbb{A}$ matrix ([1], Sect. 5.4) of the triple $\Gamma 1_G \Gamma$.

If Γ is a *third-kind* irrep ([1], Sect. 5.2), it will be assigned just one j value, and $\bar{\Gamma}$ will be assigned the same value j. Since

$$\begin{pmatrix} j & 0 & j \\ \Gamma\gamma & 1_G 0 & \bar{\Gamma}\gamma' \end{pmatrix} = (-1)^{2j} \begin{pmatrix} j & 0 & j \\ \bar{\Gamma}\gamma' & 1_G 0 & \Gamma\gamma \end{pmatrix} \tag{4.4.2}$$

by ([1], Eq. (6.8) or Eq. (6.9)), we have for the 3-Γ symbols:

$$\begin{pmatrix} \Gamma & 1_G & \bar{\Gamma} \\ \gamma & 0 & \gamma' \end{pmatrix} = (-1)^{2j} \begin{pmatrix} \bar{\Gamma} & 1_G & \Gamma \\ \gamma' & 0 & \gamma \end{pmatrix}. \tag{4.4.3}$$

(In the cases we have dealt with, there is never any branching multiplicity for a primary j-value.) Recalling the fact that $(-1)^{2j} = +1$ when $\mathscr{D}^{[j]}$ (and thus Γ) is a vector irrep (Sect. 2) and $(-1)^{2j} = -1$ when $\mathscr{D}^{[j]}$ (and thus Γ) is a spin irrep, we may draw the following two important conclusions:

Firstly, the phase $\pi(\Gamma 1_G \bar{\Gamma})$ (see [1], Sect. 4) satisfies the relations

$$\pi(\Gamma 1_G \bar{\Gamma}) = \begin{cases} +1 \text{ when } \Gamma \text{ is a vector irrep of the third kind} \\ -1 \text{ when } \Gamma \text{ is a spin irrep of the third kind.} \end{cases} \tag{4.4.4}$$

With the definition of $\pi(\Gamma 1_G \bar{\Gamma})$ for first- and second-kind irreps set up in ([1], Sect. 5.3.2), (4.4.4) holds for all three kinds of irreps in the non-commutative double groups thanks to the correspondence first-kind↔vector and second-kind↔spin noted in Sect. 2. An implication is that for any triple $\Gamma_1\Gamma_2\Gamma_3$ with $\dim \mathscr{F}(\Gamma_1\Gamma_2\Gamma_3) > 0$ we have

$$\pi(\Gamma_1 1_G \bar{\Gamma}_1)\pi(\Gamma_2 1_G \bar{\Gamma}_2)\pi(\Gamma_3 1_G \bar{\Gamma}_3) = +1, \tag{4.4.5}$$

in all the non-commutative double groups (cf. Sect. 2.1). This property ensures the "associativity of the invariant triple product" [1, Sect. A.4]. (Note again that (4.4.4) does not hold in the cyclic double groups. The example of C_1^* (Sect. 2) may be used also here.)

Secondly, by invoking also the above remark regarding $\bar{1}_G$, we may evaluate the $\mathbb{A}$ matrices ([1], Sect. 5.4) for the triples $\Gamma 1_G \bar{\Gamma}$ and $\bar{\Gamma} 1_G \Gamma$ when Γ is of the third kind. We note that there must be a complex phase $\omega(\Gamma, \bar{\Gamma})$ such that

$$\begin{pmatrix} \Gamma & 1_G & \bar{\Gamma} \\ \gamma & 0 & \gamma' \end{pmatrix} = \omega(\Gamma, \bar{\Gamma})(\dim \Gamma)^{-1/2}\delta(\gamma, \gamma') \quad \text{for all } \gamma \text{ and } \gamma' \tag{4.4.6}$$

