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Symmetrized *n*th powers of space group representations

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Abstract. This paper outlines the way in which the constructive method obtained for symmetrizing *n*th Kronecker powers of induced representations may be applied to space group representations. Also a step by step procedure is given for finding the symmetrized cubes of space group representations, with zinc-blende as an example, which may be used independently of the general theory.

1. Introduction

In a previous paper (Gard 1973, to be referred to as I), a constructive method was given for the reduction of the *n*th Kronecker power of an induced representation into its symmetry classes with respect to the symmetric group S_n. Here, we apply the theory directly to space group representations. This method should be compared with that of Lewis (1973) who has solved the particular problem of obtaining the totally symmetric and antisymmetric *n*th powers of a space group representation, that is the ones corresponding to the identity and alternating representations of S_n, respectively, by adapting a full group method. The subgroup technique has already been used by Bradley and Davies (1970) to work out the symmetrized squares of space group representations and so we may concentrate on giving a step by step procedure for obtaining the symmetrized cubes. This will also serve as a working example for those who may wish to apply the general results of I to find the symmetrized representations of a group corresponding to all the other representations of S_n.

In § 2 we make some remarks of a general nature about the application of the results of I to space group representations, and in § 3 we restrict attention to the case $n = 3$ and give a procedure for finding the symmetrized cubes. This is given in detail for those who may not wish to read I beyond § 1. An example is given in § 4. We conclude by comparing our method for finding totally symmetrized powers with that of Lewis (1973).

2. Space group representations

From the theory of little groups, we know that a complete set of irreducible representations of the space group G is given by $\{D_p^k \uparrow G\}$, where k is any vector in the representation domain of the first BZ (Brillouin zone) and p is a label for the particular small representation D_p^k of the little group $K = G^k$. The representation domain Φ is defined by Bradley and Cracknell (1972) to be the minimal connected subspace of the BZ such that $\Sigma_{R\in F} R\Phi$ is the whole BZ, where F is the point group corresponding to the space group G. More details about space group representations may be found in the review article by Koster (1957) and the book by Bradley and Cracknell (1972).

Suppose we wish to find the symmetrized nth power of $(D_p^k \uparrow G)$. For convenience we shall suppress the index p. First we work out a complete set of double coset representatives as defined by equation (1.8) of I which are in the standard form described immediately after theorem (2.3) of I. Consider a particular n-tuple (α) with $d_{\alpha_0} = \{E|\mathbf{0}\}$, $d_{\alpha_i} = \{R_i|\boldsymbol{w}_i\} \in \boldsymbol{G}$, where $R_i \in \boldsymbol{F}$ and $\boldsymbol{w}_i$ is either a nonprimitive translation or the zero vector $(i = 1, \ldots, n-1)$. The carrier space of the representation

$$(D^k_{\alpha_{n-1}} \otimes D^k_{\alpha_{n-2}} \otimes \ldots \otimes D^k) \downarrow \boldsymbol{K}_{n-1},$$

where $D_\alpha^k(d_\alpha l d_\alpha^{-1}) = D^k(l)$ for all $l \in \boldsymbol{G}^k$, carries a direct sum of a fixed representation of the discrete translation group $\boldsymbol{T}_3$ associated with the vector

$$\boldsymbol{q} = R_{n-1}\boldsymbol{k} + R_{n-2}\boldsymbol{k} + \ldots + R_1\boldsymbol{k} + \boldsymbol{k}.$$

Now $\boldsymbol{K}_{n-1} \subset \boldsymbol{G}^{\boldsymbol{q}}$, so in order to obtain a decomposition in terms of irreducibles, we may induce the representation of $\boldsymbol{G}$ by stages through $\boldsymbol{G}^{\boldsymbol{q}}$. This is possible in all cases since, using the notation of I,

$$P(\pi)\Delta(a_\pi^{-1} l a_\pi)P(\pi)^{-1} = \Delta(l) \tag{2.1}$$

for all $l \in \boldsymbol{K}_{n-1}$ and hence the group $\boldsymbol{M}$, defined in theorem (3.7) of I, is also contained in $\boldsymbol{G}^{\boldsymbol{q}}$. This result considerably simplifies the problem of decomposing the symmetrized powers into irreducibles.

