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1984 J. Phys. A: Math. Gen. 17 3077

(http://iopscience.iop.org/0305-4470/17/16/010)

J. Phys. A: Math Gen. 17 (1984) 3077-3089. Printed in Great Britain

Classification and determination of irreducible bases for induced representations for chains of subgroups of finite groups

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Received 16 January 1984

Abstract. The problem of classification and determination of standard irreducible bases for induced presentations of an arbitrary finite group is discussed. A general prescription for classification and determination of these bases for an arbitrary induced representation is proposed, and an extra independent prescription for the special case of primitive representations is given. Relations between appropriate transformation coefficients are investigated and, in particular, a matrix similar to the Racah recoupling matrix from theory of multiple coupling of angular momenta is introduced.

1. Introduction

Transitive permutation representations (transreps) have been recently applied to achieve a unique classification of symmetric coordinates for several clusters of material points such as molecules, or atomic shells in a crystal (Lulek 1980, Kuźma *et al* 1980, Newman 1981, Chen and Newman 1982, Chan and Newman 1983), finite crystals with periodic boundary conditions ('cyclic regions' in the terminology of Chan and Newman 1982), or infinite crystals (Litvin 1982). The key for this application is provided by a factorisation of the mechanical representation of a cluster into a permutational factor called the positional representation, and a vector one. The positional representation is either a transrep describing permutations of identical atoms under symmetry transformations of the cluster, or the direct sum of transreps. An irreducible representation (irrep) entering the positional representation constitutes an additional classification label for the symmetric coordinates of the cluster.

Newman (1981), and Chen and Newman (1982) have demonstrated that the above classification scheme yields a unique classification for some cubic clusters (with the coordination $z=6$, 8, and 12) but is insufficient for cubic clusters with $z=24$ and 48 because of repetitions of some irreps in the corresponding positional representation. These authors have proposed a unique classification for the latter cases using the so-called 'correlation theorem' (Wilson *et al* 1955, p 121), which is essentially a version of the well known Frobenius reciprocity theorem for induced representations (indreps) (cf e.g. Altmann 1977, p 148). The method relies on using irreps of members of an appropriate chain of subgroups as labels for distinguishing the repeated irreps of the symmetry group of a cluster in the positional representation. One can put a question whether there exists a unique classification of irreps for an arbitrary cluster, or more generally, for an arbitrary transrep of a finite group G. The next question, which is important in quantum applications (e.g. coupling of lattice vibrations with localised electrons of paramagnetic ions in crystals—cf e.g. Newman 1981 and references therein, or magnetic excitations in crystals, associated with a point impurity—cf Callen and Baryakhtar 1973) is a procedure for a determination of states corresponding to such a classification and transforming in a standard way according to irreps of the group G.

From the mathematical point of view it is the aim to consider a more general problem: find a unique classification scheme for irreps of a finite group G entering an indrep $\Theta\uparrow G$, where the inducing representation Θ is an arbitrary irrep of an arbitrary subgroup $H\subset G$. A transrep of G is equivalent to a particular indrep $\Theta_0\uparrow G$, where Θ_0 is the unit irrep of H. Such a generalisation can be also useful in a wide area of applications of indreps in physics (cf e.g. Barut and Rączka 1977, Altmann 1977, and references therein).

The above problem is entirely analogous to that of a classification of irreps Θ of a subgroup $H\subset G$ entering the subduced representation $\Gamma\downarrow H$, where Γ is an irrep of G. A formal description of the analogy is provided by the Frobenius reciprocity theorem, and a procedure for the determination of irreducible bases of an indrep in this way is proposed by us elsewhere (Lulek and Lulek 1984). The aim of the present paper is a discussion of ways of classification and explicit determination of the irreducible bases for an arbitrary indrep $\Theta\uparrow G$ of a finite group G, associated with possible intermediate subgroups in the chain $H\subset G$. Essentially, the classification based exclusively on irreps of intermediate subgroups is not always complete (exactly as in the case of the state-labelling problem for subduced representation). A complete classification can be, however, obtained assuming that the irreducible basis for irreps of G, adapted to the chain $H\subset G$, is already known. Then different chains of subgroups, $H\subset K\subset G$ and $H\subset K'\subset G$, $K\neq K'$, give rise to different irreducible bases, and hence to linear transformations resembling the famous Racah recoupling matrices from angular momentum theory (see e.g. Fano and Racah 1959). In the present work we propose a formal description of such transformations. We suppose that it is a necessary part of a programme of paving the way to Racah algebra for quantum theory of multicentre systems (Newman 1983).

The paper is organised as follows. In § 2 we give a formulation of the problem, which is associated with introducing the principal properties of indreps in the way of establishing the notation and terminology. We try to use the notation appropriately adjusted to the problem, which, in particular, clearly reflects the structure of sets of labels of several basis vectors. In § 3 we discuss the basis classification and determination problem for the case of three-member chain $H\subset K\subset G$ introducing a quantity associated with the structure of imprimitivity blocks for this chain, and bearing an analogy to the Racah recoupling matrix. In § 4 we describe an explicit solution of the classification and determination problem, basing on the Frobenius reciprocity theorem. In § 5 we propose a standard basis equivalent to Yamanochi basis for primitive representations, consitituting an important special case of transreps.

2. The formulation of the problem

2.1. *The notation used for irreps.*

We shall use the following notation associated with a finite group $G:\tilde{G}$ is the set of all linearly inequivalent irreps Γ of G, $[\Gamma]$ is the dimension of Γ, and $\tilde{\Gamma}=\{\gamma|\gamma=1,2,\ldots,[\Gamma]\}$ is the set of labels of a standard orthonormal irreducible basis of

Γ, so that the vectors $|\Gamma\gamma\rangle$, $\gamma\in\tilde{\Gamma}$, span a carrier space for Γ. In particular, $\Gamma_0\in\tilde{G}$ is the unit irrep of G.

The corresponding symbols have the same meaning for a subgroup $H\subset G(\tilde{H}, \Theta, [\Theta], \tilde{\Theta}, \vartheta, \Theta_0)$, a subgroup $K\subset G(\tilde{K}, \Xi, [\Xi], \tilde{\Xi}, \xi, \Xi_0)$, etc. Moreover, for an arbitrary finite set A the symbol $|A|$ denotes the number of elements of A, so that e.g. $|G|$ is the order of the group G, $|\tilde{\Gamma}|=[\Gamma]$, etc.