(cf. [1, Eq. (5.3.9)]). We then have

$$\begin{aligned} A(\Gamma 1_G \bar{\Gamma}) &= \sum_{\gamma\gamma'} \overline{\begin{pmatrix} \Gamma & 1_G & \bar{\Gamma} \\ \gamma & 0 & \gamma' \end{pmatrix}} \, \overline{\begin{pmatrix} \bar{\Gamma} & \bar{1}_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix}} \\ &= \sum_{\gamma\gamma'} \overline{\begin{pmatrix} \Gamma & 1_G & \bar{\Gamma} \\ \gamma & 0 & \gamma' \end{pmatrix}} \, \overline{\begin{pmatrix} \bar{\Gamma} & 1_G & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix}} \\ &= \pi(\Gamma 1_G \bar{\Gamma}) \sum_{\gamma\gamma'} \delta(\gamma, \gamma')\overline{\omega(\Gamma, \bar{\Gamma})}\delta(\gamma, \gamma')\overline{\omega(\Gamma, \bar{\Gamma})}(\dim \Gamma)^{-1} \\ &= \begin{cases} +(\overline{\omega(\Gamma, \bar{\Gamma})})^2 \text{ for } \Gamma \text{ a vector irrep} \\ -(\overline{\omega(\Gamma, \bar{\Gamma})})^2 \text{ for } \Gamma \text{ a spin irrep} \end{cases} \\ &= A(\bar{\Gamma} 1_G \Gamma), \end{aligned} \tag{4.4.7}$$

which shows that if our 3-Γ symbols in (4.4.6) are *real* and thus $\omega=+1$ or $\omega=-1$ – which we shall actually always have them to be – then the $\mathbb{A}$ matrix is necessarily (-1) when Γ is a spin irrep (cf. the discussion in [1], Sect. 5.4).

Two somewhat more lengthy comments have been given separate subsections below (Sect. 4.5 and 4.6), and some further remarks on the literature etc. are collected in Sect. 5.

4.5. Phase changes of subduction coefficients associated with rotation around the Z axis

Considering the 3-*j* symbol property (3.5.3), one may observe that changing a given set of subduction coefficients $s(jm, ja\Gamma\gamma)$ by choosing a real number α with $0<\alpha<2\pi$ and putting

$$s_\alpha(jm, ja\mathbb{\Gamma}\gamma)=e^{-im\alpha}s(jm, ja\mathbb{\Gamma}\gamma) \tag{4.5.1}$$

leaves the transformed 3-*j* symbols, defined as in (4.3.5), unchanged. This may appear to be of limited interest, since the subduction coefficients $s(jm, ja\mathbb{\Gamma}\gamma)$ must generally generate a matrix form of Γ different from $\mathbb{\Gamma}$. However, we shall analyse now the significance of the s_α's.

The double group G we are considering is a certain subgroup of R_3^* (Sect. 2). By specifying φ, θ, ψ for each of its elements we get, in principle, also information on the axes of rotation and angles of rotation of the ordinary rotations to which the double group elements correspond. Now consider the double group element

$$\boldsymbol{C}_{2\pi/\alpha}^{Z*}=\mathscr{D}^{[1/2]}(\alpha,0,0) \tag{4.5.2}$$

corresponding to a rotation about the Z axis through the angle α. This element is represented in the standard matrix irrep $\mathscr{D}^{[j]}$ (j being any of the numbers 1/2, 1, 3/2, 2, ...) by the matrix defined by

$$\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})_{mm'}=\delta(m,m')\,e^{-im\alpha}. \tag{4.5.3}$$

Thus the coefficients s_α defined in (4.5.1) are elements of the matrix $(\mathbb{S}_\alpha^{ja\mathbb{\Gamma}})^\dagger$, where

$$\mathbb{S}_\alpha^{ja\mathbb{\Gamma}}=\mathbb{S}^{ja\mathbb{\Gamma}}\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}. \tag{4.5.4}$$

If $\boldsymbol{g}$ is any element of G, we have, using the homomorphism property of $\mathscr{D}^{[j]}$ and then (4.3.1), that

$$\begin{aligned}
&\mathbb{S}_\alpha^{ja\mathbb{\Gamma}}\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*}\boldsymbol{g}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1})\\
&\quad=\mathbb{S}^{ja\mathbb{\Gamma}}\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})\mathscr{D}^{[j]}(\boldsymbol{g})\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}\\
&\quad=\mathbb{S}^{ja\mathbb{\Gamma}}\mathscr{D}^{[j]}(\boldsymbol{g})\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}\\
&\quad=\mathbb{\Gamma}(\boldsymbol{g})\mathbb{S}^{ja\mathbb{\Gamma}}\mathscr{D}^{[j]}(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}\\
&\quad=\mathbb{\Gamma}(\boldsymbol{g})\mathbb{S}_\alpha^{ja\mathbb{\Gamma}}.
\end{aligned} \tag{4.5.5}$$