By a consideration of the induction procedure, it follows that if $\boldsymbol{G}$ is symmorphic we need only induce the representation of the factor group $\overline{\boldsymbol{M}} = \boldsymbol{M}/\boldsymbol{T}_3$ up to $\overline{\boldsymbol{G}}^{\boldsymbol{q}}$ to obtain a representation containing small representations of the little group. The procedure for inducing is given by Bradley (1966). If the space group is asymmorphic, then it can be shown that inducing a representation of $\boldsymbol{M}$ up to $\boldsymbol{G}^{\boldsymbol{q}}$ is equivalent to inducing a projective representation of $\overline{\boldsymbol{M}}$ up to $\overline{\boldsymbol{G}}^{\boldsymbol{q}}$, and for each element $\{R|\boldsymbol{v}\} \in \boldsymbol{G}^{\boldsymbol{q}}$, multiplying the result by $\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{v})$. A complete set of tables of projective representations of three-dimensional point groups is given by Hurley (1966) and a formula for inducing projective representations is given by Backhouse and Bradley (1970). If the vector $\boldsymbol{q}$ is not equivalent to a vector in the representation domain, then the space group representation will not be given in standard form. We must apply an automorphism, as in the proof of theorem (3.1) of I, so that the transform of $\boldsymbol{q}$ is in the representation domain. This will be illustrated in the example given in § 4.

3. Prescription for symmetrized cubes

We now give a prescription for obtaining symmetrized cubes of space group representations. This may be read independently of paper I although a knowledge of the introduction may be found useful.

Let $\boldsymbol{G}$ be a space group and let $\boldsymbol{K} = \boldsymbol{G}^k$ be a little group with small representation D_p^k. We give a procedure for decomposing $(D_p^k \uparrow G) \otimes (D_p^k \uparrow G) \otimes (D_p^k \uparrow G)$ into its symmetrized powers. As before we shall suppress the index p.

(i) Work out a complete set $A_1 = \{d_{\alpha_1}\}$ of double coset representatives

$$\boldsymbol{G} = \bigcup_{\alpha_1} \boldsymbol{K} d_{\alpha_1} \boldsymbol{K}.$$

It is necessary to take one double coset representative to be $\{E|\mathbf{0}\}$. More details about double coset representatives may be found in Bradley (1966).

(ii) For *each* $d_{\alpha_1} \in A_1$, form the subgroup $\boldsymbol{K}_1(\alpha_1) = \boldsymbol{K} \cap d_{\alpha_1}\boldsymbol{K}d_{\alpha_1}^{-1}$ and work out a new set $A_2(\alpha_1) = \{d_{\alpha_2}\}$ of double coset representatives such that

$$\boldsymbol{G} = \bigcup_{\alpha_2} \boldsymbol{K}_1(\alpha_1)d_{\alpha_2}\boldsymbol{K}$$

which includes the previous set A_1.

In this way we obtain a complete set of standard triplets $(\alpha) = (d_{\alpha_2}, d_{\alpha_1}, d_{\alpha_0})$ for the Mackey decomposition given by equation (1.12) of I, where $d_{\alpha_0} = \{E|\mathbf{0}\}$, $d_{\alpha_1} \in A_1$ and $d_{\alpha_2} \in A_2(\alpha_1)$.

(iii) Form the triplets into orbits under the action of the symmetric group $\boldsymbol{S}_3$ by applying permutations to the positions of the elements in the triplet. Write the new triplets obtained in the usual form so that $(d_{\alpha_{\pi(2)}}, d_{\alpha_{\pi(1)}}, d_{\alpha_{\pi(0)}})$ becomes $(d_{\alpha_{\pi(0)}}^{-1}d_{\alpha_{\pi(2)}}, d_{\alpha_{\pi(0)}}^{-1}d_{\alpha_{\pi(1)}}, \{E|\mathbf{0}\})$. Reduce this to a standard triplet (β) by finding elements $p_0, k_0 \in \boldsymbol{K}$ such that $p_0 d_{\alpha_{\pi(0)}}^{-1}d_{\alpha_{\pi(1)}}k_0 = d_{\beta_1} \in A_1$ and elements $k_1 \in \boldsymbol{K}$, $p_1 \in \boldsymbol{K} \cap d_{\beta_1}\boldsymbol{K}d_{\beta_1}^{-1}$ such that $p_1 p_0 d_{\alpha_{\pi(0)}}^{-1}d_{\alpha_{\pi(2)}}k_1 = d_{\beta_2} \in A_2(\beta_1)$. This is in accordance with the definition of the equivalence relation $\sim$ given by equation (2.1) of I. Then $(\{E|\mathbf{0}\}, \{E|\mathbf{0}\}, \{E|\mathbf{0}\})$ will form an orbit on its own. For a triplet with two entries the same, it follows from theorem (3.5) of I that the orbit will have order three. Finally, if the three entries in the triplet are distinct, the orbit may have order 1, 2, 3 or 6.

