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nth symmetrized powers of space group representations: subgroup formulae

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Abstract. The paper outlines a full group method to obtain subgroup formulae enabling one to calculate nth symmetrized powers of space group representations. Attention is given to the practical cases of $n = 2, 3$, and a comparison drawn with work of Bradley and Bradley and Davies on direct and symmetrized squares.

1. Introduction

The object is to present subgroup formulae enabling one to calculate nth direct and symmetrized powers of space group representations by using a full-group formulation. The special cases of $n = 2, 3$ are examined as special cases of the general theory, and as yet are the only powers which are specifically used in physical situations to determine selection rules, for instance intervalley scattering, the Raman effect, and the Landau theory of second order phase transitions, which requires one to evaluate symmetrized cubes and antisymmetrized squares.

A comparison is drawn in the $n = 2$ case with the subgroup method given by Bradley (1966) and for symmetrized squares by Bradley and Davies (1970).

2. Notation

It was thought advisable to give a preliminary list of the notation adopted. For completeness some relevant information and definitions are also given.

$D_p^{\boldsymbol{k}}$ is the pth irreducible representation of a space group based on the wavevector $\boldsymbol{k}$ in the Brillouin zone.

$\chi_p^{\boldsymbol{k}}$ is the character of the representation $D_p^{\boldsymbol{k}}$.

$G^{\boldsymbol{k}}$ is the group of the wavevector $\boldsymbol{k}$, and is usually termed a 'little' group.

$\Delta_p^{\boldsymbol{k}}$ is the pth irreducible 'small', or allowed representation of the little group $G^{\boldsymbol{k}}$ of $\boldsymbol{k}$.

$\psi_p^{\boldsymbol{k}}$ is the character of $\Delta_p^{\boldsymbol{k}}$.

$D_p^{\boldsymbol{k}} = (\Delta_p^{\boldsymbol{k}} \uparrow G)$, where $\uparrow$ symbolizes the process of induction (see Bradley 1966).

R is a typical space group element and can be written as $R \equiv (S|\boldsymbol{t} + \boldsymbol{\tau}_S)$, in the Seitz notation.

$\boldsymbol{t} \in T$, the abelian group of lattice translations; $T \subseteq G^{\boldsymbol{k}}$ for all $\boldsymbol{k}$, and $\boldsymbol{\tau}_S$ is the associated nonlattice translation.

The standard formula linking the full group and the subgroup characters is given by

$$\chi_p^{\boldsymbol{k}}(R) = \sum_i \psi_p^{\boldsymbol{k}}(\alpha_i^{-1}R\alpha_i)J_{\alpha i}^{\boldsymbol{k}}(R)$$

where the sum is taken over all the coset representatives of $G^{\boldsymbol{k}}$ in G. $\psi_p^{\boldsymbol{k}}(\alpha^{-1}R\alpha) = \psi_{\alpha p}^{\boldsymbol{k}}(R)$ in shorthand notation.

$$J_\alpha^{\boldsymbol{k}}(R) \begin{array}{ll} = 1 & \text{if } \alpha^{-1}R\alpha \in G^{\boldsymbol{k}}, \text{ that is } (\alpha|\tau_\alpha)^{-1}(S|\tau_s+\boldsymbol{t})(\alpha|\tau_\alpha) \in G^{\boldsymbol{k}} \\ = 0 & \text{otherwise.} \end{array}$$

If A is a set, then define $\bar{A}$ by the isomorphism $\bar{A} \cong A/T$, that is $(S|\tau_S+\boldsymbol{t}) \in A$ implies $S \in \bar{A}$. If A is a group, $\bar{A}$ is termed the little cogroup.

$|A|$ is the order of the group (set) A.

Given the coset expansion $G = \Sigma_i \alpha_i G^{\boldsymbol{k}}$, then the set $\{\alpha_i \boldsymbol{k}\}$ is called the star of $\boldsymbol{k}$, denoted by $^\star\boldsymbol{k}$, and is a set of $|G|/|G^{\boldsymbol{k}}|$ nonequivalent wavevectors.

Two wavevectors $\boldsymbol{h}$ and $\boldsymbol{k}$ are equivalent, $\boldsymbol{h} \equiv \boldsymbol{k}$, if and only if they differ by a reciprocal lattice vector $\boldsymbol{K}$.

$^\star\boldsymbol{k}_1 \otimes {}^\star\boldsymbol{k}_2 \otimes \ldots \otimes {}^\star\boldsymbol{k}_n = \Sigma_l n_l {}^\star\boldsymbol{l}$ is a set S of WVSRS (wavevector selection rules), n_l being the frequency of $^\star\boldsymbol{l}$. A typical member of S is $\alpha_1\boldsymbol{k}_1+\alpha_2\boldsymbol{k}_2+\ldots+\alpha_n\boldsymbol{k}_n \equiv \boldsymbol{l}$. Here the α_i are arbitrary coset representatives of $G^{\boldsymbol{k}_i}$ in G.

$$\delta(\alpha_1\boldsymbol{k}_1+\alpha_2\boldsymbol{k}_2+\ldots+\alpha_n\boldsymbol{k}_n-\boldsymbol{l}) \begin{array}{ll} = 1 & \text{if and only if } \alpha_1\boldsymbol{k}_1+\alpha_2\boldsymbol{k}_2+\ldots+\alpha_n\boldsymbol{k}_n \equiv \boldsymbol{l} \\ = 0 & \text{otherwise.} \end{array}$$

The notion of a double coset $H\alpha K$, with H, K both subgroups of G is explained in Bradley (1966). We would like to emphasize that whenever a double coset appears in the following text, it is taken from a double coset decomposition with respect to G.

3. *n*th power direct products

3.1. *Derivation of method*

We examine the set S of WVSRS

$$^\star\boldsymbol{k}_1 \otimes {}^\star\boldsymbol{k}_2 \otimes \ldots \otimes {}^\star\boldsymbol{k}_n = \sum_l n_l^\star\boldsymbol{l}$$

and show how they can be combined into subsets by using various double coset expansions with respect to G, the full space group.

Choose an arbitrary member of S

$$\alpha_1\boldsymbol{k}_1+\alpha_2\boldsymbol{k}_2+\ldots+\alpha_n\boldsymbol{k}_n = \sum_i \alpha_i\boldsymbol{k}_i \equiv \boldsymbol{l} \tag{1}$$

and form the expansion

$$A = \sum_\pi z_\pi(A \wedge N_{\alpha_1\alpha_2\ldots\alpha_n})$$

where $N_{\alpha_1\alpha_2\ldots\alpha_n} = G_{\alpha_1}^{\boldsymbol{k}_1} \wedge G_{\alpha_2}^{\boldsymbol{k}_2} \wedge \ldots \wedge G_{\alpha_n}^{\boldsymbol{k}_n} = \bigcap_{i=1}^n G_{\alpha_i}^{\boldsymbol{k}_i} = N_\alpha$ with the convention $z_1 = e$, the identity. $\bar{A}$ is a subgroup of G.

Definition 1. Two WVSRS $\Sigma_i\,\alpha_i\boldsymbol{k}_i \equiv \boldsymbol{l}$ and $\Sigma_j\alpha_j'\boldsymbol{k}_j \equiv \boldsymbol{l}'$ are equivalent if and only if $\alpha_i\boldsymbol{k}_i \equiv \alpha_i'\boldsymbol{k}_i'$ for all i, and $\boldsymbol{l} \equiv \boldsymbol{l}'$. Otherwise the WVSRS are termed distinct.

Definition 2. Given a group A, and a particular set of coset representatives $\{z_\pi\}$ with respect to $A \wedge N_\alpha$, then the set of WVSRs obtained by operating with the z_π on WVSR (1) is called the 'derived set' of the 'leading' WVSR (1).

Lemma 1. Any member of the 'derived set' could be taken as a leading WVSR, and the same derived set would result.

Proof. Take as 'leading' WVSR $z_\pi \Sigma_i \alpha_i \boldsymbol{k}_i \equiv z_\pi \boldsymbol{l}$ and thus form the expansion,

$$A = \sum_\rho \omega_\rho (A \wedge N_{(z_\pi \alpha)}).$$

$\omega_\rho z_\pi (\Sigma_i \alpha_i \boldsymbol{k}_i) \equiv \omega_\rho z_\pi \boldsymbol{l}$ can be rewritten as $z_{\rho\pi}(\Sigma_i \alpha_i \boldsymbol{k}_i) = z_{\rho\pi}\boldsymbol{l}$, where $z_{\rho\pi} \in \{z_\pi\}$ for each ρ, giving the same derived set.

Lemma 2. The members of a derived set are mutually distinct, that is there are $|A|/|A \wedge N_\alpha| = d_\alpha = d_{\alpha_1 \alpha_2 \ldots \alpha_n}$ distinct WVSRs in the derived set.

Proof. Assume the contrary, then for $z_\rho, z_\sigma \in \{z_\pi\}$, we have $z_\rho \Sigma_i \alpha_i \boldsymbol{k}_i \equiv z_\sigma \Sigma_i \alpha_i \boldsymbol{k}_i$ implying $z_\sigma^{-1} z_\rho \in N_\alpha$, a contradiction.

Thus the expansion $A = \Sigma_\pi z_\pi (A \wedge N_\alpha)$ generates d_α distinct WVSRs, which are of course dependent on the choice of A.

This motivates the classification of all members of the set S of selection rules by using such expansions.

Now examine the nature of the terms in the original set. To this end consider the expansion

$$A = \sum_\lambda a_\lambda (A \wedge G^{\boldsymbol{k}_1}_{\alpha_1}) \tag{2}$$

with $|A|/|A \wedge G^{\boldsymbol{k}_1}_{\alpha_1}| = d_1$.

Lemma 3. Let $P, Q \subset G$, $P = \Sigma_\xi p_\xi (P \wedge Q_\eta)$, $Q_\eta = d_\eta Q d_\eta^{-1}$, then the $|P|/|P \wedge Q_\eta|$ left cosets of Q in the double coset $Pd_\eta Q$ (with respect to G) are those generated by the set $\{p_\xi\}$ operating on $d_\eta Q$, and in particular we can write $Pd_\eta Q = Pd_\eta Q \wedge \Sigma_\xi p_\xi d_\eta Q$ (see also Bradley 1966).

As a result of lemma 3 we write

$$A\alpha_1 G^{\boldsymbol{k}_1} = A\alpha_1 G^{\boldsymbol{k}_1} \wedge \sum_\lambda a_\lambda \alpha_1 G^{\boldsymbol{k}_1}$$

the set $\{a_\lambda\}$, $a_1 = e$, of coset representatives operating on $\alpha_1 G^{\boldsymbol{k}_1}$ generates the same cosets as are contained in the double coset $A\alpha_1 G^{\boldsymbol{k}_1}$.

This set $\{a_\lambda\}$ can be used to generate d_1 distinct WVSRs from (1), that is

$$\left\{ a_\lambda \sum_1^n \alpha_i \boldsymbol{k}_i \right\} \equiv \{a_\lambda \boldsymbol{l}\} \tag{3}$$

noting that all cosets of $G^{\boldsymbol{k}_1}$ (members of the star of $\boldsymbol{k}_1$) generated in the double coset $A\alpha_1 G^{\boldsymbol{k}_1}$ are used up in (3).

Put $\alpha_\lambda \alpha_i = \alpha_{\lambda i}$ with $a_1 \alpha_i = \alpha_{1i} = \alpha_i$. Thus consider

$$(A \wedge G^{\boldsymbol{k}_1}_{\alpha_{\lambda 1}}) = \sum_{\mu=1}^{d_{\lambda 2}} a_{\lambda\mu} (A \wedge G^{\boldsymbol{k}_1}_{\alpha_{\lambda 1}} \wedge G^{\boldsymbol{k}_2}_{\alpha_{\lambda 2}}) \tag{4}$$

for fixed λ. Using lemma (3) again

$$(A \wedge G^{k}_{\alpha_{\lambda 1}})\alpha_{\lambda 2}G^{k_2} = (A \wedge G^{k_1}_{\alpha_{\lambda 1}})\alpha_{\lambda 2}G^{k_2} \wedge \sum_{\mu=1}^{d_{\lambda 2}} a_{\lambda\mu}(a_\lambda \alpha_2 G^{k_2}) \tag{5}$$

that is the set $\{\alpha_{\lambda\mu}\}$ generates $d_{\lambda 2}$ distinct cosets from $\alpha_{\lambda 2}G^{k_2}$ being the same left cosets contained in the double coset $(A \wedge G^{k_1}_{\alpha_{\lambda 1}})\alpha_{\lambda 2}G^{k_2}$.