This calculation shows that the matrix $\mathbb{S}_\alpha^{ja\mathbb{\Gamma}}$ subduces the irrep $\mathscr{D}^{[j]}$, acting on the "rotated group" $G_\alpha=\boldsymbol{C}_{2\pi/\alpha}^{Z*}G(\boldsymbol{C}_{2\pi/\alpha}^{Z*})^{-1}$, to the matrix form $\mathbb{\Gamma}$ of Γ. The group G is obtained by rotating the axes of the R_3-elements corresponding to the elements of G through an angle α about the Z axis; it is isomorphic to G (and, as seen from its definition, in fact *conjugate*, in the subgroup sense, to G within R_3^*).

Another way of expressing the same facts is to say that by introducing the coefficients s_α, we have changed from the basis functions $|ja\Gamma\gamma\rangle$ in (4.3.2) to functions $|ja\Gamma\gamma\rangle_\alpha$ defined by

$$\begin{aligned} |ja\Gamma\gamma\rangle_\alpha &= \sum_m e^{-im\alpha} s(jm, ja\Gamma\gamma)|jm\rangle \\ &= \sum_m s(jm, ja\Gamma\gamma) \sum_{m'} \mathscr{D}^{[j(}\boldsymbol{C}^{Z^*}_{2\pi/\alpha})]_{m'm}|jm\rangle \\ &= \sum_m s(jm, ja\Gamma\gamma)\{\hat{\mathscr{P}}(\boldsymbol{C}^{Z^*}_{2\pi/\alpha})|jm\rangle\}, \end{aligned} \qquad (4.5.6)$$

i.e. obtained by "rotating the $|jm\rangle$ functions by α around the Z axis", and then performed the subduction by the matrix $\mathbb{S}^\dagger$.

Note that the functions $|ja\Gamma\gamma\rangle_\alpha$ for a given Γ may well be mixtures of functions $|j\tilde{a}\tilde{\Gamma}\gamma\rangle$ with several different $\tilde{a}$ and $\tilde{\Gamma}$. Examples where this remark is relevant will be discussed in [4, 5].

In conclusion, if we rotate the axes of the rotations corresponding to the elements of our double group about the Z axis an angle α and consider the new copy of the double group generated, we may keep our matrix irreps and transformed 3-j symbols by defining new subduction coefficients by (4.5.1). We shall make use of this in our treatment of the double groups for obtaining, by a judicious choice of coordinate system, the simplest possible subduction coefficients once the matrix irreps and transformed 3-j symbols have been decided upon ("simplest possible" referring to rules (5)–(8) in Sect. 4.4).

(The phases involved in the rotations we are discussing here seem to be a special case of the "orientation phases" discussed in [19–21].)

4.6. An orthogonality property of the subgroup-adapted 3-j symbols

Suppose G is a double group and we are constructing 3-Γ symbols for a G-irrep triple $\Gamma_1\Gamma_2\Gamma_3$ *with multiplicity* by the above procedure (Sects. 4.3–4.4). We require an *orthonormal* basis $(\mathfrak{c}_1, \ldots, \mathfrak{c}_N)$ for the fix-vector space $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ [much of our formalism depends on this requirement]. The question is whether the several triples of j-values assigned to $\Gamma_1\Gamma_2\Gamma_3$ by the rules given above automatically lead to mutually orthogonal sets of 3-Γ symbols. It turns out that this may be answered in the affirmative, and we shall now discuss this more closely.

As a matter of experience, every time we are in the situation just described, the following particular further conditions are fulfilled: Two of the irreps, Γ_1 and Γ_2 say, are "spherical" in the sense that there are irreps $\mathscr{D}^{[j_1]}$ and $\mathscr{D}^{[j_2]}$ of the rotation group which remain irreducible upon restriction to the subgroup in question and become equivalent to Γ_1 and Γ_2, respectively. Furthermore, all j-triples assigned to the irrep triple $\Gamma_1\Gamma_2\Gamma_3$ are of the particular form j_1j_2j, where D_j is a rotation group irrep yielding Γ_3 at least once when restricted to the subgroup. Thus, any set of 3-Γ symbols $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ will be constructed in the procedure by normalizing subgroup-adapted 3-j symbols of the form $(j_1j_2j_3/\Gamma_1\gamma_1\Gamma_2\gamma_2a_3\Gamma_3\gamma_3)$.