(iv) Suppose $d_{\alpha_1} = \{R_1|\boldsymbol{w}_1\}$, $d_{\alpha_2} = \{R_2|\boldsymbol{w}_2\}$, where $R_1, R_2 \in \boldsymbol{F}$ and $\boldsymbol{w}_1, \boldsymbol{w}_2$ are either nonprimitive translations or the zero vector. With each standard triplet (α) we associate the vector $\boldsymbol{q} = \boldsymbol{k} + R_1\boldsymbol{k} + R_2\boldsymbol{k}$ in the BZ. All vectors associated with triplets of a given orbit belong to the same star and so, wherever possible, we choose the representative (α) of the orbit so that the corresponding vector $\boldsymbol{q}$ is equivalent to one in the representation domain.

Having completed the analysis of the double coset representatives as described above, the next step is to apply the theory of I to *one* representative (α) from each orbit to work out the symmetrized representations. We denote the three symmetry classes by $\Omega^{[3]}$, $\Omega^{[2,1]}$ and $\Omega^{[1^3]}$ where $[3]$, $[1^3]$ are the identity and alternating representations of $\boldsymbol{S}_3$, respectively. They carry representations $\Gamma^{[3]}$, $\Gamma^{[2,1]}$ and $\Gamma^{[1^3]}$ respectively. Note, we have defined $\Omega^{[2,1]}$ so that the whole space $\Omega = \Omega^{[3]} \oplus \Omega^{[2,1]} \oplus \Omega^{[1^3]}$.

(v) If $d_{\alpha_2} = d_{\alpha_1} = d_{\alpha_0} = \{E|\mathbf{0}\}$, then $\boldsymbol{S}_3(\alpha) = \boldsymbol{E}_3(\alpha) = \boldsymbol{S}_3$ and so, by equation (6.28) of I,

$$\Gamma^{[3]} \text{ contains } (D^{\boldsymbol{k}})^{[3]} \uparrow \boldsymbol{G},$$

$$\Gamma^{[2,1]} \text{ contains } 2(D^{\boldsymbol{k}})^{[2,1]} \uparrow \boldsymbol{G},$$

$$\Gamma^{[1^3]} \text{ contains } (D^{\boldsymbol{k}})^{[1^3]} \uparrow \boldsymbol{G},$$

where $(D^{\boldsymbol{k}})^{[3]}$ means the totally symmetrized cube of $D^{\boldsymbol{k}}$, etc. The characters of powers of a representation are to be found in Lyubarskii (1960).

(vi) If $d_{\alpha_r} = d_{\alpha_s} \neq d_{\alpha_t}$, where $r, s, t \in \{0, 1, 2\}$, $r \neq s \neq t$, then $\boldsymbol{S}_3(\alpha) = \boldsymbol{E}_3(\alpha) \cong \boldsymbol{S}_2$ and so

$$\Gamma^{[3]} \text{ contains } \{[(D^{\boldsymbol{k}}_{\alpha_r})^{[2]} \otimes D^{\boldsymbol{k}}_{\alpha_t}] \downarrow \boldsymbol{K}_2\} \uparrow \boldsymbol{G}.$$

$$\Gamma^{[2,1]} \text{ contains } 2[(D^{\boldsymbol{k}}_{\alpha_r} \otimes D^{\boldsymbol{k}}_{\alpha_r} \otimes D^{\boldsymbol{k}}_{\alpha_t}) \downarrow \boldsymbol{K}_2] \uparrow \boldsymbol{G},$$

$$\Gamma^{[1^3]} \text{ contains } \{[(D^{\boldsymbol{k}}_{\alpha_r})^{[1^2]} \otimes D^{\boldsymbol{k}}_{\alpha_t}] \downarrow \boldsymbol{K}_2\} \uparrow \boldsymbol{G},$$

where $\boldsymbol{K}_2 = \boldsymbol{K} \cap d_{\alpha_1}\boldsymbol{K}d_{\alpha_1}^{-1} \cap d_{\alpha_2}\boldsymbol{K}d_{\alpha_2}^{-1}$.