2.2. The notation for indreps.

Let

$$G=\bigcup_{r\in\tilde{R}(G:H)} g_r H \tag{1}$$

be the decomposition of the group G into left cosets with respect to its subgroup H, so that $\{g_r|r\in\tilde{R}(G:H)\}$ is the set of arbitrarily chosen, but fixed left coset representatives. The formula

$$R^{G:H}(x)=\begin{pmatrix} g_r H \\ xg_r H\end{pmatrix}, \qquad r\in\tilde{R}(G:H), \qquad x\in G, \tag{2}$$

defines the transrep $R^{G:H}$ (the ground representation in the terminology of Altmann 1977, ch 10), acting on the orbit (the homogeneous space) $\tilde{R}(G:H)$. The linear analogue of the permutation representation $R^{G:H}$ is determined by matrices $D^{G:H}(x)$, $x\in G$, with elements

$$D^{G:H}_{r'r}(x)=\begin{cases}1 & \text{if } xg_r\in g_{r'}H,\\ 0 & \text{otherwise,}\end{cases} \qquad r, r'\in\tilde{R}(G:H). \tag{3}$$

The set

$$B^{\Theta\uparrow G}_{\text{nat}}=\{r\vartheta|r\in\tilde{R}(G:H),\ \vartheta\in\tilde{\Theta}\}\cong\tilde{R}(G:H)\times\tilde{\Theta}, \tag{4}$$

where the cross '$\times$' denotes the cartesian product of sets, constitutes the natural basis of the indrep $\Theta\uparrow G$ of the group G. The corresponding operators $D^{\Theta}(x)$, $x\in G$, are defined by their action on vectors $|\Theta\uparrow Gr\vartheta\rangle$, $(r\vartheta)\in B^{\Theta\uparrow G}_{\text{nat}}$, according to a formula

$$D^{\Theta\uparrow G}(x)|\Theta\uparrow Gr\vartheta\rangle=\sum_{r'\in\tilde{R}(G:H)}\ \sum_{\vartheta'\in\tilde{\Theta}} D^{G:H}_{r'r}(x)D^{\Theta}_{\vartheta'\vartheta}(h_r(x))|\Theta\uparrow Gr'\vartheta'\rangle, \tag{5}$$

where $D^{\Theta}_{\vartheta'\vartheta}(h)$, $h\in H$, $\vartheta'\in\tilde{\Theta}$, $\vartheta\in\tilde{\Theta}$, is the Wigner matrix element of the inducing representation Θ, and $h_r(x)\in H$ is the subelement of the element $x\in G$ under the representative g_r (cf Altmann 1977, p 133), i.e. the element of H, defined uniquely by $xg_r=g_{r''}h_r(x)$, with $g_{r''}$ being an appropriate representative in the decomposition (1). As a matter of fact, Θ in equations (4)–(5) can be substituted by an arbitrary finite-dimensional representation of H (not necessarily an irrep) providing that $\tilde{\Theta}$ is the corresponding complete set of basis labels for Θ. The transrep $R^{G:H}$ is linearly equivalent to the indrep $\Theta_0\uparrow G$, and

$$B^{\Theta_0\uparrow G}_{\text{nat}}\cong\tilde{R}(G:H), \tag{6}$$

i.e. the orbit of the transrep $R^{G:H}$ corresponds to the natural basis of the indrep $\Theta_0\uparrow G$.

2.3. *The irreducible basis of an indrep*

The indrep $\Theta\uparrow\mathrm{G}$ is, in general, reducible in G. Let

$$\Theta\uparrow\mathrm{G}\simeq\sum_{\Gamma\in\tilde{\mathrm{G}}}\oplus n(\Theta\uparrow\mathrm{G},\Gamma)\Gamma, \tag{7}$$

where '$\oplus$' denotes the direct sum, be the decomposition of $\Theta\uparrow\mathrm{G}$ into irreps Γ of G, so that $n(\Theta\uparrow\mathrm{G},\Gamma)$ is the multiplicity of Γ in $\Theta\uparrow\mathrm{G}$. Using standard methods of finite groups representation theory (cf. e.g. Lyubarskii 1960, § 26) one can determine the standard irreducible basis in a carrier space of $\Theta\uparrow\mathrm{G}$. Such a basis can be labelled by the elements of the set

$$\begin{aligned} B_{\mathrm{irr}}^{\Theta\uparrow\mathrm{G}} &= \{\Gamma w\gamma|\Gamma\in\tilde{\mathrm{G}},\ w\in\tilde{W}(\Theta,\Gamma),\ \gamma\in\tilde{\Gamma}\} \\ &\cong\bigcup_{\Gamma\in\tilde{\mathrm{G}}}\tilde{W}(\Theta,\Gamma)\times\tilde{\Gamma}, \end{aligned} \tag{8}$$

where

$$\tilde{W}(\Theta,\Gamma)=\{w|w=1,2,\ldots,n(\Theta\uparrow\mathrm{G},\Gamma)\} \tag{9}$$

is the set of repetition indices for Γ in $\Theta\uparrow\mathrm{G}$. Hence, the irreducible basis for $\Theta\uparrow\mathrm{G}$ can be written as

$$|\Theta\uparrow\mathrm{G}\Gamma w\gamma\rangle=\sum_{(r\vartheta)\in B_{\mathrm{nat}}^{\Theta\uparrow\mathrm{G}}}b^{\Theta}_{r\vartheta,\Gamma w\gamma}|\Theta\uparrow\mathrm{G}r\vartheta\rangle,\qquad(\Gamma w\gamma)\in B_{\mathrm{irr}}^{\Theta\uparrow\mathrm{G}}. \tag{10}$$