Also

$$d_{\lambda 2} = \frac{|A \wedge G^{k_1}_{\alpha_{\lambda 1}}|}{|A \wedge G^{k_1}_{\alpha_{\lambda 1}} \wedge G^{k_2}_{\alpha_{\lambda 2}}|} = \frac{|A \wedge G^{k_1}_{\alpha_1}|}{|A \wedge G^{k_1}_{\alpha_1} \wedge G^{k_2}_{\alpha_2}|} = d_{12} = d_2$$

that is $d_{\lambda 2} = d_2$ is independent of λ.

Note that

$$\begin{aligned}(A \wedge G^{k_1}_{\alpha_{\lambda 1}})\alpha_{\lambda 2}G^{k_2} &= (A \wedge a_\lambda G^{k_1}_{\alpha_1}a_\lambda^{-1})a_\lambda\alpha_2 G^{k_2} = a_\lambda[(A \wedge G^{k_1}_{\alpha_1})\alpha_2 G^{k_2}] \\ &= a_\lambda\left[(A \wedge G^{k_1}_{\alpha_1}) \wedge \sum_{\mu'=1}^{d_2} a_{1\mu'}\alpha_2 G^{k_2}\right].\end{aligned} \tag{6}$$

Hence from (5), the set of d_2 cosets of G^{k_2} generated from $a_\lambda\alpha_2 G^{k_2}$ by $\{a_{\lambda\mu}\}$, that is $\{a_{\lambda\mu}a_\lambda\alpha_2 G^{k_2}\}$ is the same as the set generated in (6), $a_\lambda\{a_{1\mu'}\alpha_2 G^{k_2}\} \equiv a_\lambda\{a_{1\mu}\alpha_2 G^{k_2}\}$.

Without loss of generality we can make the identification $a_\lambda a_{1\mu'} = a_{\lambda\mu}a_\lambda$, that is $a_{\lambda\mu} = a_\lambda a_{1\mu'}a_\lambda^{-1} \in G^{k_1}_{\alpha_{\lambda 1}}$. Using the set $\{a_{\lambda\mu}\}$ for each a_λ, we generate d_2 new distinct WVSRS, that is

$$a_\lambda a_1 \boldsymbol{k}_1 + \left\{a_{\lambda\mu}a_\lambda \sum_{i=2}^{n} \alpha_i \boldsymbol{k}_i\right\} \equiv \{a_{\lambda\mu}a_\lambda \boldsymbol{l}\}.$$

Set $a_{\lambda\mu}a_\lambda\alpha_i = \alpha_{\lambda\mu i}$. Note again, that for the terms $\{a_{\lambda\mu}a_\lambda\alpha_2\boldsymbol{k}_2\}$ the members of the star generated by the $a_{\lambda\mu}$ are exactly equivalent to the cosets generated in the double coset $(A \wedge G^{k_1}_{\alpha_{\lambda 1}})\alpha_{\lambda 2}G^{k_2}$ which is in turn equal to $a_\lambda((A \wedge G^{k_1}_{\alpha_1})\alpha_2 G^{k_2})$ giving a very convenient link, as of course

$$\sum_\lambda \alpha_\lambda\{(A \wedge G^{k_1}_{\alpha_1})\alpha_2 G^{k_2}\} = \left(\sum_\lambda a_\lambda(A \wedge G^{k_1}_{\alpha_1})\right)\alpha_2 G^{k_2} = A\alpha_2 G^{k_2}. \tag{7}$$

We now examine the pth step in this procedure. For notational purposes adopt ν, ξ, σ as the $(p-2)$th, $(p-1)$th and pth symbols in a string of Greek letters.

Definition 3.

$$M^{(p-1)}_{\lambda\mu\ldots\nu\xi} = A \wedge G^{k_1}_{\alpha_{\lambda 1}} \wedge G^{k_2}_{\alpha_{\lambda\mu 2}} \wedge \ldots \wedge G^{k_{p-1}}_{\alpha_{\lambda\mu\ldots\nu\xi p-1}}.$$

Definition 4.

$$a_{\lambda\mu\ldots\xi\sigma}\alpha_{\lambda\mu\ldots\nu\xi i} \to \alpha_{\lambda\mu\ldots\xi\sigma i}.$$

For notational convenience we shall denote a string of Greek symbols by bracketing the last member, for example $a_{\lambda\mu} = a_{(\mu)}$, $M^{(p-1)}_{\lambda\mu\ldots\nu\xi} = M^{(p-1)}_{(\xi)}$, etc. This convention will be used only when no confusion can arise.

Consider

$$M^{(p-1)}_{(\xi)} = \sum_{\sigma=1}^{d_{(\xi)p}} a_{(\sigma)}(M^{(p-1)}_{(\xi)} \wedge G^{k_p}_{\alpha_{(\xi)p}}) \tag{8}$$

in relation to the double coset $(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p}$. Using lemma 3

$$(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} = (M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} \wedge \sum_{\sigma=1}^{d_{(\xi)p}} a_{(\sigma)}\alpha_{(\xi)p}G^{k_p} \tag{9}$$

that is the $d_{(\xi)p}$ left cosets of G^{k_p} are generated by the $\{a_{(\sigma)}\}$ operating on $\alpha_{(\xi)p}G^{k_p}$, so for fixed (ξ), $d_{(\xi)p}$ cosets (members of $^\star\boldsymbol{k}_p$) appear in combination with

$$a_{(\lambda)}\alpha_1\boldsymbol{k}_1 + a_{(\mu)}a_{(\lambda)}\alpha_2\boldsymbol{k}_2 + \ldots + a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)}\alpha_{p-1}\boldsymbol{k}_{p-1}.$$

Lemma 4.

$$M^{(p-1)}_{(\xi)} = a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)}M^{(p-1)}_{11\ldots1}a^{-1}_{(\lambda)}a^{-1}_{(\mu)}\ldots a^{-1}_{(\nu)}a^{-1}_{(\xi)}.$$

Proof.

$$\begin{aligned} M^{(p-1)}_{(\xi)} &= A \wedge G^{k_1}_{\alpha_{(\lambda)1}} \wedge G^{k_2}_{\alpha_{(\mu)2}} \wedge \ldots \wedge G^{k_{p-1}}_{\alpha_{(\xi)p-1}} \\ &= A \wedge a_{(\lambda)}G^{k_1}_{\alpha_1}a^{-1}_{(\lambda)} \wedge a_{(\mu)}a_{(\lambda)}G^{k_2}_{\alpha_2}a^{-1}_{(\lambda)}a^{-1}_{(\mu)} \wedge a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)}G^{k_{p-1}}_{\alpha_{p-1}}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\xi)} \\ &= a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)}(A \wedge G^{k_1}_{\alpha_1} \wedge G^{k_2}_{\alpha_2} \wedge \ldots \wedge G^{k_{p-1}}_{\alpha_{p-1}})a^{-1}_{(\lambda)}a^{-1}_{(\mu)}\ldots a^{-1}_{(\xi)} \end{aligned}$$

using the properties of the coset representatives.

Lemma 5.

$$d_{(\xi)p} = d_{\lambda\mu\ldots\nu\xi p} = d_{11\ldots11p} = d_p$$

that is, the number of cosets in the double coset $(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p}$ is independent of (ξ).

Proof.

$$d_{(\xi)p} = \frac{|M^{(p-1)}_{(\xi)}|}{|M^{(p-1)}_{(\xi)} \wedge G^{k_p}_{\alpha_{(\xi)p}}|}.$$

From lemma 4, $|M^{(p-1)}_{(\xi)}| = |A \wedge N_{\alpha_1\alpha_2\ldots\alpha_{p-1}}|$. Consequently

$$|M^{(p-1)}_{(\xi)} \wedge G^{k_p}_{\alpha_{(\xi)p}}| = |A \wedge N_{\alpha_1\alpha_2\ldots\alpha_{p-1}} \wedge G^{k_p}_{\alpha_p}| = |A \wedge N_{\alpha_1\alpha_2\ldots\alpha_p}|.$$

Thus

$$d_{(\xi)p} = \frac{|A \wedge N_{\alpha_1\ldots\alpha_{p-1}}|}{|A \wedge N_{\alpha_1\ldots\alpha_p}|} = d_p.$$

Lemma 6.

$$(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} = (a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)})((M^{(p-1)}_{11\ldots1})\alpha_pG^{k_p}).$$

The proof follows immediately from previous lemmas.

Lemma 7. The same left cosets of G^{k_p} are generated in the set $\{a_{(\sigma)}\alpha_{(\xi)p}G^{k_p}\}$ as in the set $\{a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots1\sigma}\alpha_pG^{k_p}\}$. The proof is immediate from the previous lemma.

Lemma 8.

$$a_{(\sigma)} = a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots1\sigma}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\nu)}a^{-1}_{(\xi)}.$$

Proof

$$M^{(p-1)}_{11\ldots1} = \sum_{\sigma} a_{11\ldots1\sigma}(M^{(p-1)}_{11\ldots1} \wedge G^{k_p}_{\alpha_p})$$

and by lemma 6, and equation 10

$$a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}M^{(p-1)}_{11\ldots 1}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\nu)}a^{-1}_{(\xi)}$$
$$= \sum_{\sigma}(a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots 1\sigma}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\nu)}a^{-1}_{(\xi)})$$
$$\times (M^{(p-1)}_{(\xi)} \wedge a_{(\xi)}\ldots a_{(\lambda)}G^{k_p}_{\alpha_p}\alpha^{-1}_{(\lambda)}\ldots a^{-1}_{(\xi)})$$
$$= M^{(p-1)}_{(\xi)} = \sum_{\sigma} a_{(\sigma)}(M^{(p-1)}_{(\xi)} \wedge a_{(\xi)}\ldots a_{(\lambda)}G^{k_p}_{\alpha_p}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\xi)}).$$

Hence we can make the identification

$$a_{(\sigma)} = a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots 1\sigma}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\nu)}a^{-1}_{(\xi)}.$$

Lemma 9.

$$a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)} = a_{\lambda\mu\ldots\nu\xi}a_{\lambda\mu\ldots\nu}\ldots a_{\lambda\mu}a_{\lambda} = a_{\lambda}a_{1\mu}\ldots a_{11\ldots 1\xi}.$$

Proof. By lemma 8

$$a_{(\xi)} = a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots 1\xi}a^{-1}_{(\lambda)}\ldots a^{-1}_{(\nu)}.$$

Therefore

$$a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)} = a_{(\nu)}\ldots a_{(\lambda)}a_{11\ldots 1\xi}.$$

Next substitute for $a_{(\nu)}$ using lemma 8, and the final result is evident.

Hence we can rewrite the set

$$\{a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)}a_{11\ldots 1\sigma}\alpha_p G^{k_p}\}$$

as

$$\{a_{\lambda}a_{1\mu}\ldots a_{11\ldots 1\xi}a_{11\ldots 1\sigma}\alpha_p G^{k_p}\}.$$

This now gives us a convenient method for linking the derived set with a set of double cosets; for as we have noted already the only terms appearing in the derived set in combination with

$$a_{(\lambda)}\alpha_1\boldsymbol{k}_1 + a_{(\mu)}a_{(\lambda)}\alpha_2\boldsymbol{k}_2 + \ldots + a_{(\xi)}a_{(\nu)}\ldots a_{(\lambda)}\alpha_{p-1}\boldsymbol{k}_{p-1}$$

are those, and only those appearing in the double coset

$$(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} = (a_{(\xi)}a_{(\nu)}\ldots a_{(\mu)}a_{(\lambda)})(M^{(p-1)}_{11\ldots 11})\alpha_p G^{k_p}$$
$$= (a_{\lambda}a_{1\mu}\ldots a_{11\ldots 1\xi})(M^{(p-1)}_{11\ldots 1})\alpha_p G^{k_p} \quad (11)$$

giving a direct association between

$$(M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} \qquad \text{and} \qquad (M^{(p-1)}_{11\ldots 1})\alpha_p G^{k_p}$$

using the coset representatives $a_{\lambda}, a_{1\mu}, \ldots, a_{11\ldots 1\xi}$ etc, where $\{z_\pi\} = \{a_{\lambda}a_{1\mu}\ldots a_{11\ldots 1\omega}\}$, the order of the RHS being $d_1 d_2 \ldots d_{n-1} = d_{\alpha_1\alpha_2\ldots\alpha_n}$ as required.

A typical member of the derived set can be written as

$$a_{\lambda}(\alpha_1\boldsymbol{k}_1 + a_{1\mu}(\alpha_2\boldsymbol{k}_2 + \ldots + a_{11\ldots 1\omega}\alpha_n\boldsymbol{k}_n))\ldots) = a_{\lambda}a_{1\mu}\ldots a_{11\ldots 1\omega}\boldsymbol{l}.$$

Lemma 10.

$$\sum_{\lambda,\mu,\ldots,\nu,\xi}{}' (M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} = A\alpha_p G^{k_p}$$

where Σ' implies the sum is restricted to those indices that appear in the expansions (8).