(vii) If all the double coset representatives are distinct, apply the theory given in § 5 of I:

(*a*) If the orbit has order 6, then $S_3(\alpha) = E_3(\alpha) = \{1\}$ and

$$\Gamma^{[3]} \text{ contains } [(D^k_{\alpha_2} \otimes D^k_{\alpha_1} \otimes D^k)\downarrow K_2]\uparrow G,$$

$$\Gamma^{[2,1]} \text{ contains } 4[(D^k_{\alpha_2} \otimes D^k_{\alpha_1} \otimes D^k)\downarrow K_2]\uparrow G,$$

$$\Gamma^{[1^3]} \text{ contains } [(D^k_{\alpha_2} \otimes D^k_{\alpha_1} \otimes D^k)\downarrow K_2]\uparrow G.$$

(*b*) If the orbit has order 3, find

$$a \in K \cap d_{\alpha_2} K d_{\alpha_1}^{-1} \cap d_{\alpha_1} K d_{\alpha_2}^{-1}$$

and induce up to the group M generated by $K_2(\alpha)$ and a. We write $M = \langle K_2(\alpha), a\rangle$.

(*c*) If the orbit has order 2, find

$$b \in K d_{\alpha_1}^{-1} \cap d_{\alpha_2} K \cap d_{\alpha_1} K d_{\alpha_2}^{-1}$$

and induce up to $M = \langle K_2(\alpha), b\rangle$.

(*d*) If the orbit has order 1, we find a, b as defined above and induce up to

$$M = \langle K_2(\alpha), a, b\rangle.$$

In cases (*b*), (*c*) and (*d*) the representation of the group M is given by equation (5.14) of I. Hence the characters at the appropriate elements of the group M are given by

$$\theta^{\pm}(l) = \chi(l)\chi(d_{\alpha_1}^{-1} l d_{\alpha_1})\chi(d_{\alpha_2}^{-1} l d_{\alpha_2})$$

$$\theta^{\pm}(bl) = \chi[(bl)^3]$$

$$\theta^{\pm}(b^2 l) = \chi[(b^2 l)^3]$$

$$\theta^{\pm}(al) = \pm\chi(al)\chi[d_{\alpha_1}^{-1}(al)^2 d_{\alpha_1}]$$

$$\theta^{\pm}(abl) = \pm\chi[d_{\alpha_2}^{-1}(abl)d_{\alpha_2}]\chi[(abl)^2]$$

$$\theta^{\pm}(ab^2 l) = \pm\chi[d_{\alpha_1}^{-1}(ab^2 l)d_{\alpha_1}]\chi[(ab^2 l)^2],$$

where $\theta^{\pm}$ are the characters of the totally symmetrized and antisymmetrized cubes on M, χ is the character of the small representation D^k_p, and $l \in K_2(\alpha)$. Hence $\Gamma^{[3]}$ and $\Gamma^{[1^3]}$ contain representations with characters $\theta^{\pm}\uparrow G$, respectively.

In case (vii) (*b*), (*c*), (*d*) the remaining contribution to $\Gamma^{[2,1]}$ is obtained as follows: with the element $a \in M$ associate the transposition $\pi_a = (1\ 2) \in S_3$, and with $b \in M$ associate the cycle $\pi_b = (1\ 0\ 2) \in S_3$ (see theorem (3.6) of I). Any element of K_2 is associated with the identity operation and so the coset abK_2 corresponds to the permutation

$$\pi_{ab} = (1\ 2)(1\ 0\ 2) = (1\ 0) \quad \text{etc}$$

where the multiplication is from right to left in accordance with the action of the elements of M on the triplets. To obtain the character $\theta^{[\nu]}(m)$ of $m \in M$, multiply $\theta^+(m)$ by $f_\nu[\nu](\pi_m)$ where $f_\nu = \dim[\nu]$. The character table of S_3 may be found in Hamermesh (1964, chap 7). So if $[\nu] = [1^3]$, then $f_\nu = 1$ and $[\nu](\pi_m) = (-1)^{\pi_m}$ as obtained above. If $[\nu] = [2, 1]$, then $f_\nu = 2$ and so

$$\theta^{[2,1]}(l) = 4\theta^+(l)$$

$$\theta^{[2,1]}(bl) = -2\theta^+(bl)$$

$$\theta^{[2,1]}(b^2 l) = -2\theta^+(b^2 l).$$

The value of the character is zero on the remaining elements of M. The representation $\Gamma^{[2,1]}$ contains a representation with character $\theta^{[2,1]} \uparrow G$.