The problem of determination of the irreducible basis for the indrep $\Theta\uparrow\mathrm{G}$ consists in evaluation the matrix b^{Θ} of the transformation (10), with rows and columns labelled by the natural and irreducible basis, respectively. The problem of classification of identical Γ's in $\Theta\uparrow\mathrm{G}$ is the first step of the determination problem, and consists in a definite choice of sets $\tilde{W}(\Theta,\Gamma)$, with $\Gamma\in\tilde{\mathrm{G}}$, that is, the choice of the system of repetition indices. A solution of the determination problem for the case of a two-member chain of subgroups $\mathrm{H}\subset\mathrm{G}$, based on the Frobenius reciprocity theorem, has been given elsewhere (Lulek and Lulek 1984, cf § 4). This solution does not exploit, however, the intermediate subgroups, which is one of aims of the present paper. The generalisation of the problem of a unique classification, investigated by Newman (1981) and Chan and Newman (1982), can be now formulated as a question whether it is possible to find, for each triad $(\mathrm{G},\mathrm{H},\Theta)$, such sets $\tilde{W}(\Theta,\Gamma)$, $\Gamma\in\tilde{\mathrm{G}}$, all elements of which are constructed exclusively of irreps $\Xi\in\tilde{\mathrm{K}}$ for some intermediate sugroups K, so that $\mathrm{H}\subset\mathrm{K}\subset\mathrm{G}$.

2.4. *The space of intertwining operators*

It has been shown by Edwards (1980), that the classification problem can be nicely formulated in terms of a choice of an orthonormal basis in the space $\mathrm{Hom}_{\mathrm{G}}(\Gamma,\Theta\uparrow\mathrm{G})$ of operators which intertwine Γ with $\Theta\uparrow\mathrm{G}$ in the group G, i.e. the linear operators B carrying vectors of the carrier space of Γ into the carrier space of $\Theta\uparrow\mathrm{G}$ and satisfying the conditions

$$BD^{\Gamma}(x)=D^{\Theta\uparrow\mathrm{G}}(x)B,\qquad x\in\mathrm{G}. \tag{11}$$

The irreducible basis of $\Theta\uparrow\mathrm{G}$, defined by equations (8)–(10) is associated with operators

$$B_w=\sum_{\gamma\in\tilde{\Gamma}}|\Theta\uparrow\mathrm{G}\Gamma w\gamma\rangle\langle\Gamma\gamma|,\qquad w\in\tilde{W}(\Theta,\Gamma), \tag{12}$$

with the property

$$B_w|\Gamma\gamma\rangle = |\Theta\uparrow \mathrm{G}\Gamma w\gamma\rangle, \qquad \gamma \in \tilde{\Gamma}. \tag{13}$$

Operators B_w, $w \in \tilde{W}(\Theta, \Gamma)$, form a basis in $\mathrm{Hom}_\mathrm{G}(\Gamma, \Theta\uparrow \mathrm{G})$, orthonormal with respect to the scalar product

$$(B_1, B_2) = \frac{1}{[\Gamma]} \mathrm{Tr}\, B_1^+ B_2 = \frac{1}{[\Gamma]} \sum_{\gamma\in\tilde{\Gamma}} \langle \Gamma\gamma|B_1^+ B_2|\Gamma\gamma\rangle, \tag{14}$$

where B_1, $B_2 \in \mathrm{Hom}_\mathrm{G}(\Gamma, \Theta\uparrow \mathrm{G})$. Such a formulation allows for an immediate and full use of the Frobenius reciprocity theorem, which will be demonstrated in § 4.

3. A three-member chain of subgroups

Now we consider a three-member chain $\mathrm{H} \subset \mathrm{K} \subset \mathrm{G}$ of subgroups. A comparison of definitions given by equations (2) and (5) yields

$$R^{\mathrm{G:H}} \simeq (R^{\mathrm{K:H}})\uparrow \mathrm{G} \tag{15}$$

and

$$\tilde{R}(\mathrm{G:H}) \cong \tilde{R}(\mathrm{G:K}) \times \tilde{R}(\mathrm{K:H}), \tag{16}$$

i.e. the transrep $R^{\mathrm{G:H}}$ is equivalent to the representation, induced from the transrep $R^{\mathrm{K:H}}$ of the intermediate subgroup K, and the corresponding orbit is equivalent to the cartesian product of orbits $\tilde{R}(\mathrm{G:K})$ and $\tilde{R}(\mathrm{K:H})$, associated with the links of the chain. In more detail, the orbit $\tilde{R}(\mathrm{K:H})$ of the representation $R^{\mathrm{K:H}}$ consists of those left cosets of G with respect to H, which constitute the intermediate subgroup K, i.e.

$$\mathrm{K} = \bigcup_{r_2 \in \tilde{R}(\mathrm{K:H})} g_{r_2}\mathrm{H}, \tag{17}$$

and

$$\mathrm{G} = \bigcup_{r_1 \in \tilde{R}(\mathrm{G:K})} g_{r_1}\mathrm{K}. \tag{18}$$

A comparison of equations (17) and (18) with (1) yields a natural one-to-one mapping ψ: $\tilde{R}(\mathrm{G:K}) \times \tilde{R}(\mathrm{K:H}) \rightarrow \tilde{R}(\mathrm{G:H})$, given by

$$\psi(r_1, r_2) = r \Leftrightarrow g_{r_1} g_{r_2}\mathrm{H} = g_r\mathrm{H}. \tag{19}$$

The situation described above can be interpreted as such that the intermediate subgroup K defines a decomposition of the orbit $\tilde{R}(\mathrm{G:H})$ into subsets called imprimitivity systems (cf e.g. Burnside 1911, p 191 or Hall 1959, § 5,6) which transform as a whole one into another under permutations $R^{\mathrm{G:H}}(x)$, $x \in \mathrm{G}$. It can be also described as a 'coarsening' of the transrep $R^{\mathrm{G:H}}$ to $R^{\mathrm{G:K}}$ (cf a similar situation in a paper of Mucha and Lulek 1983).