Suppose that two triples j_1j_2j' and j_1j_2j'' with corresponding branching multiplicity indices a_3' and a_3'' correspond to two different multiplicity indices β' and β''. We wish to show that the coefficients $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_{\beta'}$ and $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_{\beta''}$ form mutually orthogonal sets, i.e. that

$$\sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{\beta'}} \begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{\beta''} = 0. \tag{4.6.1}$$

Now, the left-hand side of (4.6.1) is, by the construction, proportional to

$$\sum_{\gamma_1\gamma_2\gamma_3} \overline{\begin{pmatrix}j_1 & j_2 & j_3\\ \Gamma_1\gamma_1 & \Gamma_2\gamma_2 & a_3'\Gamma_3\gamma_3\end{pmatrix}} \begin{pmatrix}j_1 & j_2 & j''\\ \Gamma_1\gamma_1 & \Gamma_2\gamma_2 & a_3''\Gamma_3\gamma_3\end{pmatrix}. \tag{4.6.2}$$

By convention (1) in Sect. 4.4, we have $j' \neq j''$. Then an argument completely analogous to the one leading to Eq. (A.3.3) in [1], applied here to the involved rotation group irreps D_{j_1}, D_{j_2}, $D_{j'}$, and $D_{j''}$ in their subgroup-adapted matrix forms, shows that (4.6.2) is zero, as desired, and in fact even that

$$\sum_{\gamma_1\gamma_2} \overline{\begin{pmatrix}j_1 & j_2 & j'\\ \Gamma_1\gamma_1 & \Gamma_2\gamma_2 & a_3'\Gamma_3\gamma_3\end{pmatrix}} \begin{pmatrix}j_1 & j_2 & j''\\ \Gamma_1\gamma_1 & \Gamma_2\gamma_2 & a_3''\Gamma_3\gamma_3\end{pmatrix} = 0 \tag{4.6.3}$$

for every γ_3.

This orthogonality property of the subgroup-adapted 3-j symbols not only has interest for the reasons already mentioned; it is also invoked in the proof needed in several multiplicity cases that the subgroup triple coefficients constructed actually *do* form sets of 3-Γ symbols (see, e.g. the discussion of 3-Γ symbols for the tetrahedral triple TTT in [3]).

5. Concluding remarks

The procedure which we have discussed above for obtaining double group 3-Γ symbols has also been described by Lulek [14] and has been used by Kibler et al. [22] in the case of the hierarchy $R_3^* \supset O^* \supset D_4^* \supset D_2^*$; formulas like (4.3.5) also appear with König and Kremer [16] and Butler [17]. In Lulek's nomenclature the subgroup-adapted 3-j symbols of (4.3.5) are called 3j symbols [14] or $3j\Gamma\gamma$ symbols [23].

In [16] it is claimed – and the same idea seems to be present in [23] – that it is essential for the permutational properties of the resulting subgroup 3-Γ symbols that a *positive* normalization constant is used in Eq. (4.3.6). This is evidently not so; we suggest a positive number to have a *definite* procedure, but a common phase on *all* numbers in a given set of 3-Γ symbols would not alter its permutational properties.

When actually carrying out the procedure outlined in Sect. 4, for the groups discussed in [2–5], we of course needed concrete basis functions of the type (4.3.2). There is a rather vast literature dealing with methods for the construction of such basis functions, but we shall not discuss that here; in all our cases, basis functions were either obtainable by immediate inspection or could be obtained by suitable manipulation from the functions already given in the literature. (See, though, a remark in [24, § 8] regarding necessity of having basis functions for high j-values.)

The discussion towards the end of Sect. 4.3 clearly demonstrates that one has to distinguish between the *standard basis functions* we choose and functions which *just transform the standard way.* In multiplicity cases like the triple UT_2U of the octahedral double group mentioned there, it may have rather dramatic consequences to replace the standard functions, *in casu* $|\frac{3}{2}U\gamma\rangle$, by other functions transforming correctly, like $|\frac{5}{2}U\gamma\rangle$. In multiplicity-free groups, the difference can never amount to more than a phase change (if the two function sets being compared both generate non-zero subgroup triple coefficients and thus 3-Γ symbols). On the other hand, in some cases phase differences *inevitably* occur between 3-Γ symbols corresponding to independent choices of basis functions transforming the standard way; this follows from the unitarity of matrices of isoscalar factors (see [6] for a discussion of specific examples). Quite the contrary seems to be assumed in [25].