This method may also be used to work out the Kronecker cube of a space group representation. Take *one* representative (α) from each orbit and work out

$$[(D^{k}_{\alpha_2} \otimes D^{k}_{\alpha_1} \otimes D^{k}) \downarrow K_2] \uparrow G.$$

Then the cube contains this representation t times, where t is the order of the orbit. This provides a partial check of the results computed for symmetrized cubes of a given representation since the sum of the contributions to the symmetrized representations from a given orbit is the same as the contribution to the cube.

As noted in § 2, if we wish to express the symmetrized power as a sum of irreducible representations of G, we induce the representation of M through the little group G^{q} and reduce at this stage. To obtain the space group representations in standard form, it may be necessary to conjugate the elements of G^{q} to obtain a character of

$$G^{Rq} = \{R|v\}G^{q}\{R|v\}^{-1},$$

where Rq is equivalent to a vector in the representation domain. It follows from the theory of induced representations that this leads to an equivalent representation of G.

4. Example

Take G to be the space group T_{d}^{2} corresponding to the zinc-blende structure. This is the same example as that used by Bradley and Davies (1970) to discuss the case $n = 2$. The notation for the elements of the cubic group is given by Altmann and Cracknell (1965).

The direct lattice for zinc-blende is face-centred cubic with basic translation vectors

$$t_1 = \tfrac{1}{2}a(0, 1, 1), \qquad t_2 = \tfrac{1}{2}a(1, 0, 1), \qquad t_3 = \tfrac{1}{2}a(1, 1, 0),$$

where a is the length of a cube edge. The corresponding reciprocal lattice vectors are

$$g_1 = \frac{2\pi}{a}(-1, 1, 1), \qquad g_2 = \frac{2\pi}{a}(1, -1, 1), \qquad g_3 = \frac{2\pi}{a}(1, 1, -1).$$

Let k be any vector in reciprocal space, then we write

$$k = (\lambda, \mu, \nu) = \lambda g_1 + \mu g_2 + \nu g_3.$$

We shall consider the point of symmetry $L(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$ which has little cogroup

$$C_{3v} = \{E, C_{31}^{+}, C_{31}^{-}, \sigma_{db}, \sigma_{de}, \sigma_{df}\}.$$

Note that we are using the active convention whereby the group elements move the field and leave the axes fixed. A picture of the Brillouin zone for T_{d}^{2} with all the special points and lines marked is figure (3.14) of Bradley and Cracknell (1972). It is also possible to adapt their table (1.5) to obtain a group multiplication table for the point group T_d by the substitution $C_{2p} \rightarrow IC_{2p} = \sigma_{dp}$ $(p = a, b, \ldots, f)$ and $C_{4m}^{\pm} \rightarrow IC_{4m}^{\pm} = S_{4m}^{\mp}$ $(m = x, y, z)$, where I is the inversion operator.

The character table of the point group C_{3v} is:

L	E	$C_{31}^{\pm}$	$\{\sigma_{db}, \sigma_{de}, \sigma_{df}\}$
L^1	1	1	1
L^2	1	1	-1
L^3	2	-1	0

A standard set of double coset representatives is the following:

	d_{α_0}	d_{α_1}	d_{α_2}	q	$\bar{K}_1(\alpha_1)$	$\bar{K}_2(\alpha)$
(i)	E	E	E	k_L	C_{3v}	C_{3v}
(ii)	E	E	C_{2x}	$C_{2x}k_L$	$\{E, \sigma_{df}\}$	$\{E, \sigma_{df}\}$
	E	C_{2x}	E	$C_{2x}k_L$	$\{E, \sigma_{df}\}$	$\{E, \sigma_{df}\}$
	E	C_{2x}	C_{2x}	k_L	$\{E, \sigma_{df}\}$	$\{E, \sigma_{df}\}$
(iii)	E	C_{2x}	S_{4x}^{+}	$S_{4x}^{-}k_L$	$\{E, \sigma_{df}\}$	$\{E\}$

The vector q may be found by using the picture of the BZ directly. Alternatively, the action of R_i on $k = (\lambda, \mu, \nu)$ is given in table (3.4) of Bradley and Cracknell (1972). It is a peculiarity of this example that all the orbits are associated with the vector k_L.