Let us now consider a representation which is induced in two stages, i.e. $(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}$. The natural basis of this representation,

$$\begin{aligned} B_{\mathrm{nat}}^{(\Theta\uparrow\mathrm{K})\uparrow\mathrm{G}} &= \{r_1 r_2 \vartheta | r_1 \in \tilde{R}(\mathrm{G:K}),\ r_2 \in \tilde{R}(\mathrm{K:H}),\ \vartheta \in \tilde{\Theta}\} \\ &\simeq \tilde{R}(\mathrm{G:K}) \times \tilde{R}(\mathrm{K:H}) \times \tilde{\Theta} \cong B_{\mathrm{nat}}^{\Theta\uparrow\mathrm{G}}, \end{aligned} \tag{20}$$

is clearly equivalent to the natural basis of $\Theta\uparrow \mathrm{G}$, with the mapping of elements determined by ψ of equation (19). The irreducible basis can be obtained using (10) twice: first for the link $\mathrm{H} \subset \mathrm{K}$, and then for $\mathrm{K} \subset \mathrm{G}$, so that

$$B_{\mathrm{irr}}^{(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}} = \{\Gamma \Xi w_1 w_2 \gamma | \Gamma \in \tilde{\mathrm{G}}, \Xi \in \tilde{\mathrm{K}}, w_1 \in \tilde{W}(\Xi, \Gamma), w_2 \in \tilde{W}(\Theta, \Xi), \gamma \in \tilde{\Gamma}\}$$
$$\simeq \bigcup_{\Gamma \in \tilde{\mathrm{G}}} \tilde{W}_K(\Theta, \Gamma) \times \tilde{\Gamma}, \tag{21}$$

where

$$\tilde{W}_K(\Theta, \Gamma) = \bigcup_{\Xi \in \tilde{K}} \tilde{W}(\Theta, \Xi) \times \tilde{W}(\Xi, \Gamma) \tag{22}$$

is the set determining the system of repetitions of Γ in $(\Theta \uparrow \mathrm{K}) \uparrow \mathrm{G}$. It is evident that the problem of unique classification of Γ in $\Theta \uparrow \mathrm{G}$ by means of irreps Ξ has a solution only when there exists such an intermediate subgroup K that

$$|\tilde{W}(\Theta, \Xi)| \leqslant 1, \qquad |\tilde{W}(\Xi, \Gamma)| \leqslant 1 \qquad \forall \Xi \in \tilde{\mathrm{K}}, \tag{23}$$

i.e. each of these sets contains not more than one element. When one of these conditions is not fulfilled, say $|\tilde{W}(\Theta, \Xi)| = 1$ but $|\tilde{W}(\Xi, \Gamma)| > 1$, then one can look for a new intermediate subgroup K_1, so that $\mathrm{H} \subset \mathrm{K} \subset \mathrm{K}_1 \subset \mathrm{G}$, consider a three-stage induction $((\Theta \uparrow \mathrm{K}) \uparrow \mathrm{K}_1) \uparrow \mathrm{G}$ etc, ending either on a satisfactory solution, or on exhaustion of the set of possible subgroups. If there exists a solution for a given chain $\mathrm{H} \subset \mathrm{K}_1 \subset \ldots \subset \mathrm{K}_f \subset \mathrm{G}$, then the corresponding set of labels can be written as

$$\tilde{W}_{\mathrm{H} \subset \mathrm{K}_1 \subset \ldots \subset \mathrm{K}_f \subset \mathrm{G}}(\Theta, \Gamma) = \{\Xi_1 \Xi_2 \ldots \Xi_f | \Xi_i \in \tilde{\mathrm{K}}_i\},$$
$$n(\Theta \uparrow \mathrm{K}, \Xi_1) = n(\Xi_f \uparrow \mathrm{G}, \Gamma) = 1, \qquad n(\Xi_{i-1} \uparrow \mathrm{K}_i, \Xi_i) = 1 \qquad \text{for } i = 1, 2, \ldots, f. \tag{24}$$

If there is no solution, then for each chain of subgroups linking H with G there exists such a two-member subchain $\mathrm{K}_{i-1} \subset \mathrm{K}_i$ and such $\Gamma \in \tilde{\mathrm{G}}$ that K_{i-1} is maximal in K_i (that is, that there is no non-trivial intermediate subgroup between K_{i-1} and K_i, cf Hall 1959, § 5.6), and $n(\Xi_{i-1} \uparrow K_i, \Xi_i) > 1$ for a pair (Ξ_{i-1}, Ξ_i), $\Xi_{i-1} \in \tilde{\mathrm{K}}_{i-1}$, $\Xi_i \in \tilde{\mathrm{K}}_i$. It turns out that the solution of the form (24) does not always exist. A counter example is provided by the case $\mathrm{G} = \mathrm{K}$, the group of rotations of a regular icosahedron, $\mathrm{H} = \mathrm{D}_3$ (a dihedral point group), and $\Theta = E$ (the two-dimensional irrep of D_3). We have $E \uparrow \mathrm{K} \simeq T_1 \oplus T_2 \oplus U \oplus 2V (T_1, T_2, U, V \in \tilde{\mathrm{K}})$, and the repetition of $V \in \tilde{\mathrm{K}}$ in $E \uparrow \mathrm{K}$ cannot be resolved by means of any intermediate subgroup since D_3 is maximal in K (notation for the irreps of the icosahedral group K is given from Griffith 1964). Nevertheless, for a very important family consisting of the primitive representations, i.e. the transreps $R^{\mathrm{G}:\mathrm{H}}$ for which H is maximal in G, the solution does exist. It will be considered in § 5.

Vectors of the irreducible basis (21) of $(\Theta \uparrow \mathrm{K}) \uparrow \mathrm{G}$ can be expressed in terms of the natural basis (20) as

$$|(\Theta \uparrow \mathrm{K}) \uparrow \mathrm{G} \Gamma \Xi w_1 w_2 \gamma\rangle$$
$$= \sum_{(r_1 r_2 \vartheta) \in B_{\mathrm{nat}}^{(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}}} b_{r_1 r_2 \vartheta, \Gamma \Xi w_1 w_2 \gamma}^{(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}} |(\Theta \uparrow \mathrm{K}) \uparrow \mathrm{G} r_1 r_2 \vartheta\rangle,$$
$$(\Gamma \Xi w_1 w_2 \gamma) \in B_{\mathrm{irr}}^{(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}}, \tag{25}$$

where

$$b_{r_1 r_2 \vartheta, \Gamma \Xi w_1 w_2 \gamma}^{(\Theta\uparrow \mathrm{K})\uparrow \mathrm{G}} = \sum_{\xi \in \tilde{\Xi}} g_{r_1 \xi, \Gamma w_1 \gamma}^{\Xi} b_{r_2 \vartheta, \Xi w_2 \xi}^{\Theta}. \tag{26}$$