Proof.

$$\sum_{\lambda,\mu,\ldots,\nu,\xi}' (M^{(p-1)}_{(\xi)})\alpha_{(\xi)p}G^{k_p} = \sum_{\lambda,\mu,\ldots,\nu,\xi}' (a_\lambda a_{1\mu}\ldots a_{11\ldots1\xi})(M^{(p-1)}_{11\ldots11})\alpha_p G^{k_p}$$

by lemmas 4 and 9. Now

$$\sum_{\xi}' a_{11\ldots1\xi}M^{(p-1)}_{11\ldots11} = M^{(p-2)}_{11\ldots11}$$

and

$$\sum_{\nu}' a_{11\ldots1\nu}M^{(p-2)}_{11\ldots1} = M^{(p-3)}_{11\ldots1}$$

etc, and the result follows.

This lemma tells us that within the derived set framework all the cosets of G^{k_p} in $A\alpha_p G^{k_p}$ are used up, and only these are used.

We can sum up in a theorem.

Theorem 1. Associated with a leading WVSR $\Sigma\,\alpha_i \boldsymbol{k}_i \equiv \boldsymbol{l}$ there exists a unique set (n-tuple) of double cosets $\{(M^{(p-1)}_{11\ldots1})\alpha_p G^{k_p}\}^n_{p=1}$ that completely specify the nature of the derived set, in the sense that all relevant information is obtainable by using these double cosets and various coset representatives outlined in the above lemmas.

As a result of the theorem, to obtain a new leading WVSR, one has to consider at least one new double coset in the above n-tuplet

Consider the following expansions

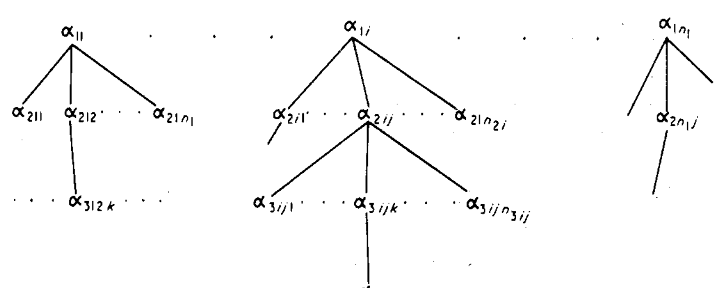
$$G = \sum_{i}^{n_1}{}' A\alpha_{1i}G^{k_1} \tag{12a}$$

$$G = \sum_{j}^{n_{2i}} (A \wedge G^{k_1}_{\alpha_{1i}})\alpha_{2ij}G^{k_2} \qquad \text{for each } i \tag{12b}$$

$\vdots$

$$G = \sum_{l}^{n_{pij\cdots k}} (A \wedge G^{k_1}_{\alpha_{1i}} \wedge \ldots \wedge G^{k_{p-1}}_{\alpha_{p-1ij\ldots k}})\alpha_{pij\ldots kl}G^{k_p} \tag{12c}$$

with the convention that $\alpha_{p11\ldots11} = \alpha_p$. Now given $\alpha_{1i}, \alpha_{2ij}, \ldots, \alpha_{p-1ij\ldots k}$, the expansions tell us the possible α's that appear in 'combination', that is the set of double coset representatives $\{\alpha_{pij\ldots kl}\}$. This can be represented pictorially as follows



defining a series of paths, each of which gives us a 'leading' WVSR.

For example to obtain a new leading WVSR, change say the pth member in the set $\{(M^{(p-1)}_{11\ldots 11})\alpha_p G^{k_p}\}$, that is alter $\alpha_p = \alpha_{p11\ldots 1}$ to $\alpha_{p1\ldots 1l}$ say. See equation 12(c). This effectively moves us onto a new path in the diagram, and one now continues along this new path making sure not to cross onto any other. Care must be taken, of course, if we decide to change the nth entry, in that the new choice must 'complete' a path.

We can check up on the completeness of the procedure as follows. From equation 12(a),

$$\sum_i{}' \frac{|A|}{|A \wedge G^{k_1}_{\alpha_{1i}}|} = \frac{|G|}{|G^{k_1}|}.$$

Similarly

$$\sum_j{}' \frac{|A \wedge G^{k_1}_{\alpha_{1i}}|}{|A \wedge G^{k_1}_{\alpha_{1i}} \wedge G^{k_2}_{\alpha_{2ij}}|} = \frac{|G|}{|G^{k_2}|}$$

for fixed i. Multiply both sides by $|A|/|A \wedge G^{k_1}_{\alpha_{1i}}|$ and sum over i, that is

$$\sum_{i,j}{}' \frac{|A|}{|A \wedge G^{k_1}_{\alpha_{1i}} \wedge G^{k_2}_{\alpha_{2ij}}|} = \frac{|G|}{|G^{k_2}|} \sum_i{}' \frac{|A|}{|A \wedge G^{k_1}_{\alpha_{1i}}|} = \frac{|G|^2}{|G^{k_1}||G^{k_2}|}.$$

The procedure is continued, until eventually

$$\sum_{i,j,\ldots,k,\ldots m}{}' \frac{|A|}{|A \wedge N_{ij\ldots m}|} = \frac{|G|^n}{\Pi^n_{i=1} |G^{k_i}|} \tag{13}$$

$$N_{ij\ldots k\ldots m} = G^{k_1}_{\alpha_{1i}} \wedge G^{k_2}_{\alpha_{2ij}} \wedge \ldots \wedge G^{k_p}_{\alpha_{pij\ldots k}} \wedge \ldots \wedge G^{k_n}_{\alpha_{nij\ldots k\ldots m}}.$$

The sum $\Sigma'_{i,j,\ldots k,\ldots m}$ is over precisely the same double coset formation discussed above in association with the derived set.

Now from the collection of selection rules (set S)

$$\star\boldsymbol{k}_1 \otimes \star\boldsymbol{k}_2 \otimes \ldots \otimes \star\boldsymbol{k}_n = \sum_l n_l \star\boldsymbol{l} \tag{14}$$

the identity equation

$$\frac{|G|}{\Pi^n_{i=1}|G^{k_i}|} = \sum_l n_l \frac{|G|}{|G^{l}|} \tag{15}$$

relates the number of terms on each side of equation (14) and therefore from equations (13), (15)

$$\sum_{i,j,\ldots,m}{}' \frac{|A|}{|A \wedge N_{ij\ldots m}|} = \sum_l n_l \frac{|G|}{|G^l|} \tag{16}$$

which is independent of the choice of A.

But $|A|/|A \wedge N_{ij\ldots m}| = d_{ij\ldots m}$ is precisely the same number of WVSRs that are grouped together via the coset representatives $\{z_\pi\}$, so that the set of derived sets (being mutually exclusive), exhaust the set $S(\Sigma n_l \star \boldsymbol{l})$. The size and nature of the derived set of course depends on A.

Note that the group A operating on a vector $\boldsymbol{l}$, can only send $\boldsymbol{l}$ into a member of $\star\boldsymbol{l}$. As each pair of derived sets are mutually distinct, then there exists a subset of the set of derived sets which is associated only with members of $\star\boldsymbol{l}$, and so

$$\sum_{i,j,\ldots,m}{}'' d_{ij\ldots m} = n_l \frac{|G|}{|G^l|}$$

Σ'' implying that the sum is restricted to those leading WVSRs combining to give a member of $^{\star}\boldsymbol{l}$.

If $A = G^{l}$, then $\eta \in G^{l}$ will be such that $\eta \boldsymbol{l} \rightarrow \boldsymbol{l}$, thus

$$\sum_{i,j,\dots,m}''' d_{ij\dots m} = n_{l} \tag{17}$$

Σ''' being the restriction to that subset of leading WVSRs combining to give $\boldsymbol{l}$.

To illustrate some of the above ideas, we take as an example of the triple power of $^{\star}\boldsymbol{W}$ from the asymmorphic space group $Fd3m$. For details on notation etc, we refer the reader to tables in Davies and Lewis (1971).

Now $^{\star}\boldsymbol{W} \otimes {}^{\star}\boldsymbol{W} \otimes {}^{\star}\boldsymbol{W} = 16{}^{\star}\boldsymbol{W} + 12{}^{\star}\boldsymbol{\Delta} + 12{}^{\star}\boldsymbol{L}$

$$\begin{aligned}
{}^{\star}\boldsymbol{W} &= (\boldsymbol{W}, C_{2z}\boldsymbol{W}, C_{31}^{+}\boldsymbol{W}, C_{31}^{-}\boldsymbol{W}, C_{33}^{+}\boldsymbol{W}, C_{33}^{-}\boldsymbol{W}) \\
{}^{\star}\boldsymbol{\Delta} &= (\boldsymbol{\Delta}, C_{2x}\boldsymbol{\Delta}, C_{31}^{+}\boldsymbol{\Delta}, C_{31}^{-}\boldsymbol{\Delta}, C_{34}^{+}\boldsymbol{\Delta}, C_{34}^{-}\boldsymbol{\Delta}) \\
{}^{\star}\boldsymbol{L} &= (\boldsymbol{L}, C_{2x}\boldsymbol{L}, C_{2y}\boldsymbol{L}, C_{2z}\boldsymbol{L}).
\end{aligned}$$

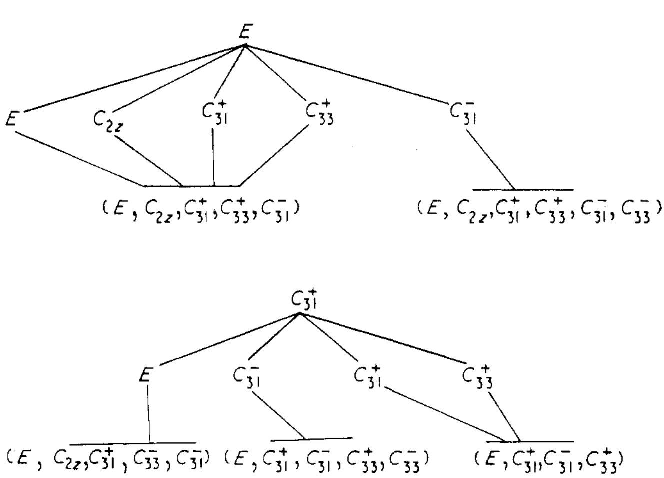
Take $\boldsymbol{W} + \boldsymbol{W} + \boldsymbol{W} \equiv C_{2z}\boldsymbol{W}$ as our starting leading WVSR, with $A = G^{\Delta}$ say. So consider (a): $G = \Sigma_{i} G^{\Delta}\alpha_{1i}G^{\boldsymbol{W}}$, compare (12$a$), $\alpha_{11} = E$, $\alpha_{12} = C_{31}^{+}$ where

$$\begin{aligned}
G^{\Delta}EG^{\boldsymbol{W}} &= (E, C_{2z}, C_{31}^{-}, C_{33}^{-})G^{\boldsymbol{W}} \\
G^{\Delta}C_{31}^{+}G^{\boldsymbol{W}} &= (C_{31}^{+}, C_{33}^{+})G^{\boldsymbol{W}}.
\end{aligned}$$

Next (b): $G = \Sigma_{j}(G^{\Delta} \wedge G_{i}^{\boldsymbol{W}})\alpha_{2ij}G^{\boldsymbol{W}}$, compare (12$b$), with $G_{i}^{\boldsymbol{W}} = \alpha_{1i}G^{\boldsymbol{W}}\alpha_{1i}^{-1}$, giving $\{\alpha_{21j}\} = \{E, C_{2z}, C_{31}^{+}, C_{33}^{+}, C_{31}^{-}\}$, $\{\alpha_{22j}\} = (E, C_{31}^{+}, C_{31}^{-}, C_{33}^{+})$.

(c): $$G = \sum_{k}(G^{\Delta} \wedge G_{i}^{\boldsymbol{W}} \wedge G_{ij}^{\boldsymbol{W}})\alpha_{3ijk}G^{\boldsymbol{W}}; \qquad G_{ij}^{\boldsymbol{W}} = \alpha_{2ij}G^{\boldsymbol{W}}\alpha_{2ij}^{-1}.$$

We quote results in the following diagram.



These diagrams define $26+18 = 44$ leading WVSRs, for example, from

$$W+W+W \equiv C_{2z}W$$

change the second entry $W \to C_{31}^{-}W$, then we have a choice of five entries; take $C_{31}^{-}W$. So $W+C_{31}^{+}W+C_{31}^{-}W \equiv L$ is another leading WVSR.

To avoid confusion one must use the original labels for double coset representatives; for example, one could take $W+C_{33}^{+}W+C_{33}^{-}W$ as a leading WVSR, as long as $W+C_{33}^{+}W+C_{31}^{-}W$ is excluded from the list. As $C_{33}^{-} \in (G^{\Delta} \wedge G^{W} \wedge G^{W}_{C_{33}^{+}})C_{31}^{-}G^{W}$, both are in the same derived set.