A computer program has been developed which calculates the subgroup-adapted 3-j symbols according to (4.3.5), using for $(j_1 j_2 j_3 / m_1 m_2 m_3)$ the explicit formula (e.g., [26], Eq. (1.5)), and the normalization constant in (4.3.6) according to its defining expression. The results are expressed by square roots of rational numbers when the subduction coefficients are of this form. An analogous programme for the exact calculation of coupling coefficients of R_3^* in such a root-rational-fraction form has been described in [27].

[A word may be in place on the calculation of the normalization constant in (4.3.6). Formulae exist [28] which, in principle, allow one to calculate such quantities – at least in the case of no branching multiplicities, that is, the a_i in (4.3.6) superfluous – as a combined integral over the group R_3^* and summation over the finite group in question, using only the *characters* of the six irreps involved. These formulae did not to us seem suitable, if applicable at all, for computer calculations.]

Ongoing work aims at making the programme calculate also Derome–Sharp $\mathbb{A}$ and $\mathbb{B}^i$ matrices ([1], Sect. 5.4) and coupling coefficients according to ([1], formula (5.3.16)) and further to calculate 6-Γ and 9-Γ symbols and recoupling coefficients as they are defined in the formalism under development [24, 29].

It is worth noting that the exposition we have given in [1] and in the present paper descends through a hierarchy of levels of generality. One may stop at any level desired and use the results established until there. Thus the generalities of [1] and Sects. 2 and 3 above together with the general procedure outlined in Sect.

4.3 provide a framework which is applicable whether or not one would like to use our suggestions for choices of basis functions in Sect. 4.4.

Especially the phase choices on the basis functions are, of course, somewhat arbitrary; we ourselves shall feel free to make other phase choices in the future if this seems useful. The important feature to us is the fundamental fact that the procedure we describe *fixes the phases for the entire Wigner–Racah algebra in one step* by fixing the phases of the basis functions. This is evident because of the "Aufbau" way we construct the algebra with 3-Γ symbols as the basic quantity (see [1] in combination with [24, 29] for the 6-Γ and 9-Γ symbols and recoupling coefficients). This is to be contrasted with the almost "orthogonal" approach adopted by Butler [30, 21] (which he himself calls a "building up principle" [31]) which of course should lead to an equivalent apparatus in the last end. With Butler, the basis functions, the matrix irreps they generate, and the "3-*jm* symbols" (normalized triple coefficients in our terminology) are the last things to be calculated, not the first ones, and pieces of information such as placement of coordinate system and matrix irreps are only obtainable through a very involved discussion. The initial steps are the calculation of "6-*j* symbols" and "3-*jm* factors" (the latter being quantities related to our normalization constant in (4.3.6)) by a recursive procedure. The phase fixations begin here and are made in a not very transparent way; at least their connection with the "3-*jm* symbols" – which are to represent (through the Wigner–Eckart theorem ([1], Sect. 2)) the operators whose phases we are really interested in – is not clear.

We further point out that the basis functions really only play a dummy role in our procedure. What matters is the subduction coefficients and the explicit knowledge of the matrix irreps and 3-Γ symbols of the parent group R_3^*, and wherever this kind of information is present for a group and a subgroup of it, the procedure may, in principle, be applied. (See remarks on studies of new groups in [24, § 6.1].)

Appendix

In this appendix we give some mathematical arguments which are relevant to the discussion of various sufficient conditions for the existence of real 3-Γ symbols (see Sect. 3.2).

Suppose that Γ_1, Γ_2, Γ_3 are unitary matrix reps of a group G. If the linear space $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ of column fix-vectors for $\bar{\Gamma}_1\otimes\bar{\Gamma}_2\otimes\bar{\Gamma}_3$ has dimension at least one and is stable under complex conjugation, or, for short, $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ is conjugation stable [meaning that $\mathfrak{c}\in\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)\Rightarrow\bar{\mathfrak{c}}\in\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$], then there exists – and *only* then does there exist – an orthonormal basis for $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ consisting of *real* column vectors. This again ensures the existence of real 3-Γ symbols ([1], Sect. 4) for $\Gamma_1\Gamma_2\Gamma_3$ (provided the triple is simple phase ([1], Sect. 3.2) if $\Gamma_1=\Gamma_2=\Gamma_3$).