It follows from (26) (and the fact that $(\Theta\uparrow K)\uparrow G$ is linearly equivalent to $\Theta\uparrow G$) that the knowledge of irreducible bases for each link of the chain $H\subset K\subset G$ allows us to determine an irreducible basis for the carrier space of $\Theta\uparrow G$ by immediate induction. The bases $B_{\rm irr}^{\Theta\uparrow G}$ and $B_{\rm irr}^{(\Theta\uparrow K)\uparrow G}$, however, do not necessarily coincide since the choice of sets $\tilde{W}(\Theta,\Gamma)$, $\Gamma\in\tilde{G}$ (equation (10)) is *a priori* independent of the construction of the sets $\tilde{W}_K(\Theta,\Gamma)$, $\Gamma\in\tilde{G}$ (equation (22)). In general, we have

$$b^{(\Theta\uparrow K)\uparrow G}_{r_1r_2\vartheta,\Gamma\Xi w_1w_2\gamma}=\sum_{w\in\tilde{W}(\Theta,\Gamma)} Q_{w,\Xi w_1w_2}(\Theta,\Gamma)\,b^{\Theta}_{r_1r_2\vartheta,\Gamma w\gamma}, \tag{27}$$

where the coefficients $Q_{w,\Xi w_1w_2}(\Theta,\Gamma)$ are independent of the indices of bases r_1, r_2, ϑ, γ, and form a unitary matrix $Q(\Theta,\Gamma)$, describing the linear transformation between two systems of repetition indices for Γ in $\Theta\uparrow G$, characterised by $B_{\rm irr}^{(\Theta\uparrow K)\uparrow G}$ and $B_{\rm irr}^{\Theta\uparrow G}$. The coefficients $Q_{w,\Xi w_1w_2}(\Theta,\Gamma)$ play here a role similar to Racah recoupling matrices for a change in sequence of coupling of several angular momenta (cf e.g. Fano and Racah 1959, cf also Wybourne 1974 § 19.11 for some generalisations), to isoscalar factors associated with Racah's lemma (Racah 1949, cf also Wybourne 1974, § 19.15), or to Derome–Sharp matrices associated with the permutational symmetry of Clebsch–Gordan coefficients (Derome and Sharp 1965, Derome 1966, cf also Chatterjee and Lulek 1982, Mucha and Lulek 1983).

Using the orthogonality properties of matrices b^{Θ} one can obtain from (27) a direct expression for $Q_{w,\Xi w_1w_2}(\Theta,\Gamma)$, namely

$$Q_{w,\Xi w_1w_2}(\Theta,\Gamma)=\sum_{(r_1r_2\vartheta)\in B_{\rm nat}^{\Theta\uparrow G}} b^{(\Theta\uparrow K)\uparrow G}_{r_1r_2\vartheta,\Gamma\Xi w_1w_2\gamma}\left(b^{\Theta}_{r_1r_2\vartheta,\Gamma w\gamma}\right)^*, \tag{28}$$

where $w\in\tilde{W}(\Theta,\Gamma)$, $(\Xi w_1w_2)\in\tilde{W}_K(\Theta,\Gamma)$. The dependence of the right-hand side of (28) on γ is apparent for the reason of Schur's lemma. In fact, the coefficients $Q_{w,\Xi w_1w_2}(\Theta,\Gamma)$ are values of some scalar products in the space $\mathrm{Hom}_G(\Gamma,\Theta\uparrow G)$, namely

$$Q_{w,\Xi w_1w_2}(\Theta,\Gamma)=(B_w,B_{\Xi w_1w_2}), \tag{29}$$

where B_w and $B_{\Xi w_1w_2}$ are intertwining operators defined according to equation (12).

4. The classification based on the Frobenius reciprocity theorem

Now we are going to discuss a particular system of classification of irreps of an indrep, related to the known Frobenius reciprocity theorem (cf e.g. Altmann 1977, p 148). Let $\Gamma\uparrow H$ be the subduced representation, and let

$$\Gamma\downarrow H\simeq\sum_{\Theta\in\tilde{H}}\oplus\, n(\Gamma\downarrow H,\Theta)\Theta \tag{30}$$

be its decomposition into irreps of H, and let

$$\tilde{V}(\Gamma,\theta)=\{v|v=1,2,\ldots,n(\Gamma\downarrow H,\Theta)\} \tag{31}$$

be the set determining the system of repetition indices of $\Theta\in\tilde{H}$ in $\Gamma\downarrow H$, so that the vectors

$$|\Gamma\downarrow H\Theta v\vartheta\rangle=\sum_{\gamma\in\tilde{\Gamma}} a^{\Gamma\gamma}_{\Theta v\vartheta}|\Gamma\gamma\rangle \tag{32}$$

with $\Theta\in\tilde{H}$, $v\in\tilde{V}(\Gamma,\Theta)$, $\vartheta\in\tilde{\Theta}$, constitute an orthonormal standard complete basis in a carrier space of the representation Γ. Then, as we have shown elsewhere (Lulek and

Lulek 1984), one can choose the system of repetition indices of Γ in $\Theta\uparrow \mathrm{G}$ putting

$$\tilde{W}(\Theta, \Gamma) = \tilde{V}(\Gamma, \Theta) \tag{33}$$

for each $\Gamma \in \tilde{\mathrm{G}}$, so that the elements of the corresponding matrix b^{Θ} (11) have the form

$$b^{\Theta}_{r\vartheta, \Gamma v \gamma} = \left(\frac{|H|[\Gamma]}{|\mathrm{G}|[\Theta]}\right)^{1/2} \sum_{\gamma' \in \tilde{\Gamma}} (a^{\Gamma\gamma'}_{\Theta v \vartheta})^* D^{\Gamma}_{\gamma\gamma'}(g_r)^*. \tag{34}$$

The formulae (33)–(34) express in fact a generalisation of the Frobenius reciprocity theorem

$$n(\Theta\uparrow \mathrm{G}, \Gamma) = n(\Gamma\downarrow \mathrm{H}, \Theta), \qquad \Gamma \in \tilde{\mathrm{G}}, \qquad \Theta \in \tilde{\mathrm{H}}, \tag{35}$$

on the level of irreducible bases, similarly as in the paper of Edwards (1980).