To check the completeness of this procedure, work out $|G^{\Delta}|/|G^{\Delta} \wedge G_i^{W} \wedge G_{ij}^{W}|$, and sum over the 44 leading WVSRs. In fact

$$\sum_{i,j}{}' \frac{|G^{\Delta}|}{|G^{\Delta} \wedge G_i^{W} \wedge G_{ij}^{W}|} = 216 = \sum_{l} n_l \frac{|G|}{|G^{l}|},$$

compare (16), as required.

Let us now examine the case $l = L$, with again $A = G^{\Delta}$, and consider the nature of the derived set.

An appropriate leading WVSR is

$$W+C_{31}^{+}W+C_{31}^{-}W \equiv L, \qquad \bar{A} = \bar{G}^{\Delta} = (E, C_{2y}, C_{4y}^{+}, \sigma_{x,z}, \sigma_{dc/e}).$$

Form the expansion

$$G^{\Delta} = \sum_{\pi} z_{\pi}(G^{\Delta} \wedge G^{W} \wedge C_{31}^{+}G^{W}C_{31}^{-} \wedge C_{31}^{-}G^{W}C_{31}^{+} \wedge G^{L}) = \sum_{\pi} z_{\pi}E.$$

Hence $\{z_{\pi}\} = G^{\Delta}$.

The derived set thus consists of 8 WVSRs, which are

$$\begin{array}{ll}
W+C_{31}^{+}W+C_{31}^{-}W \equiv L & C_{31}^{-}W+C_{31}^{+}W+C_{2z}W \equiv C_{2z}L \\
W+C_{31}^{+}W+C_{33}^{-}W = C_{2z}L & C_{31}^{-}W+C_{33}^{+}W+W \equiv C_{2y}L \\
C_{2z}W+C_{31}^{+}W+C_{33}^{-}W \equiv C_{2y}L & C_{33}^{-}W+C_{33}^{+}W+C_{2z}W \equiv L \\
C_{2z}W+C_{31}^{+}W+C_{31}^{-}W = C_{2x}L & C_{33}^{-}W+C_{33}^{+}W+W \equiv C_{2x}L.
\end{array}$$

Note also that the frequency of each member of the star of L is the same. This is in fact a general result, even if not all members of $*l$ appear.

The structure is further emphasized by using

$$G = G^{\Delta}(E, C_{2z}, C_{31}^{-}, C_{33}^{-})G^{W} + G^{\Delta}(C_{31}^{+}, C_{33}^{+})G^{W}.$$

This shows clearly that columns 1 and 3 contain only $(E, C_{2z}, C_{31}^{-}, C_{33}^{-})W$ while the second column contains only, $(C_{31}^{+}, C_{33}^{+})W$.

Consider $G^{\Delta} = \Sigma_{\lambda} a_{\lambda}(G^{\Delta} \wedge G^{W})$, see equations (2), (8), with $\{\alpha_{\lambda}\} = \{E, C_{2y}, C_{4y}^{\pm}\}$, that is, there are four different entries in the first column, with

$$C_{2y}W \equiv C_{2z}W, \qquad C_{4y}^{+}W \equiv C_{31}^{-}W, \qquad C_{4y}^{-}W \equiv C_{33}^{-}W.$$

For each λ, examine

$$G^{\Delta} \wedge G^{W}_{a_{\lambda}} = \sum_{\mu}^{d_2} a_{\lambda\mu}(G^{\Delta} \wedge G^{W}_{a_{\lambda}} \wedge G^{W}_{a_{\lambda}C_{31}^{+}})$$

compare (4), (8), and in this case $\{a_{\lambda\mu}\} = E$ only, for all λ. Hence for each λ, $(G^{\Delta} \wedge G^{W}_{\alpha_{\lambda}\alpha_1})a_{\lambda}\alpha_2 G^{W}$ contains only one left coset of G^{W}, (see equations (7), (12)), telling us that with each $a_\lambda W$ there is only one term appearing in combination—this can clearly be seen from the example.

Also

$$\sum_\lambda a_\lambda\{(G^\Delta \wedge G^W)C_{31}^+G^W\} = G^\Delta C_{31}^+G^W$$

(see equation (7) and lemma 10). Finally for each $\lambda\mu$,

$$M_{\lambda\mu}^{(2)} = \sum_\nu^{d_3} a_{\lambda\mu\nu}(M_{\lambda\mu}^{(2)} \wedge G^W_{a_{\lambda\mu}C_{31}^-})$$

(see equation (8)), we shall quote the results, that is $d_3 = 2, a_{111} = a_{211} = a_{311} = a_{411} = E$, $a_{112} = a_{212} = \sigma_z, a_{312} = a_{412} = \sigma_x$.

From these results we see that in combination with $W + C_{31}^+W$ in the derived set, we can have both $EC_{31}^-W \equiv C_{31}^-W$ and $\sigma_z C_{31}^-W \equiv C_{33}^-W$, which ties up with the example.

Similar results can be generated for the other cases. We can show how the cosets link up. For example with $\lambda = 3$, $\mu = 1$, $a_\lambda = C_{4y}^+$, $a_{1\mu} = E$, (see equation (12)).

$$(M_{\lambda\mu}^{(2)})\alpha_{\lambda\mu 3}G^W = (M_{31}^{(2)})\alpha_{313}G^W = (M_{31}^{(2)})a_{31}a_3\alpha_3G^W.$$

Now

$$M_{31}^{(2)} = G^\Delta \wedge G^W_{C_{31}^-} \wedge G^W_{C_{33}^+} = \sum_\nu a_{31\nu}(M_{31}^{(2)} \wedge G^W_{C_{4x}^-})$$

where $a_{31}a_3\alpha_3 = C_{4y}^+C_{31}^- = C_{4x}^-$. Therefore

$$(M_{31}^{(2)})a_{31}a_3\alpha_3G^W = (E, C_{2z})G^W.$$

Compare with

$$a_3a_{11}((M_{11}^{(2)})C_{31}^-G^W) = C_{4y}^+(C_{31}^-G^W, C_{33}^-G^W) = (E, C_{2z})G^W.$$

A relevant practical example could be considered by taking $A = G^\Delta, l = \Delta$. One could then scan through the 44 leading WVSRs to find one giving Δ, that is,

$$W + W + C_{33}^+W = \Delta.$$

As $|G^\Delta|/|G^W \wedge G^W_{C_{33}^+} \wedge G^\Delta| = 4$, the derived set contains 4 members with

$$\{z_\pi\} = (E, C_{2y}, C_{4y}^\pm),$$

and the derived set is

$$W + W + C_{33}^+W \equiv \Delta$$

$$C_{2z}W + C_{2z}W + C_{33}^+W \equiv \Delta$$

$$C_{31}^-W + C_{31}^-W + C_{31}^+W \equiv \Delta$$

$$C_{33}^-W + C_{33}^-W + C_{31}^+W \equiv \Delta.$$

To find a new leading WVSR change the second entry from W to C_{33}^+W say, and clearly a possibility is $W + C_{33}^+W + W \equiv \Delta$ for a second leading WVSR. Again the order of the derived set is 4.

Now an obvious practical choice for a third (and final) leading WVSR would be $C_{33}^+W + W + W$ but this does not appear explicitly in the scheme of paths, but will appear as $C_{31}^+W + C_{31}^-W + C_{31}^-W \equiv \Delta$, a member of its derived set as

$$C_{4y}^+C_{31}^+W \rightarrow C_{33}^+W, \qquad C_{4y}^+C_{31}^-W \rightarrow W.$$

So these three leading WVSRs have (by coincidence) derived sets of order 4, and so as the frequency of $^*\mathbf{\Delta}$ is 12, they are sufficient.

There are no more paths giving $\mathbf{\Delta}$, for if there were the overall completeness would not be guaranteed.

3.2. *Application of method*

To calculate nth direct powers, we have to evaluate the coefficients

$$C = C^{k_1 k_2 \dots k_n l}_{p_1 p_2 \dots p_n \nu} = \frac{1}{|G|} \sum_{R \in G} \prod_{i=1}^{n} \chi^{k_i}_{p_i}(R) \chi^{*l}_{\nu}(R).$$

Use the usual substitution to express the character in terms of characters of the appropriate small representation, that is,

$$\chi^{k}_{p}(R) = \sum_{\alpha} \psi^{k}_{\alpha p}(R) J^{k}_{\alpha}(R). \tag{18}$$

So

$$C = \frac{1}{|G|} \sum_{R \in G} \sum_{\alpha_1 \alpha_2, \dots, \alpha_n, \delta} \left(\prod_{i=1}^{n} \psi^{k_i}_{\alpha_i p_i}(R) J^{k_i}_{\alpha_i}(R) \right) \psi^{*l}_{\delta \nu}(R) J^{l}_{\delta}(R).$$

As one can interchange the summation, this allows the sum over the translation terms to be carried out. Put $R = (S|\boldsymbol{\tau}_s + \boldsymbol{t})$, thus

$$C = \frac{|T|}{|G|} \sum_{\alpha_1, \alpha_2, \dots, \alpha_n, \delta} \sum_{S \in \bar{N}_{\alpha_1 \alpha_2 \dots \alpha_n \delta}} \prod_{i=1}^{n} \psi^{k_i}_{\alpha_i p_i}\{(S|\boldsymbol{\tau}_S)\} \psi^{*l}_{\delta \nu}\{(S|\boldsymbol{\tau}_S)\} \, \delta\left(\sum_{j=1}^{n} \alpha_j \boldsymbol{k}_j - \boldsymbol{l} \right)$$

where $\bar{N}_{\alpha_1 \dots \alpha_n \delta}$ is the little co-group of $N_{\alpha_1 \alpha_2 \dots \alpha_n \delta} = G^{k_1}_{\alpha_1} \wedge \dots \wedge G^{k_n}_{\alpha_n} \wedge G^{l}_{\delta}$. We write

$$C = \frac{|T|}{|G|} \sum_{\alpha_1, \alpha_2, \dots, \alpha_n, \delta} A_{\alpha_1 \alpha_2 \dots \alpha_n \delta}. \tag{19}$$

The definition of $A_{\alpha_1 \dots \alpha_n \delta}$ is obvious from (19).

Lemma 11.

$$A_{\alpha_1 \alpha_2 \dots \alpha_n \delta} = A_{\beta_1 \beta_2 \dots \beta_n e}, \qquad \text{with } \beta_i = \delta^{-1} \alpha_i.$$

Proof.

$$A_{\alpha_1 \alpha_2 \dots \alpha_n \delta} = \sum_{S \in \bar{N}_{\alpha_1 \dots \alpha_n \delta}} \prod_{i=1}^{n} \psi^{k_i}_{p_i}\{(\alpha_i|\boldsymbol{\tau}_{\alpha_i})^{-1}(S|\boldsymbol{\tau}_s)(\alpha_i|\boldsymbol{\tau}_{\alpha_i})\} \psi^{*l}_{\nu}\{(\delta|\boldsymbol{\tau}_\delta)^{-1}(S|\boldsymbol{\tau}_s)(\delta|\boldsymbol{\tau}_\delta)\}$$
$$\times \delta\left(\sum_{j=1}^{n} \alpha_j \boldsymbol{k}_j - \boldsymbol{l} \right).$$

In order to rewrite this expression consider

$$(\alpha|\boldsymbol{\tau}_\alpha)^{-1}(S|\boldsymbol{\tau}_S)(\alpha|\boldsymbol{\tau}_\alpha) = (\alpha|\boldsymbol{\tau}_\alpha)^{-1}(\delta|\boldsymbol{\tau}_\delta)(\delta|\boldsymbol{\tau}_\delta)^{-1}(S|\boldsymbol{\tau}_S)(\delta|\boldsymbol{\tau}_\delta)(\delta|\boldsymbol{\tau}_\delta)^{-1}(\alpha|\boldsymbol{\tau}_\alpha);$$

putting

$$(\delta|\boldsymbol{\tau}_\delta)^{-1}(\alpha|\boldsymbol{\tau}_\alpha) = (\beta|\boldsymbol{\tau}_\beta + \boldsymbol{t}_\beta)$$

where

$$\boldsymbol{\tau}_\beta + \boldsymbol{t}_\beta = \delta^{-1}(\boldsymbol{\tau}_\alpha - \boldsymbol{\tau}_\delta),$$

and $\boldsymbol{t}_\beta$ is a lattice translation vector. Also $(\delta|\boldsymbol{\tau}_\delta)^{-1}(S|\boldsymbol{\tau}_S)(\delta|\boldsymbol{\tau}_\delta) = (U|\boldsymbol{\tau}_U + \boldsymbol{t}_U)$ with $\boldsymbol{t}_U + \boldsymbol{\tau}_U = \delta^{-1}(U\boldsymbol{\tau}_\delta + \boldsymbol{\tau}_U - \boldsymbol{\tau}_\delta)$, and $\boldsymbol{t}_U$ a translation vector. As $U = \delta^{-1}S\delta$, then