The fact that conjugation stability implies the existence of a real orthonormal basis for $\mathscr{F}=\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3)$ is easily ascertained: Since the Gram–Schmidt orthonormalization procedure applied to a real basis will yield a real orthonormal basis, it is sufficient to show that there exists a real basis for $\mathscr{F}$. To see that *this* is true, start by picking any vector $\mathbb{c}_1 \neq \mathbb{0}$ in $\mathscr{F}$. Since $\mathbb{c}_1 \in \mathscr{F}$, the *real* vectors $\mathbb{c}_1 + \bar{\mathbb{c}}_1$ and $i(\mathbb{c}_1 - \bar{\mathbb{c}}_1)$ are also in $\mathscr{F}$, and these two vectors together span the same subspace of $\mathscr{F}$ as do $\mathbb{c}_1$ and $\bar{\mathbb{c}}_1$ together. Continue by picking a vector $\mathbb{c}_2 \neq \mathbb{0}$ in the orthogonal complement in $\mathscr{F}$ to this subspace .... At the end, a real vector-set $(\mathbb{c}_1 + \bar{\mathbb{c}}_1,\ i(\mathbb{c}_1 - \bar{\mathbb{c}}_1),\ \mathbb{c}_2 + \bar{\mathbb{c}}_2,\ i(\mathbb{c}_2 - \bar{\mathbb{c}}_2), \ldots)$ generating $\mathscr{F}$ is obtained, and from this a real *basis* may be selected. Q.E.D.

The condition that $\mathscr{F}(\mathbb{\Gamma}_1\mathbb{\Gamma}_2\mathbb{\Gamma}_3)$ is conjugation stable is, for example, fulfilled in the following two particular situations:

(1) There is a generating set $M \subseteq G$ such that for each $R \in M$, the matrix $\mathbb{\Gamma}_1(R) \otimes \mathbb{\Gamma}_2(R) \otimes \mathbb{\Gamma}_3(R)$ is *real.* (The conjugation stability is here evident).

As a special case of this we note the situation where the $\mathbb{\Gamma}_i$ are all *real* matrix reps.

(2) There is a generating set $M \subseteqq G$ such that for each $R \in M$, the matrices $\mathbb{\Gamma}_1(R)$, $\mathbb{\Gamma}_2(R)$, and $\mathbb{\Gamma}_3(R)$ are all *symmetric.* Proof of the conjugation stability in this situation: Suppose that $\mathbb{c} \in \mathscr{F}$. We have to show that $\bar{\mathbb{c}} \in \mathscr{F}$, i.e., that

$$[\bar{\mathbb{\Gamma}}_1(R) \otimes \bar{\mathbb{\Gamma}}_2(R) \otimes \bar{\mathbb{\Gamma}}_3(R)]\bar{\mathbb{c}} = \bar{\mathbb{c}} \quad \text{for all } R \in G. \tag{A.1}$$

Now, given $R \in G$, we know from the facts that $R^{-1} \in G$ and $\mathbb{c} \in \mathscr{F}$ that

$$[\bar{\mathbb{\Gamma}}_1(R^{-1}) \otimes \bar{\mathbb{\Gamma}}_2(R^{-1}) \otimes \bar{\mathbb{\Gamma}}_3(R^{-1})]\mathbb{c} = \mathbb{c}. \tag{A.2}$$

Conjugating on both sides of this equation and using the unitarity and the assumed transposition symmetry of the $\mathbb{\Gamma}_i(R)$, we get

$$\begin{aligned} \bar{\mathbb{c}} &= [\mathbb{\Gamma}_1(R^{-1}) \otimes \mathbb{\Gamma}_2(R^{-1}) \otimes \mathbb{\Gamma}_3(R^{-1})]\bar{\mathbb{c}} \\ &= [\overline{\mathbb{\Gamma}_1(R)}^T \otimes \overline{\mathbb{\Gamma}_2(R)}^T \otimes \overline{\mathbb{\Gamma}_3(R)}^T]\bar{\mathbb{c}} \\ &= [\bar{\mathbb{\Gamma}}_1(R) \otimes \bar{\mathbb{\Gamma}}_2(R) \otimes \bar{\mathbb{\Gamma}}_3(R)]\bar{\mathbb{c}}, \end{aligned} \tag{A.3}$$

as desired.

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