Equations (33) and (34) provide, respectively, a solution of the problem of classification and determination of the irreducible bases of the indrep $\Theta\uparrow \mathrm{G}$, $\Theta \in \tilde{\mathrm{H}}$ for the chain $\mathrm{H} \subset \mathrm{G}$ under the assumption that both problems for the subduced representations $\Gamma\downarrow \mathrm{H}$, $\Gamma \in \tilde{\mathrm{G}}$ are already solved, i.e. that the sets $\tilde{V}(\Gamma, \Theta)$ and bases (32) are known. At this point it is worth observing that the repetition indices $v \in \tilde{V}(\Gamma, \Theta)$ originate essentially from the set of basis functions of Γ, adapted to the chain $\mathrm{H} \subset \mathrm{G}$, where $\gamma \in \tilde{\Gamma}$ is replaced by $\Theta v \vartheta$, $\Theta \in \tilde{\mathrm{H}}$, $v \in \tilde{V}(\Gamma, \Theta)$, $\vartheta \in \tilde{\Theta}$. It is especially clear for the case of the regular representations

$$D^{\mathrm{reg}} \simeq D^{\mathrm{G}:\{e\}} \cong \Theta_{0e}\uparrow \mathrm{G}, \tag{36}$$

where Θ_{0e} is the unit irrep of the group {e}, since we have

$$\tilde{W}(\Theta_{0e}, \Gamma) = \tilde{V}(\Gamma, \Theta_{0e}) = \tilde{\Gamma}, \tag{37}$$

as a direct result of the well known decomposition of the group algebra into matrix units (cf e.g. Matsen 1975).

We proceed to evaluate the matrices $Q(\Theta, \Gamma)$, defined by (27) for the case when both systems of repetition indices are associated with the Frobenius reciprocity theorem, applied to two three-member chains of subgroups: $\mathrm{H} \subset \mathrm{K} \subset \mathrm{G}$ and $\mathrm{H} \subset \mathrm{K}' \subset \mathrm{G}$. One can substantially simplify awkward calculations based on (28), using (29) and the Frobenius reciprocity theorem at the level of bases (Edwards 1980). For this purpose we introduce, in an analogy to § 2.4, the space $\mathrm{Hom_H}(\Gamma\downarrow \mathrm{H}, \Theta)$ of operators which intertwine $\Gamma\downarrow \mathrm{H}$ with Θ in the group H, i.e. such linear operators A which carry the vectors of a carrier space of Γ into a carrier space of Θ and satisfy the conditions

$$AD^{\Gamma}(h) = D^{\Theta}(h)A, \qquad h \in \mathrm{H}. \tag{38}$$

Vectors (32) correspond in this space to operators

$$A_v = \sum_{\vartheta \in \tilde{\Theta}} |\Theta\vartheta\rangle\langle\Gamma\Theta v\vartheta|, \qquad v \in \tilde{V}(\Gamma, \Theta), \tag{39}$$

with the property

$$A_v|\Gamma\Theta v\vartheta\rangle = |\Theta\vartheta\rangle, \qquad \vartheta \in \tilde{\Theta}. \tag{40}$$

Vectors A_v, $v \in \tilde{V}(\Gamma, \Theta)$ constitute a basis in $\mathrm{Hom_H}(\Gamma\downarrow \mathrm{H}, \Theta)$, which is orthonormal with respect to the scalar product

$$(A_1, A_2) = \frac{1}{[\Theta]} \operatorname{Tr} A_1^+ A_2 = \frac{1}{[\Theta]} \sum_{\gamma \in \tilde{\Gamma}} \langle \Gamma\gamma | A_1^+ A_2 | \Gamma\gamma \rangle, \tag{41}$$

where $A_1, A_2 \in \operatorname{Hom}_{\mathrm{H}}(\Gamma \downarrow \mathrm{H}, \Theta)$.

The Frobenius reciprocity theorem, given by (35), can be also formulated at the level of irreducible bases as follows (Naimark 1976 II.4.3, cf also Edwards (1980) and references given therein): there exists such an isomorphism

$$\varkappa : \operatorname{Hom}_{\mathrm{G}}(\Gamma, \Theta \uparrow \mathrm{G}) \to \operatorname{Hom}_{\mathrm{H}}(\Gamma \downarrow \mathrm{H}, \Theta) \tag{42}$$

between both spaces of intertwining operators which is a linear mapping satisfying the conditions

$$\varkappa(B_v) = A_v, \qquad v \in \tilde{V}(\Gamma, \Theta), \tag{43}$$

(so that bases $|\Theta \uparrow \mathrm{G}\Gamma v\gamma\rangle$ and $|\Gamma\Theta v\vartheta\rangle$ are mutually reciprocal in the terminology of Edwards 1980) and

$$(\varkappa(B_1), \varkappa(B_2)) = (B_1, B_2),\ B_1, B_2 \in \operatorname{Hom}_{\mathrm{G}}(\Gamma, \Theta \uparrow \mathrm{G}), \tag{44}$$

where the scalar products of the left- and right-hand side are given by equations (14) and (41), respectively. The operator $\varkappa(B) \in \operatorname{Hom}_{\mathrm{H}}(\Gamma \downarrow \mathrm{H}, \Theta)$, with $B \in \operatorname{Hom}_{\mathrm{G}}(\Gamma, \Theta \uparrow \mathrm{G})$ is then defined by the formula

$$\varkappa(\mathrm{B})(D^{\Gamma}(g^{-1})l) = \left(\frac{[\Theta]}{[\Gamma]}\right)^{1/2} (Bl)(g), \qquad g \in \mathrm{G}, \tag{45}$$

where l is an arbitrary vector of the carrier space of Γ (so that Bl is an element of the carrier space of $\Theta \uparrow \mathrm{G}$), and the carrier space of $\Theta \uparrow \mathrm{G}$ is realised in a standard way as the space of functions on the group G with the values in the carrier space of Θ satisfying the conditions $D^{\Theta}(h)(Bl)(g) = (Bl)(gh^{-1})$ for each $h \in \mathrm{H}$ (so that $([\Theta]/[\Gamma])^{1/2}(Bl)(g)$ is an element of the carrier space of Θ).