$U \in \bar{N}_{\beta_1\beta_2\ldots\beta_n}$. Thus

$$(\alpha|\tau_\alpha)^{-1}(S|\tau_S)(\alpha|\tau_\alpha) = (E|\beta^{-1}(Ut_\beta - t_\beta + t_U))(\beta|\tau_\beta)^{-1}(U|\tau_U)(\beta|\tau_\beta).$$

Therefore

$$\psi_p^{k}\{(\alpha|\tau_\alpha)^{-1}(S|\tau_S)(\alpha|\tau_\alpha)\} = \psi_p^{k}\{(\beta|\tau_\beta)^{-1}(U|\tau_U)(\beta|\tau_\beta)\} \exp\{-\mathrm{i}k \cdot \beta^{-1}(Ut_\beta + t_U - t_\beta)\}$$

by using the properties of ψ_p^k as a small representation. Because $U \in G_\beta^k$, then $U^{-1}\beta k \equiv \beta k$, and we have

$$\exp[\mathrm{i}k \cdot \{\beta^{-1}(Ut_\beta + t_U - t_\beta)\}] = \exp(-\mathrm{i}\beta k \cdot t_U).$$

By substituting similar results, the expression becomes

$$A_{\alpha_1\alpha_2\ldots\alpha_n\delta} = \sum_{U \in \bar{N}_{\beta_1\beta_2\ldots\beta_n}} \prod_{i=1}^{n} \psi_{\beta_i p_i}^{k_i}\{(U|\tau_U)\}\psi_\nu^{*l}\{(U|\tau_U)\}\delta\left(\sum_j \alpha_j k_j - \delta l\right)$$
$$\times \exp\left\{-\mathrm{i}\left(\sum_m \beta_m k_m - l\right) \cdot t_U\right\}.$$

Now

$$\delta\left(\sum_j \alpha_j k_j - \delta l\right) \exp\left\{-\mathrm{i}\left(\sum_m \beta_m k_m - l\right) \cdot t_U\right\} = \delta\left(\sum_j \beta_j k_j - l\right)$$

so that

$$A_{\alpha_1\alpha_2\ldots\alpha_n\delta} = A_{\beta_1\ldots\beta_n e} = A_{\beta_1\ldots\beta_n}$$

with $\bar{N}_{\beta_1\ldots\beta_n} = \delta\bar{N}_{\alpha_1\ldots\alpha_n\delta}\delta^{-1}$.

The lemma shows that we can concentrate specifically on the WVSR $\Sigma_j\beta_j k_j \equiv l$, and the sum (19) is split into $|G|/|G^l|$ equal portions, that is,

$$C = \frac{|T|}{|G^l|}\sum_{\beta_1\beta_2\ldots\beta_n} A_{\beta_1\beta_2\ldots\beta_n}. \tag{20}$$

As we can concentrate specifically on the WVSRs $\Sigma_{i=1}^{n}\beta_i k_i \equiv l$ we are dealing with the case $A = G^l$ mentioned above. So, consider the expansion

$$G^l = \sum_\pi z_\pi \bar{N}_{\beta_1\ldots\beta_n} \tag{21}$$

with the set of coset representatives $\{z_\pi\}$ having the properties outlined in lemmas 1, 2.

As each z_π gives a different WVSR of the derived set, denote $z_\pi\beta_j$ by $\beta_{\pi j}$ and $A_{\beta_{\pi1}\beta_{\pi2}\ldots\beta_{\pi n}}$ by $A^{(\pi)}_{\beta_1\beta_2\ldots\beta_n}$.

Lemma 12.

$$A^{(e)}_{\beta_1\ldots\beta_n} = A^{(\pi)}_{\beta_1\ldots\beta_n}.$$

Proof.

$$A^{(\pi)}_{\beta_1\ldots\beta_n} = \sum_{S \in \bar{N}^{(\pi)}_{\beta_1\ldots\beta_n}} \prod_{i=1}^{n} \psi_{\beta_i p_i}^{k_i}\{(z_\pi|\tau_\pi)^{-1}(S|\tau_S)(z_\pi|\tau_\pi)\}\psi_\nu^{*l}\{(z_\pi|\tau_\pi)^{-1}(S|\tau_S)(z_\pi|\tau_\pi)\}$$
$$\times \delta\left(\sum_i z_\pi\beta_i k_i - l\right)$$
$$\bar{N}^{(\pi)}_{\beta_1\ldots\beta_n} = z_\pi\bar{N}_{\beta_1\ldots\beta_n}z_\pi^{-1}.$$

Denote $z_\pi^{-1} S z_\pi$ by S_π, then $(z_\pi|\boldsymbol{\tau}_\pi)^{-1}(S|\boldsymbol{\tau}_S)(z_\pi|\boldsymbol{\tau}_\pi) = (S_\pi|\boldsymbol{\tau}_{S_\pi}+\boldsymbol{t})$ where

$$\boldsymbol{t} = z_\pi^{-1}(-\boldsymbol{\tau}_\pi+\boldsymbol{\tau}_S+S\boldsymbol{\tau}_\pi)-\boldsymbol{\tau}_{S\pi}.$$

So

$$A^{(\pi)}_{\beta_1\ldots\beta_n} = \sum_{S_\pi\in\bar{N}_{\beta_1\ldots\beta_n}} \prod_{i=1}^{n} \psi^{\boldsymbol{k}_i p}_{\beta_i p_i}\{(S_\pi|\boldsymbol{\tau}_{S_\pi})\}\psi^{*\boldsymbol{l}}_{\nu}\{(S_\pi|\boldsymbol{\tau}_{S_\pi})\} \exp\left\{-i\boldsymbol{t}\cdot\left(\sum_i \beta_i\boldsymbol{k}_i-\boldsymbol{l}\right)\right\}$$
$$\times\delta\left(\sum_i z_\pi\beta_i\boldsymbol{k}_i-\boldsymbol{l}\right)$$

using the properties of small representations. Now as $z_\pi \in G^{\boldsymbol{l}}$, then

$$\exp\left\{-i\boldsymbol{t}\cdot\left(\sum_i \beta_i\boldsymbol{k}_i-\boldsymbol{l}\right)\right\}\delta\left(\sum_i z_\pi\beta_i\boldsymbol{k}_i-\boldsymbol{l}\right) = \delta\left(\sum_i \beta_i\boldsymbol{k}_i-\boldsymbol{l}\right).$$

Thus finally

$$A^{(\pi)}_{\beta_1\beta_2\ldots\beta_n} = A^{(e)}_{\beta_1\ldots\beta_n}.$$

The lemma shows that the sum (20) can be split into various portions based on the leading WVSRs and the completeness of this approach has been guaranteed previously in this section, that is, by

$$\sum_{(\beta)} d_{\beta_1\ldots\beta_n} = n_l,$$

(compare (17)). $\Sigma_{(\beta)}$ is the restriction to those leading WVSRs combining to give $\boldsymbol{l}$. The procedure for finding the relevant leading WVSRs has been laid down, where we have $G^{\boldsymbol{l}}$ for A. Thus

$$C = \sum_{(\beta)} \frac{|T|}{|N_{\beta_1\ldots\beta_n}|} A_{\beta_1\ldots\beta_n},$$

or in the final form

$$C^{\boldsymbol{k}_1\boldsymbol{k}_2\ldots\boldsymbol{k}_n\boldsymbol{l}}_{p_1p_2\ldots p_n\nu} = \sum_{(\beta)}{}' \frac{|T|}{|N_{\beta_1\ldots\beta_n}|} \sum_{S\in\bar{N}_{\beta_1\ldots\beta_n}} \prod_{i=1}^{n} \psi^{\boldsymbol{k}_i}_{\beta_i p_i}\{(S|\boldsymbol{\tau}_S)\}\psi^{*\boldsymbol{l}}_{\nu}\{(S|\boldsymbol{\tau}_S)\} \tag{22}$$

where Σ' signifies that the $\delta(\Sigma_i\beta_i\boldsymbol{k}_i-\boldsymbol{l})$ term is automatically allowed for.

The result is identical to one obtainable by a natural extension of Bradley's (1966) work, but has been obtained by a totally different approach.

4. Symmetrized *n*th powers

We now wish to calculate the coefficient

$$[C^{\boldsymbol{kl}}_{p\nu}]^{(n)} = \frac{1}{|G|}\sum_{R\in G}[\chi^{\boldsymbol{k}}_p]^{(n)}(R)\chi^{*\boldsymbol{l}}_\nu(R)$$

$[\chi^{\boldsymbol{k}}_p]^{(n)}$ being the character of the nth symmetrized power. It will be shown in § 5 that one can concentrate specifically on a portion of the sum

$$C^{\boldsymbol{kl}}_{p\nu}(n) = \frac{1}{n}\frac{1}{|G|}\sum_{R\in G}\chi^{\boldsymbol{k}}_p(R^n)\chi^{*\boldsymbol{l}}_\nu(R).$$

Make the usual substitution to reduce to the character of the small representations (see equation (18)):

$$C^{kl}_{p\nu}(n) = \frac{1}{n}\frac{1}{|G|}\sum_{R\in G}\sum_{\alpha_1,\delta}\psi^{k}_{\alpha_1 p}(R^n)\psi^{*l}_{\delta\nu}J^{k}_{\alpha_1}(R^n)J^{l}_{\delta}(R).$$

Put $R = (S|\tau_S+t)$, so that $R^n = (S^n|\tau_S+t+S(\tau_S+t)+\ldots+S^{n-1}(\tau_S+t))$, and sum over the translation group noting that

$$(\alpha|\tau_\alpha)^{-1}(S|\tau_S+t)^n(\alpha|\tau_\alpha) = \left(E\middle|\alpha^{-1}\left(\sum_{j=1}^{n-1}S^j\right)t\right)\times(\alpha|\tau_\alpha)^{-1}(S|\tau_S)^n(\alpha|\tau_\alpha).$$

Hence

$$C^{kl}_{p\nu}(n) = \frac{1}{n}\sum_{\alpha_1,\delta}\frac{|T|}{|G|}\sum_{S\in\bar{Q}_{\alpha_1\delta}}{}' \psi^{k}_{\alpha_1 p}\{(S|\tau_S)^n\}\psi^{*l}_{\delta\nu}\{(S|\tau_S)\}$$

where $\bar{Q}_{\alpha_1\delta}$ is defined by: (i) $S^n\in\bar{G}^{k}_{\alpha_1}$, (ii) $S\in\bar{G}^{l}_{\delta}$, (iii) $(1+S+\ldots+S^{n-1})\alpha_1 k\equiv\delta l$ and the Σ' is included to show that the WVSR of condition (iii) must be satisfied. Write

$$C^{kl}_{p\nu}(n) = \frac{1}{n}\sum_{\alpha_1,\delta}\frac{|T|}{|G|}B_{\alpha_1\delta}$$

with $B_{\alpha_1\delta}$ defined in the obvious way, then:

Lemma 13.

$$B_{\alpha_1\delta} = B_{\beta_1 e}, \qquad \beta_1 = \delta^{-1}\alpha_1.$$

The proof is straightforward along the lines of Lemma 11.

Using lemma 13 we have

$$C^{kl}_{p\nu}(n) = \frac{1}{n}\sum_{\beta_1}{}'\frac{|T|}{|G^l|}B_{\beta_1}, \qquad (B_{\beta_1} = B_{\beta_1 e})$$

and

$$B_{\beta_1} = \sum_{S\in\bar{Q}_{\beta_1}}\psi^{k}_{\beta_1 p}\{(S|\tau_S)^n\}\psi^{*l}_{\nu}\{(S|\tau_S)\} \tag{23}$$

where $\bar{Q}_{\beta_1}$ is defined as:

(i) $S^n\in\bar{G}^{k}_{\beta_1}$, (ii) $S\in\bar{G}^{l}$, (iii) $(1+S+\ldots+S^{n-1})\beta_1 k\equiv l$.

We note that either (i), (iii) or (ii), (iii) would suffice to define the set.

Write $S^{j-1}\beta_1 = \beta_j$ and consider the expansion $G^l = \Sigma_\pi z_\pi N_{\beta_1\ldots\beta_n}$, proceeding in exactly the same way as for ordinary powers by using the notion of leading and derived sets of WVSRs, and splitting the sums into sets of order $|G^l|/|N_{\beta_1\ldots\beta_n}|$ (see lemma 12), and so we have the analogous lemma:

Lemma 14.

$$B^{(\pi)}_{\beta_1} = B^{(e)}_{\beta_1}.$$

The proof is straightforward. Thus we can write

$$C^{kl}_{p\nu}(n) = \frac{1}{n}\sum_{(\beta)}{}''\frac{|T|}{|N_{\beta_1\ldots\beta_n}|}\sum_{S\in\bar{Q}(\beta)}\psi^{k}_{\beta_1 p}\{(S|\tau_S)^n\}\psi^{*l}_{\nu}\{(s|\tau_S)\}. \tag{24}$$

(β) or $\beta_1(\beta_2 \ldots \beta_n)$ implies summing over all leading WVSRs. The symbol $\beta_1(\beta_2 \ldots \beta_n)$ is included to emphasize that all β_1 must be considered, that is, $\beta_2 \ldots \beta_n$ could be, and often is, different for the same β. Σ'' signifies that although we sum over the same leading WVSRs as for ordinary products, not all of these will contribute to $C^{kl}_{p\nu}(n)$ because of the special form that the WVSR must take, that is, its obvious dependence on S. So, faced with the various leading WVSRs one must endeavour to find a routine that will help identify those that contribute.