The formulae (42)-(45) for the isomorphism $\varkappa$ agree with the corresponding formulae of Edwards (1980) after appropriate changes in notation and taking into account both the change of the 'direction of twinning' (he used $\operatorname{Hom}_{\mathrm{H}}(\Theta, \Gamma \downarrow \mathrm{H})$ instead of our $\operatorname{Hom}_{\mathrm{H}}(\Gamma \downarrow \mathrm{H}, \Theta)$) and the change of the direction of arrow in equation (42); the definitions (1)-(5), associated with the realisation of the homogeneous space $\tilde{R}(\mathrm{G}:\mathrm{H})$ on left (not right!) cosets remain the same in both papers. Using equations (43) and (44) we obtain from (29)

$$Q_{\Xi v_1 v_2, \Xi' v_1' v_2'}(\Theta, \Gamma) = (A_{\Xi v_1 v_2}, A_{\Xi' v_1' v_2'}), \tag{46}$$

where the scalar product is related to the space $\operatorname{Hom}_{\mathrm{H}}(\Gamma \downarrow \mathrm{H}, \Theta)$. Using equations (39) and (32) for appropriate chains of subgroups we finally obtain

$$Q_{\Xi v_1 v_2, \Xi' v_1' v_2'}(\Theta, \Gamma) = \frac{1}{[\Theta]} \sum_{\gamma \in \tilde{\Gamma}} \sum_{\xi \in \tilde{\Xi}} \sum_{\xi' \in \tilde{\Xi}'} \sum_{\vartheta \in \tilde{\Theta}} a^{\Gamma\gamma}_{\Xi v_1 \xi} a^{\Xi\xi}_{\Theta v_2 \vartheta} (a^{\Gamma\gamma}_{\Xi' v_1' \xi'})^* (a^{\Xi'\xi'}_{\Theta v_2' \vartheta})^*. \tag{47}$$

We finish this section with an example of the matrix Q for the case of chains of point groups $\mathrm{O} \supset D_4 \supset \mathrm{C}_2'$ and $\mathrm{O} \supset \mathrm{D}_3 \supset \mathrm{C}_2'$, where O is the group of rotations of a cube, and $\mathrm{C}_2' = \{E, U\}$, with E and U being the unit element and the two-fold rotation around the axis $e_x - e_y$ in the cartesian system of four-fold axes of the cube. The principal axes of the dihedral groups D_4 and D_3 are oriented along vectors e_z and $e_x + e_y + e_z$, respectively. The decomposition matrices a (equation (32)) for the chains $D_4 \subset O$, $D_3 \subset O$ are given in Griffith (1964, table A 17), and we take $a_{\Theta}^{\Xi} = 1$ for one-dimensional representations Ξ of D_4 and D_3, $|EA\rangle = 2^{-1/2}(|Ex\rangle - |Ey\rangle)$, $|EB\rangle = 2^{-1/2}(|Ex\rangle + |Ey\rangle)$, and $|EA\rangle = |E\Theta\rangle$, $|EB\rangle = |E\varepsilon\rangle$ for two-dimensional representation $\Xi = E$ in the group D_4 and D_3, respectively (the representation and basis functions for O, D_4 and D_3 are labelled according to Griffith 1964, and A and B is the unit and antisymmetric irrep of C_2', respectively). With this notation and conventions, the indreps $\Theta \uparrow O$ of the group C_2' have the form

$$A \uparrow O \simeq A_1 \oplus E \oplus T_1 \oplus 2T_2$$
$$B \uparrow O \simeq A_2 \oplus E \oplus 2T_1 \oplus T_2,$$

and a complete classification of repeated irreps (T_2 in $A \uparrow O$ and T_1 in $B \uparrow O$) is fully provided by a representation Ξ of each of the intermediate subgroup, D_4 and D_3. In table 1 we give the decomposition coefficients for the chain $C_2' \subset O$ for $\Gamma = T_1$ and T_2, evaluated by equation (32) in two steps for both three-member chains. The matrices $Q(B, T_1)$ and $Q(A, T_2)$, evaluated by equation (47), are listed in table 2.

5. Primitive representations

It is difficult to derive general analytic formulae for irreducible bases of an arbitrary indrep $\Theta \uparrow G$, for the reason of an arbitrariness in choice of the systems of repetition indices for the corresponding subduced representations $\Gamma \downarrow H$. It can be done, however, in an important special case of primitive representations. It is well known (cf e.g. Hall 1959, Theorem 16.6.15), that the decomposition (7) for a primitive representation $R^{G:H}$ has the simple form

$$R^{G:H} \simeq \Theta_0 \uparrow G \simeq \Gamma_0 \oplus \Gamma, \qquad \text{H maximal in G.} \tag{48}$$

Table 1. The decomposition coefficients $a_{\Theta\Xi}^{\Gamma\gamma}$ for three-dimensional irreps of the group O ($\Gamma = T_1, T_2$) for the chains $C_2' \subset K \subset O$, $K = D_4, D_3$.

K = D_4

$T_1 \downarrow C_2'$	Θ	A	B	
γ	Ξ	E	A_2	E
x		$1/\sqrt{2}$	0	$1/\sqrt{2}$
y		$-1/\sqrt{2}$	0	$1/\sqrt{2}$
z		0	1	0

$T_2 \downarrow C_2'$	Θ	A		B
γ	Ξ	B_2	E	E
x		0	$1/\sqrt{2}$	$1/\sqrt{2}$
y		0	$1/\sqrt{2}$	$-1/\sqrt{2}$
z		1	0	0

K = D_3

$T_1 \downarrow C_2'$	Θ	A	B	
γ	Ξ	E	A_2	E
x		$1/\sqrt{2}$	$1/\sqrt{3}$	$1/\sqrt{2.3}$
y		$-1/\sqrt{2}$	$1/\sqrt{3}$	$1/\sqrt{2.3}$
z		0	$1/\sqrt{3}$	$-\sqrt{2}/\sqrt{3}$

$T_2 \downarrow C_2'$	Θ	A		B
γ	Ξ	A_1	E	E
x		$1/\sqrt{3}$	$1/\sqrt{2.3}$	$1/\sqrt{2}$
y		$1/\sqrt{3}$	$1/\sqrt{2.3}$	$-1/\sqrt{2}$
z		$1/\sqrt{3}$	$-\sqrt{2}/\sqrt{3}$	0

Table 2. Two-dimensional matrices $Q(\Theta, \Gamma)$ for the chain $C_2' \subset O$. Ξ and Ξ' denote the irreps of D_4 and D_3, respectively.

$Q(B, T_1) =$

$\Xi \backslash \Xi'$	A_2	E
A_2	$1/\sqrt{3}$	$-\sqrt{2}/\sqrt{3}$
E	$\sqrt{2}/\sqrt{3}$	$1/\sqrt{3}$

$Q(A, T_2) =$

$\Xi \backslash \Xi'$	A_2	E
B_2	$1/\sqrt{3}$	$-\sqrt{2}/\sqrt{3}$
E	$\sqrt{2}/\sqrt{3}$	$1/\sqrt{3}$

Evidently, the carrier space of Γ_0 is spanned on the vector

$$|\Theta_0 \uparrow \mathrm{G}\Gamma_0\rangle = \left(\frac{|\mathrm{H}|}{|\mathrm{G}|}\right)^{1/2} \sum_{r \in \tilde{R}(\mathrm{G}:\mathrm{H})} |\Theta_0 \uparrow \mathrm{G}r\rangle, \tag{49}$$

and the orthogonal completion in the carrier space of $D^{\Theta_0 \uparrow \mathrm{G}}$ is the carrier space of Γ, where the basis can be chosen arbitrarily. A simple universal choice is given by the formula

$$|\Theta_0 \uparrow \mathrm{G}\Gamma_j\rangle = [j(j-1)]^{1/2} \left(\sum_{r=1}^{j-1} |\Theta_0 \uparrow \mathrm{G}r\rangle - (j-1)|\Theta_0 \uparrow \mathrm{G}j\rangle \right), \tag{50}$$

where $j \in \tilde{R}(\mathrm{G}:\mathrm{H})$, $j \neq 1$. Evidently, each representation $\Gamma \in \tilde{\mathrm{G}}$, associated with a maximal subgroup of the group G by equation (48), has an orthonormal irreducible basis labelled by the elements of the orbit $\tilde{R}(\mathrm{G}:\mathrm{H})$ with the exception of element $r = 1$, i.e.

$$\tilde{\Gamma} \simeq \tilde{\mathrm{R}}(\mathrm{G}:\mathrm{H}) \diagdown \{1\}. \tag{51}$$

It is easy to observe that the basis (49)–(50) coincides with the standard Yamanauchi basis (cf e.g. Hamermesh 1962) for the irreps entering the primitive representation decomposition

$$R^{\Sigma_N : \Sigma_{N-1}} \simeq \{N\} \oplus \{N-1, 1\} \tag{52}$$

of the symmetric group Σ_N, where $N = |\mathrm{G}|/|\mathrm{H}|$, and $\{N\}$ and $\{N-1, 1\}$ are Young diagrams labelling irreps of Σ_N.

6. Final remarks and conclusions

We have considered the problem of classification and determination of irreducible bases of indreps of finite groups. Using the results of another of our papers (Lulek and Lulek 1984) we have proposed a universal classification originated from the Frobenius reciprocity theorem on the level of bases (Edwards 1980), assuming the knowledge of irreducible bases for subduced representations. Such a classification uses, in fact, the labels of irreducible bases adapted to a chain of subgroups to distinguish the repeated irreps.

We have also discussed in general the problem of classification for a three-member chain of subgroups assuming that this problem for each link of the chain is already known. We have proposed the form of some matrices Q (equation (27)) which describe the linear transformation between two systems of repetition indices for such chains and are analogues of Racah recoupling matrices in angular momentum theory. We gave general formulae (28) and (29) for elements of these matrices. Moreover, for the case of classification based on the Frobenius reciprocity theorem for two chains $\mathrm{H} \subset \mathrm{K} \subset \mathrm{G}$ and $\mathrm{H} \subset \mathrm{K}' \subset \mathrm{G}$, we expressed these coefficients in terms of decomposition coefficients for appropriate subduced representations (equations (46)–(47)), using the notion of reciprocal basis sets introduced by Edwards (1980).

If a subgroup H is maximal in G, it is difficult to propose any general classification scheme in cases when the multiplicity of Γ in $\Theta \uparrow \mathrm{G}$ is larger than one. Nevertheless, we have discussed a special case of primitive representations, where not only a unique classification exists provided by equation (48), but also universal prescription for the determination of some standard bases of irreps, coinciding with the Yamanouchi basis for the irrep $\{N-1, 1\}$ of the symmetric group Σ_N, can be proposed.

From the mathematical point of view, it proved to be a useful extension of transreps, suggested by direct physical applications, into indreps since it assures completeness of the formalism. For example, the matrices b^{Θ_0}, determining the irreducible basis for the transrep $R^{\mathrm{G:H}}$ for the chain $\mathrm{H} \subset \mathrm{K} \subset \mathrm{G}$ can be expressed, according to equation (26) by matrices b^{Ξ}, where, in general, $\Xi \neq \Xi_0$, thus by matrices corresponding to some indreps for the chain $\mathrm{K} \subset \mathrm{G}$, and not only to the transrep $R^{\mathrm{G:K}} \cong \Xi_0 \uparrow \mathrm{G}$.

The structure of the set of the natural basis of an indrep for a three-member chain of subgroups (equations (15)–(20)) was known in mathematics a long time ago (cf e.g. Burnside 1911, p 191). It was rediscovered in quantum chemistry (cf Wilson *et al* 1955, p 121) as the so-called 'correlation theorem', constituting essentially the Frobenius reciprocity theorem, modified for the case when the inducing representation is a permutation representation of a subgroup $\mathrm{H} \subset \mathrm{G}$.

Acknowledgments

The authors wish to thank to Professors D T Newman from The University of Hong Kong for making accessible the papers of his group before publication. Thanks are also due to Dr M Mucha for valuable discussions and a careful reading of the manuscript.

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