We emphasize that in the portion of the sum B_{β_1} (equation (23)) we are concerned with *one* WVSR, and clearly $\bar{Q}_{\beta_1} = \bar{Q}_{(\beta)}$ has to be non-empty.

Lemma 15.

$$S\bar{N}_{\beta_1\beta_2\ldots\beta_n} = \bar{Q}_{\beta_1(\beta_2\ldots\beta_n)}(= \bar{Q}_{(\beta)}).$$

That is, $\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)}$ is the coset of $\bar{N}_{\beta_1\ldots\beta_n}$ with respect to G^{l}.

Proof.

If $S, T \in Q_{(\beta)}$ then

$$\sum_{i=0}^{n-1} S^i\beta_1\boldsymbol{k} \equiv \boldsymbol{l}, \qquad \sum_{i=0}^{n-1} T^i\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$$

and $T^p\beta_1\boldsymbol{k} \equiv S^p\beta_1\boldsymbol{k}$ for all p, that is,

$$TT^{p-1}\beta_1\boldsymbol{k} \equiv SS^{p-1}\beta_1\boldsymbol{k}$$

implying

$$S^{-1}T\beta_p\boldsymbol{k} \equiv \beta_p\boldsymbol{k}, \qquad \forall p.$$

Thus

$$S^{-1}T \in N_{\beta_1\ldots\beta_n},$$

that is,

$$T \in SN_{\beta_1\ldots\beta_n}.$$

As a consequence $|\bar{Q}_{(\beta)}| = |\bar{N}_{\beta_1\ldots\beta_n}|$.

Lemma 16.

$$\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)} = \bigcap_{p=1}^{n} \beta_{p+1}G^k\beta_p^{-1}, \qquad (\beta_{n+1}G^k \equiv \beta_1 G^k).$$

Proof.

If $S \in \bar{Q}_{(\beta)}$ then

(*a*) $S\beta_p G^k \mapsto \beta_{p+1}G^k, \qquad \forall p$
(*b*) $S^n \in G^k_{\beta_1}$.

Condition (*a*) replacing $\Sigma S^i\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$.

From (*a*) $\beta_{p+1}^{-1}S\beta_p \in G^k$, $\forall p$, that is, $S \in \beta_{p+1}G^k\beta_p^{-1}$, so $S \in \cap_p\beta_{p+1}G^k\beta_p^{-1}$.

Conversely if $S \in \cap_p\beta_{p+1}G^k\beta_p^{-1}$, then (*a*) $S \in \beta_{p+1}G^k\beta_p^{-1}$, $\forall p$ implying $S\beta_p\boldsymbol{k} \to \beta_{p+1}\boldsymbol{k}$; and (*b*) $S^n \in \beta_1 G^k\beta_n^{-1}\beta_n G^k\beta_{n-1}^{-1} \ldots \beta_3 G^k\beta_2^{-1}\beta_2 G^k\beta_1^{-1} \in G^k_{\beta_1}$. Hence $S \in \bar{Q}_{(\beta)}$.

Alternatively we can write

$$\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)} = (n, n-1, \ldots, 2, 1)\bar{N}_{\beta_1\ldots\beta_n}; \qquad (n, n-1, \ldots, 2, 1)$$

being a permutation symbol meaning $S(\beta_1 \ldots \beta_n) \mapsto (\beta_2 \ldots \beta_n \beta_1)$.

Lemma 17.

If $\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)} \neq \phi$ then $G^l\beta_i G^k = G^l\beta_j G^k$, $\qquad \forall i,j.$

Proof.

Assume $\bar{Q}_{(\beta)} \neq \phi$, then $\exists S$ so that $S^{i-1}_{\beta_1 k} \equiv \beta_1 \boldsymbol{k}$ implying $\beta_i \in G^l\beta_1 G^k$, $\forall i$. Hence $G^l\beta_i G^k \equiv G^l\beta_j G^k$, $\forall i,j$. Certainly if $G^l\beta_i G^k \neq G^l\beta_j G^k$ then $\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)} = \phi$.

Now there may exist an integer $i \leqslant n$ for which $S^i \in G^k_{p_1}$. There are three cases:

(i) $i = n$, that is, $S^n \in G^k_{\beta_1}$, and is the least such n. If we assume that there exist integers $p, q < n$ such that $S^p\beta_1\boldsymbol{k} \equiv S^q\beta_1\boldsymbol{k}$ implying $S^{p-q} \in G^k_{\beta_1}$ we arrive at a contradiction as $p - q < n$. Hence all the coset representatives β_1 to β_n involved in the WVSR must be distinct.

(ii) $i = 1$, that is, $S \in G^k_{\beta_1}$ and $\beta_i = \beta_j$ for all $i, j \leqslant n$.

The WVSR can be written as $n\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$ with $\bar{Q}_{(\beta)} = \bar{G}^{k_1}_{\beta_1}$.

(iii) $i < n$, with $i \neq 1$, so that $S^i \in G^k_{\beta_1}, S^{i-1} \notin G^k_{\beta_1}$. Choose i to be the least such integer. For integers $p, q < i$, $S^p\beta_1\boldsymbol{k} \equiv S^q\beta_1\boldsymbol{k}$.

Lemma 18.

i divides n.

Proof.

This is obvious in cases (i), (ii). In case (iii) we assume not. Then $n = p \bmod i$, $p < i$. But as $S^n \in G^k_{\beta_1}$, and $S^i \in G^k_{\beta_1}$ then $S^p \in G^k_{\beta_1}$. This is a contradiction as i was assumed to be the smallest such integer.

As a result each WVSR has a unique factorization and can be written as

$$(1+S+\ldots+S^{i-1})\beta_1\boldsymbol{k}+\ldots+(1+S+\ldots+S^{i-1})\beta_1\boldsymbol{k} \equiv \boldsymbol{l}\,(j \text{ times}),$$

or formally as $j(1+S+\ldots+S^{i-1})\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$, $(ij = n)$. The group of this equation is $G^l \wedge G^k_{\beta_1} \wedge \ldots \wedge G^k_{\beta_i}$ and not $G^l \wedge G^{jk}_{\beta_1} \wedge \ldots \wedge G^{jk}_{\beta_i}$.

Lemma 19.

If a leading WVSR has j blocks of 'size' i, then all members of the derived set have the same structure.

For a leading WVSR written in the form $j(\beta_1 + \ldots + \beta_i)\boldsymbol{k} \equiv \boldsymbol{l}$, then

$$\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)} = \bar{Q}_{\beta_1(\beta_2\ldots\beta_i)} = \bigcap_{p=1}^{i} \beta_{p+1}G^k\beta_p^{-1}.$$

Again we have the permutation property in the sense that $S(\beta_1\beta_2\ldots\beta_i) \to (\beta_2\beta_3\ldots\beta_i\beta_1)$.

We now sum up. Presented with a leading WVSR $\Sigma_i\,\beta_i\boldsymbol{k} \equiv \boldsymbol{l}$ in conjunction with the sum (24), then the WVSR contributes only if $\bar{Q}_{\beta_1(\beta_2\ldots\beta_n)}(= \bar{Q}_{\beta_1} = \bar{Q}_{(\beta)}) \neq \phi$. $\bar{Q}_{(\beta)}$ can be defined as a set of elements S, such that

(i) $S \in G^l$ $\qquad$ (ii) $S^n \in G^k_{\beta_1}$ $\qquad$ (iii) $(1+S+\ldots+S^{n-1})\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$, or can be calculated directly from

$$\bar{Q}_{(\beta)} = \bigcap_{p=1}^{n} \beta_{p+1} G^k \beta_p^{-1}.$$

When in block form

$$\bar{Q}_{(\beta)} = \bigcap_{p=1}^{i} \beta_{p+1} G^k \beta_p^{-1}.$$

The following points are useful practically: (*a*) $\bar{Q}_{(\beta)} \neq \phi$ only if $G^l \beta_i G^k = G^l \beta_j G^k$, $\forall ij$, (but not conversely). (*b*) If $\beta_p \boldsymbol{k}$, $\beta_q \boldsymbol{k}$, $\beta_p \boldsymbol{k} \not\equiv \beta_q \boldsymbol{k}$ appear in the leading WVSR, then the frequency of appearance of both must be the same if the leading WVSR is to contribute (hence block structure). (*c*) If (*b*) is satisfied, then G^l must contain elements of order i, with $ij = n$. (*d*) If (*a*) is satisfied, and we have a block structure, then

$$G^l \beta_1 G^k = G^l \beta_m G^k, \qquad 1 \leqslant m \leqslant i.$$

Hence $|G^l|/|G^l \wedge G^k_{\beta_1}| \geqslant i$.

For space groups one can draw further simple conclusions.

(i) As space groups contain only 2, 3, 4 or 6 fold rotational elements, for $n > 6$, the leading WVSRs must split in the manner indicated above. If n is prime, and $n > 6$, then we need only concern ourselves with cases $n\boldsymbol{k} \equiv \boldsymbol{l}$.

(ii) For $n = 12$, $(g|\tau_g) \in G$, then $g^{12} = E$ always, which leads to great simplifications. Similar conclusions can sometimes be drawn for powers less than 12, depending on the nature of the space group.

We take as an example the fourth symmetrized power of $^\star X$ in $Fm3m$ (see Chen *et al* 1968, Davies and Lewis 1971 for notational details). Now

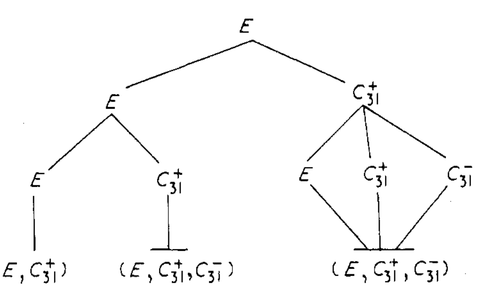
$$^\star X \otimes {}^\star X \otimes {}^\star X \otimes {}^\star X = 21\,^\star\Gamma + 20\,^\star X,$$

$$^\star X Ⓢ\, {}^\star X Ⓢ\, {}^\star X Ⓢ\, {}^\star X = 6\,^\star\Gamma + 3\,^\star X.$$

We start by taking $A = G^\Gamma$, and

$$X + X + X + X \equiv \Gamma$$

as a typical leading WVSR. We can set up the following diagram



defining 14 leading WVSRs. We can pick out the 4 relevant leading WVSRs

$$X + X + X + X \equiv \Gamma, \qquad X + X + C_{31}^+ X + C_{31}^+ X \equiv \Gamma,$$

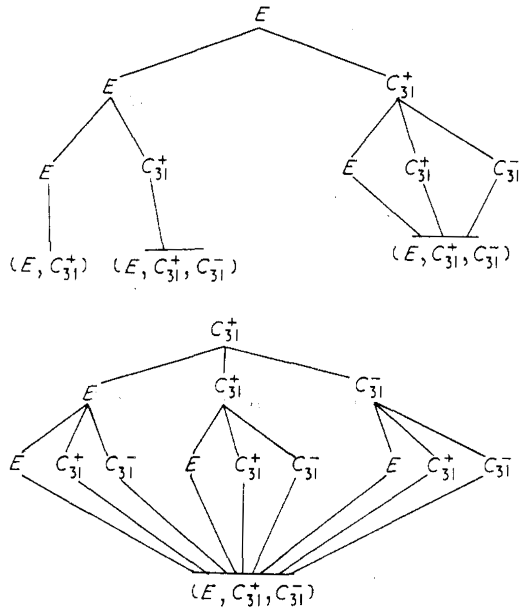
$$X + C_{31}^+ X + X + C_{31}^+ X \equiv \Gamma, \qquad X + C_{31}^+ X + C_{31}^+ X + X \equiv \Gamma.$$

Note that the orders of the derived sets are respectively 3, 6, 6, 6, giving a total of 21, as required.

Now take $A = G^{X}$, starting again from

$$\boldsymbol{X}+\boldsymbol{X}+\boldsymbol{X}+\boldsymbol{X} \equiv \boldsymbol{\Gamma}$$

the following diagram is produced



defining $12+27 = 41$ leading WVSRs.

The following are the leading WVSRs giving X:

$$(E+E+C_{31}^{+}+C_{31}^{+})X, \qquad (E+C_{31}^{+}+E+C_{31}^{-})X,$$
$$(E+C_{31}^{+}+C_{31}^{-}+E)X, \qquad (C_{31}^{+}+E+E+C_{31}^{-})X,$$
$$(C_{31}^{+}+C_{31}^{-}+E+E)X, \qquad (C_{31}^{+}+E+C_{31}^{-}+E)X,$$
$$(C_{31}^{+}+C_{31}^{+}+C_{31}^{+}+C_{31}^{-})X, \qquad (C_{31}^{+}+C_{31}^{-}+C_{31}^{+}+C_{31}^{+})X,$$
$$(C_{31}^{+}+C_{31}^{+}+C_{31}^{-}+C_{31}^{+})X, \qquad (C_{31}^{+}+C_{31}^{-}+C_{31}^{-}+C_{31}^{-})X.$$

All 10 have derived sets of order 2, giving $n_{X} = 20$ as required.

Let us now consider the evaluation of $(X_1 \uparrow G)\circledS(X_1 \uparrow G)\circledS(X_1 \uparrow G)\circledS(X_1 \uparrow G) = H_4$, $(X_1 = X_1^{+})$. Adopt the notation

$$H_1 = X_1 \uparrow G, \qquad H_2 = (X_1 \uparrow G)\circledS(X_1 \uparrow G),$$
$$H_3 = (X_1 \uparrow G)\circledS(X_1 \uparrow G)\circledS(X_1 \uparrow G), \qquad H_iH_j = H_i \otimes H_j.$$

All H_1, H_2, H_3 are known. Analysis of the character relations gives us

$$H_4 = \tfrac{1}{4}H_1^4 + C(4) - H_1^2H_2 + H_1H_3 + \tfrac{1}{2}H_2^2.$$

$C(4)$ is the total contribution from terms such as (24). Using results in Chen *et al* (1968) we get

$$H_4 = C^{\Gamma}(4)+C^{X}(4)+\tfrac{3}{2}\Gamma^1+\tfrac{1}{4}\Gamma^2+\tfrac{7}{4}\Gamma^{12}+2(X_1\uparrow G)+X_2\uparrow G.$$

where $C^{\Gamma}(4) = \frac{1}{4}\Sigma_\nu C^{X\Gamma}_{1\nu}(4)\Gamma^\nu$, $C^{X}(4) = \frac{1}{4}\Sigma_\mu C^{XX}_{1\mu}(4)(X_\mu \uparrow G)$.

Firstly let us deal with $C^{\Gamma}(4)$, clearly the only leading WVSRs that contribute are $4X \equiv \boldsymbol{\Gamma}$ and $2(X+C^{+}_{31}X) \equiv \boldsymbol{\Gamma}$ the latter being in the block form $2(E+C_{2f})X$. For the former $\bar{Q}_{(\beta)} = \bar{G}^{X}$, for the latter $\bar{Q}_{(\beta)} = C^{+}_{31}G^{X} \wedge G^{X}C^{-}_{31} = (C_{2d}, C_{2f}, C^{\pm}_{4x})\otimes(E, I) = \bar{Q}$. Note $C_{2f}X \equiv C^{+}_{31}X$, where we associate $S = C_{2f}$, $S^2 = E$. Then

$$C^{X\Gamma}_{1\nu} = \tfrac{1}{4}\left(\tfrac{1}{16}\sum_{S\in\bar{G}^X}\psi^{X}_{1}(S^4)\psi^{*\Gamma}_{\nu}(S)+\tfrac{1}{8}\sum_{S\in\bar{Q}}\psi^{X}_{1}(S^4)X^{*\Gamma}_{\nu}(S)\right)$$

$$= \tfrac{1}{4}\left(\tfrac{1}{16}\sum_{S\in\bar{G}^X}\psi^{\Gamma}_{\nu}(S)+\tfrac{1}{8}\sum_{S\in\bar{Q}}\psi^{\Gamma}_{\nu}(S)\right),$$

giving

$$C^{\Gamma}(4) = \tfrac{1}{4}(\Gamma^1+\Gamma^{12}+\Gamma^1-\Gamma^2)$$
$$= \tfrac{1}{2}\Gamma^1-\tfrac{1}{4}\Gamma^2+\tfrac{1}{4}\Gamma^{12}.$$

Clearly none of the leading WVSRs giving X will contribute to $C^{X}(4)$.

Hence

$$H_4 = 2\Gamma^1+2\Gamma^{12}+2(X_1\uparrow G)+X_2\uparrow G.$$

Note the dimensionality checks with the result

$$^{*}X \circledS\, ^{*}X \circledS\, ^{*}X \circledS\, ^{*}X = 6\, ^{*}\boldsymbol{\Gamma}+3\, ^{*}X.$$

5. Comments on evaluation of $[\chi]^{(n)}$

Using the notion of symmetric functions on the eigenvalues of a matrix, we have the following results. (The notation adopted is that in Littlewood's book (1959).)

$$[\chi]^{(n)}(R) = h_n, \qquad \{\chi\}^{(n)}(R) = a_n$$
$$\chi(R^n) = S_n,$$

$\{\ \}$ denotes symmetrized powers. Also $\chi(R) = h_1 = a_1 = S_1$.

Then

$$m!h_m = \begin{vmatrix} S_1 & -1 & 0 & \dots 0 \\ S_2 & S_1 & -2 & \dots 0 \\ \cdot & & & \vdots \\ \cdot & & \cdot & \vdots \\ \cdot & & & 0 \\ \cdot & & -m+1 & \\ S_m & S_{m-1} & & \dots S_1 \end{vmatrix}. \tag{25}$$

This is the character relation expressing $[\chi]^{(m)}(R)$ in terms of $\chi(R^j)$, $1 \leqslant j \leqslant m$. But S_p

can be expressed entirely in terms of $h_p, h_{p-1}, \ldots, h_2, h_1$ by the determinant relation

$$S_r = (-1)^{r-1} \begin{vmatrix} h_1 & 1 & 0 & 0 & \ldots & 0 \\ 2h_2 & h_1 & 1 & 0 & \ldots & 0 \\ \cdot & & & \cdot & & \vdots \\ \cdot & & & & \cdot & 0 \\ \cdot & & & & & 1 \\ ph_p & h_{p-1} & \cdot & \cdot & \cdot & h_1 \end{vmatrix} . \tag{26}$$

By using (25) and (26), h_m can be expressed completely in terms of $h_{m-1}, h_{m-2}, \ldots, h_1$ and S_m. These results are expressed in the following lemma.

Lemma 20

For all finite dimensional representations Γ_i, character χ_i, of an arbitrary group G, the nth symmetrized power can be evaluated by examining

$$C^{ij}(n) = \frac{1}{n|G|} \sum_{R \in G} \chi_i(R^n) \chi_j^*(R)$$

only, assuming that $(n-1)$th and lower symmetrized powers are known. (That is, the $h_{n-1}, h_{n-2}, \ldots, h_1$, leaving only S_n 'unknown'.)

This gives us a convenient induction technique. Further, if the dimension of the representation Γ_i is $n-1$ or less, then $a_n = 0$, that is the nth antisymmetrized power is zero, and one can express h_n completely in terms of h_p, $p < n$ by

$$a_n = 0 = \begin{vmatrix} h_1 & 1 & 0 & 0 & \ldots & 0 \\ h_2 & h_1 & 1 & 0 & \ldots & 0 \\ \cdot & & & \cdot & & \vdots \\ \cdot & & & & \cdot & 0 \\ \cdot & & & & & 1 \\ h_n & h_{n-1} & \cdot & \cdot & \cdot & h_1 \end{vmatrix} . \tag{27}$$

This has useful consequences especially if one wishes to calculate high symmetrized powers.

6. Direct square products ($n = 2$)

The result is obtained direct from the general case. Putting $\boldsymbol{k}_1 = \boldsymbol{k}$, $\boldsymbol{k}_2 = \boldsymbol{m}$, $\boldsymbol{l} = \boldsymbol{h}$ etc, equation (22) becomes

$$C^{kmh}_{pqr} = \sum_{\alpha(\beta)}{}' \frac{|T|}{|L_\alpha|} \sum_{S \in \bar{L}_\alpha} \psi^{k}_{\alpha p}\{(S|\tau_S)\} \psi^{m}_{\beta q}\{(S|\tau_S)\} \psi^{*h}_{r}\{(S|\tau_S)\} \tag{28}$$

which is based on WVSRs $\alpha\boldsymbol{k} + \beta\boldsymbol{m} \equiv \boldsymbol{h}$. The sum is taken over the relevant leading WVSRs, and indexed by $\alpha(\beta)$ showing that β is entirely dependent on α. The symbol Σ'

serves as a reminder that the various α, β must satisfy $\alpha\boldsymbol{k}+\beta\boldsymbol{m} \equiv \boldsymbol{h}$:

$$L_\alpha = G^{\boldsymbol{h}} \wedge G^{\boldsymbol{k}}_\alpha = N_{\alpha\beta} = G^{\boldsymbol{h}} \wedge G^{\boldsymbol{k}}_\alpha \wedge G^{\boldsymbol{m}}_\beta.$$

New leading WVSRs are constructed by examining the expansions $G = \Sigma_i G^{\boldsymbol{h}}\alpha_i G^{\boldsymbol{k}}$, and $G = \Sigma_j L_\alpha \beta_j G^{\boldsymbol{m}}$. The fact that $n = 2$ obviously leads to simplifications in practical examples.

These results are identical to those of Bradley's (1966), who gave a rigorous subgroup derivation based on Mackey's work.

7. Symmetrized squares

From the general equation (24)

$$C^{\boldsymbol{kh}}_{pr}(2) = \sum_\alpha{}'' \frac{|T|}{2|L_\alpha|} \sum_{S \in \bar{Q}_\alpha} \psi^{\boldsymbol{k}}_{\alpha p}\{(S|\tau_S)^2\} \psi^{*\boldsymbol{h}}_r\{(S|\tau_S)\}.$$

Define $\bar{Q}_\alpha$ by (i) $S \in \bar{G}^{\boldsymbol{h}}$, (ii) $S^2 \in \bar{G}^{\boldsymbol{k}}_\alpha$, (iii) $\alpha\boldsymbol{k}+S\alpha\boldsymbol{k} \equiv \boldsymbol{h}$, noting that (i), (ii) or (ii), (iii) would suffice to specify $\bar{Q}_\alpha$. In fact $\bar{Q}_\alpha$ is a coset of $\bar{L}_\alpha$ in $\bar{G}^{\boldsymbol{h}}$, with $\bar{Q}_\alpha = \alpha\bar{G}^{\boldsymbol{k}}\beta^{-1} \wedge G^{\boldsymbol{h}}$.

As $[\chi]^{(2)}(R) = \frac{1}{2}(\chi^2(R)+\chi(R^2))$ the $\chi^2(R)$ being presumed 'known', then the fact that $C^{\boldsymbol{kh}}_{pr}(2)$ is sufficient to determine the problem is a trivial application of § 5.

Condition (iii) must be kept in mind when running through the leading WVSRs. Those not capable of being expressed in this form will not contribute to $C^{\boldsymbol{kh}}_{pr}(2)$.

We now draw a comparison with this form of the result, to that obtained by Bradley and Davies (1970).

8. Comparison with Bradley and Davies

Initially ideas equivalent to Bradley and Davies' (BD) self- and nonself-inverse double cosets are derived, and the notion of self- and nonself-inverse WVSRs is defined. Consider the WVSRs $\alpha\boldsymbol{k}+\beta\boldsymbol{k} \equiv \boldsymbol{h}$. This is termed a self-inverse WVSR if and only if there exists $h \in G^{\boldsymbol{h}}$ such that $h\alpha\boldsymbol{k} \equiv \beta\boldsymbol{k}$. This implies $G^{\boldsymbol{h}}\alpha G^{\boldsymbol{k}} = G^{\boldsymbol{h}}\beta G^{\boldsymbol{k}}$ and can be taken as a criterion for interchangeability of the coset representatives within the WVSR framework (cf lemma 17).

Now $G^{\boldsymbol{h}}\alpha G^{\boldsymbol{k}} = G^{\boldsymbol{h}}\beta G^{\boldsymbol{k}}$ implies $G^{\boldsymbol{k}}\alpha^{-1}G^{\boldsymbol{h}} = G^{\boldsymbol{k}}\beta^{-1}G^{\boldsymbol{h}}$. So, there exists a $k' \in G^{\boldsymbol{k}}$ such that $k'\alpha^{-1}\boldsymbol{h} \equiv \beta^{-1}\boldsymbol{h}$. Rewrite $\alpha\boldsymbol{k}+\beta\boldsymbol{k} \equiv \boldsymbol{h}$ as $\boldsymbol{k}+\alpha^{-1}\beta\boldsymbol{k} \equiv \boldsymbol{h}$ or as $\beta^{-1}\alpha\boldsymbol{k}+\boldsymbol{k} \equiv \beta^{-1}\boldsymbol{h}$ and we can quickly see that we must have $G^{\boldsymbol{k}}\alpha^{-1}\beta G^{\boldsymbol{k}} = G^{\boldsymbol{k}}\beta^{-1}\alpha G^{\boldsymbol{k}}$, that is, a self-inverse double coset (cf BD).

Similarly a nonself-inverse WVSR implies $G^{\boldsymbol{h}}\alpha G^{\boldsymbol{k}} \neq G^{\boldsymbol{h}}\beta G^{\boldsymbol{k}}$ and consequently $G^{\boldsymbol{k}}\alpha^{-1}\beta G^{\boldsymbol{k}} \neq G^{\boldsymbol{k}}\beta^{-1}\alpha G^{\boldsymbol{k}}$ a nonself-inverse double coset.

Hence we have established a direct link between the two ideas.

Clearly $G^{\boldsymbol{k}}\alpha^{-1}\beta G^{\boldsymbol{k}} = G^{\boldsymbol{k}}\beta^{-1}\alpha G^{\boldsymbol{k}}$ is a necessary and sufficient condition for $\alpha G^{\boldsymbol{k}}\beta^{-1} \wedge G^{\boldsymbol{h}} = Q_\alpha$ to be non-empty. Similarly $G^{\boldsymbol{h}}\alpha G^{\boldsymbol{k}} = G^{\boldsymbol{h}}\beta G^{\boldsymbol{k}}$ implies $G^{\boldsymbol{h}} \wedge \beta G^{\boldsymbol{k}}\alpha^{-1}$ and $G^{\boldsymbol{h}} \wedge \alpha G^{\boldsymbol{k}}\beta^{-1}$ are non-empty, implying Q_α is non-empty.

The method of BD can be regarded as a 'fixed $\boldsymbol{k}$' approach, whereas the results here can be termed a 'fixed $\boldsymbol{h}$' approach. With the above observations the two approaches can be easily reconciled.

9. Symmetrized cubes

From the general theory, equation (24) gives

$$C_{p\nu}^{kl}(3) = \tfrac{1}{3}\sum_{(\beta)}'' \frac{|T|}{|N_{\beta_1\beta_2\beta_3}|} \sum_{S\in\bar{Q}_{(\beta)}} \psi_{\beta_1 p}^{k}\{(S|\tau_S)^3\}\,\psi_{\nu}^{*l}\{(S|\tau_S)\}, \tag{29}$$

$\bar{Q}_{(\beta)} = \bar{Q}_{\beta_1(\beta_2\beta_3)}$ defined by: (i) $S^3 \in \bar{G}^k_{\beta_1}$, (ii) $S \in \bar{G}^l$; (iii) $(1+S+S^2)\beta_1 \boldsymbol{k} \equiv \boldsymbol{l}$ and we can write

$$\bar{Q}_{\beta_1(\beta_2\beta_3)} = (132)\bar{N}_{\beta_1\beta_2\beta_3} = \beta_1\bar{G}^k\beta_3^{-1} \wedge \beta_3\bar{G}^k\beta_2^{-1} \wedge \beta_2\bar{G}^k\beta_1^{-1}.$$

In this case $\bar{Q}_{(\beta)} \neq \phi$ only if (cf lemmas 15, 16, 17): (i) $\beta_1 G^k = \beta_2 G^k = \beta_3 G^k$ or (ii) $\beta_1 G^k$, $\beta_2 G^k$, $\beta_3 G^k$ are all different cosets of G^k within the double coset $G^l\beta_1 G^k$. Hence $|G^l|/|G^l \wedge G^k_{\beta_1}| \geqslant 3$.

Note: (*a*) there could be several leading WVSRs with the same value of β_1. (*b*) If $S \in \bar{Q}_{(\beta)}$, then $S^2 \in \bar{Q}'(\beta)$, which performs a (123) permutation on the coset representatives in the WVSR $\beta_1\boldsymbol{k}+\beta_2\boldsymbol{k}+\beta_3\boldsymbol{k} \equiv \boldsymbol{l}$:

$$\bar{Q}'_{(\beta)} = \beta_1\bar{G}^k\beta_2^{-1} \wedge \beta_2\bar{G}^k\beta_3^{-1} \wedge \beta_3\bar{G}^k\beta_1^{-1}$$

and is also a coset of $\bar{N}_{\beta_1\beta_2\beta_3}$ with respect to $\bar{G}^l$. $\bar{Q}' \neq Q$ unless $S \in G^k_{\beta_1}$. (*c*) There is no necessity for $(1+S+S^2)\beta_1\boldsymbol{k} \equiv \boldsymbol{l}$ and $(1+S^2+S)\beta_1\boldsymbol{k} = \boldsymbol{l}$ to be related; indeed they could be different leading WVSRs.

Lemma 21.

If $S \in \bar{Q}_{(\beta)}$, then $S^{3p} = E$, (p integer).

Proof.

Assume this is not true, then:

(*a*) ∃ integer x such that $S^x = E$, with $x = 1$ (mod 3) or (*b*) ∃ integer y such that $S^y = E$ with $y = 2$ (mod 3). For (*a*) $S^x = E = S^{3m+1}$, m integer. But as $S^3 \in G^k_{\beta_1}$ then $S^{3m} \in G^k_{\beta_1}$, implying $S^x \in SG^k_{\beta_1}$ a contradiction. Similarly for (*b*). Hence $S^{3p} = E$.

This is sometimes of use in practical examples, for instance, if G^l does not contain a three-fold rotational element, then $\bar{Q}_{(\beta)}$ is automatically empty.

The full problem is evaluated by noting (see § 5)

$$[\chi_i]^{(3)}(R) = \tfrac{1}{2}\chi_i(R)(\chi_i^2(R)+\chi_i(R^2))+\tfrac{1}{3}\chi_i(R^3)-\tfrac{1}{3}\chi_i^3(R).$$

Hence

$$\Gamma_i \circledS \Gamma_i \circledS \Gamma_i = \Gamma_i \otimes [\Gamma_i \circledS \Gamma_i] - \tfrac{1}{3}(\Gamma_i \otimes \Gamma_i \otimes \Gamma_i) + \sum_j C^{ij}(3)\Gamma_j, \tag{30}$$

Γ_i is the representation, χ_i the character.

As an example we briefly outline a calculation based on the space group $Fd3m$. See Davies and Lewis (1971) for the notation, tables and references.

Now $^{\star}\boldsymbol{X} \otimes {}^{\star}\boldsymbol{X} \otimes {}^{\star}\boldsymbol{X} = 6\,{}^{\star}\boldsymbol{\Gamma} + 7\,{}^{\star}\boldsymbol{X}$, and $^{\star}\boldsymbol{X} \circledS {}^{\star}\boldsymbol{X} \circledS {}^{\star}\boldsymbol{X} = {}^{\star}\boldsymbol{\Gamma} + 3\,{}^{\star}\boldsymbol{X}$. Therefore to calculate $(X_2 \uparrow G) \circledS (X_2 \uparrow G) \circledS (X_2 \uparrow G)$, $\boldsymbol{l}$ can be $\boldsymbol{\Gamma}$ or X. $G = (E, C_{31}^+, C_{31}^-)G^{\boldsymbol{X}}$.

For $\boldsymbol{l} = \boldsymbol{\Gamma}$ a leading WVSR is $\boldsymbol{X} + C_{31}^+\boldsymbol{X} + C_{31}^-\boldsymbol{X} \equiv \boldsymbol{\Gamma}$.

$\bar{Q}_{(\beta)} = (C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-) \otimes (E, I)$, $\qquad N_{\beta_1\beta_2\beta_3} = (E, C_{2x}, C_{2y}, C_{2z}) \otimes (E, I)$.

Now as $n_{\boldsymbol{\Gamma}} = 6$, and $(|G^{\boldsymbol{\Gamma}}|/|N_{\beta_1\beta_2\beta_3}|) = 6$, only one leading WVSR is needed.

So equation (29) becomes

$$C_{2v}^{X\Gamma}(3) = \frac{1}{3}\frac{1}{|\bar{N}_{\beta_1\beta_2\beta_3}|}\sum_{S\in\bar{Q}_{(\beta)}} \psi_2^X\{(S|\tau_S)^3\}\,\psi_v^{*\Gamma}\{S|\tau_S)\}.$$

The 'Γ' contribution is thus $C^\Gamma(3) = \frac{1}{3}(\Gamma^{1\pm}+\Gamma^{2\pm}-\Gamma^{12\pm})$.

For $l = X$, we have 4 leading WVSRs $X+X+X$, $C_{31}^+X+C_{31}^+X+X$, $C_{31}^+X+X+C_{31}^+X$, $X+C_{31}^+X+C_{31}^+X$. (Note $G = G^XEG^X+G^X(C_{31}^+, C_{31}^-)G^X$). Clearly only the first of these will contribute; and for this $\bar{Q}_{(\beta)} = \bar{N}_{\beta_1\beta_2\beta_3} = \bar{G}^X$. Therefore

$$C_{2v}^{XX}(3) = \frac{1}{48}\sum_{S\in\bar{G}^X} \psi_2^X\{(S|\tau_S)^3\}\psi_v^{*X}\{(S|\tau_S)\}.$$

The total 'X' contribution $C^X(3) = \frac{1}{3}(X_2 \uparrow G)$

$$C^\Gamma(3)+C^X(3) = \tfrac{1}{3}(\Gamma^{1\pm}+\Gamma^{2\pm}-\Gamma^{12\pm}+X_2\uparrow G).$$

Now $(X_2\uparrow G)\otimes(X_2\uparrow G)\otimes(X_2\uparrow G)$ and $-\frac{1}{3}(X_2\uparrow G)\otimes[(X_2\uparrow G)\circledS(X_2\uparrow G)]$ can be easily obtained from known tables.

Finally using (30) where $\Sigma_j C^{ij}(3)\Gamma_j = C^\Gamma(3)+C^X(3)$

$$(X_2\uparrow G)\circledS(X_2\uparrow G)\circledS(X_2\uparrow G) = \Gamma^{1-}+\Gamma^{2+}+\Gamma^{15+}+\Gamma^{25-}+2(X_1\uparrow G) +4(X_2\uparrow G)+X_3\uparrow G+X_4\uparrow G.$$

10. Discussion

The calculation of selection rules for crystallographic processes is a well known problem, and in this paper subgroup formulae have been derived from the standard full-group formulation. As mentioned, this is in contrast to the subgroup technique used by Bradley (1966) and Bradley and Davies (1970) in adapting Mackey's work on direct and symmetrized squares.

Zak (1966) was the first to make an attempt at deriving subgroup formulae from the fullgroup approach, and the error in his work (on direct squares) is corrected here by including a completeness relation (see § 3). Hence the notion of a double coset is introduced and its utility in practical examples is evident, (eg the diagrams in §§ 3, 4) especially in the work on symmetrized powers. Streitwolf (1969) has also derived results from $n = 2$ using a similar approach to this paper. Raghavacharyulu (1964) also obtains formulae of a similar type, but his work contains some errors, for example equation A, p 10, and equation 22, p 15.

The general case (arbitrary n) proved illuminating in that the method emphasized the similarities between the problem for symmetrized squares and symmetrized cubes, and demonstrated its usefulness in that only one term (the $\chi(R^n)$) remains to be evaluated (see § 5).

For higher power calculations, the facility of choosing leading WVSRs is crucial to the practicality of the method. The double coset diagrams of §§ 3, 4 could often get too unwieldy to handle (especially for points of low symmetry in the Brillouin zone), and the optimum approach in solving an actual problem is to keep in mind both subgroup and full-group approaches, the latter outlined by Birman (1962). Of course, one also has to keep in mind possible 'short cuts' in all cases. For example, in the text we used

${}^{\star}W \otimes {}^{\star}W \otimes {}^{\star}W$ with $A = G^{\mathrm{A}}$, which has 44 leading WVSRS, of which only 3 are needed for the relevant portion of the sum. These can often be chosen by a more *ad hoc* approach; the general method only to be relied upon in difficult situations.

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References

Birman J L 1962 *Phys. Rev.* **127** 1093
Bradley C J 1966 *J math. Phys.* **7** 1145
Bradley C J and Davies B L 1970 *J math. Phys.* **11** 1536
Chen L-C, Berenson R and Birman J L 1968 *Phys. Rev.* **170** 639
Davies B L and Lewis D H 1971 *Phys. Stat. Solidi* A **7** 523
Littlewood D E 1959 *A University Algebra* (London: Heinemann) chap 5
Raghavacharyulu I V V 1964 *Quantum Chemistry Group, Uppsala University, Preprint* No 116
Streitwolf H W 1969 *Phys. Stat. Solids* B **33** 217
Zak J 1966 *Phys. Rev.* **151** 464