In case (i) we apply the results of § 3(v). If $D^k = L^1$, then $\Gamma^{[3]}$ contains $L^1 \uparrow G$ and there is no contribution to $\Gamma^{[2,1]}$ and $\Gamma^{[1^3]}$. In fact it is true that if D^k is one dimensional there is only a contribution to $\Gamma^{[3]}$. Hence, if $D^k = L^2$, then $\Gamma^{[3]}$ contains $L^2 \uparrow G$, only. If $D^k = L^3$, then $\Gamma^{[3]}$ contains $(L^1 \uparrow G) + (L^2 \uparrow G) + (L^3 \uparrow G)$, $\Gamma^{[2,1]}$ contains $2(L^3 \uparrow G)$ and there is no contribution to $\Gamma^{[1^3]}$.

In case (ii) we have an orbit of order 3 resulting from the action of S_3 on (C_{2x}, E, E). Note that $(0\,2)(C_{2x}, E, E) = (E, E, C_{2x})$, and multiplying through by C_{2x}, to obtain E in the zeroth place, gives the triplet (C_{2x}, C_{2x}, E) which is already in standard form. We choose this as the representative triplet of the orbit since the associated vector $q = C_{2x}k_L + C_{2x}k_L + k_L = (0, \frac{1}{2}, 0) + (0, \frac{1}{2}, 0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \equiv k_L$, and k_L is in the representation domain. We apply the results of § 3(vi). If $D^k = L^1$, then $\Gamma^{[3]}$ contains $(L^1 \uparrow G) + (L^3 \uparrow G)$ and $\Gamma^{[2,1]}$ contains $2(L^1 \uparrow G)$. If $D^k = L^2$, then $\Gamma^{[3]}$ contains $(L^2 \uparrow G) + (L^3 \uparrow G)$ and $\Gamma^{[2,1]}$ contains $2(L^2 \uparrow G)$. In both cases there is no contribution to $\Gamma^{[1^3]}$. If $D^k = L^3$, then $\Gamma^{[3]}$ contains $3(\text{reg } L) \uparrow G$ where $\text{reg } L = L^1 + L^2 + 2L^3$ is the regular representation of C_{3v}. $\Gamma^{[2,1]}$ contains $8(\text{reg } L) \uparrow G$ and $\Gamma^{[1^3]}$ contains $(\text{reg } L) \uparrow G$.

Case (iii) provides an example of a vector q which is not in the representation domain. We apply the results of § 3(vii, d) and it can be checked that we may take $a = \sigma_{de}$ and $b = C_{34}^{-}$. The characters of the symmetrized representations of M are as follows:

	E	$C_{34}^{\pm}$	$\{\sigma_{dd}, \sigma_{de}, \sigma_{da}\}$
$L^1 \rightarrow$	1	1	1
	4	-2	0
	1	1	-1
$L^2 \rightarrow$	1	1	-1
	4	-2	0
	1	1	1

$$L^3 \rightarrow \begin{cases} \begin{matrix} E & C_{34}^{\pm} & \{\sigma_{dd}, \sigma_{de}, \sigma_{da}\} \\ 8 & 2 & 0 \\ 32 & -4 & 0 \\ 8 & 2 & 0 \end{matrix} \end{cases}$$

The rows correspond to the representations [3], [2, 1] and $[1^3]$ respectively. But $G^L = S_{4x}^{+} M S_{4x}^{-}$, so we obtain character tables for G^L by conjugating the elements of M by S_{4x}^{+} in the above tables. If $D^k = L^1$, then $\Gamma^{[3]}$ contains $(L^1 \uparrow G)$, $\Gamma^{[2,1]}$ contains $2(L^3 \uparrow G)$ and $\Gamma^{[1^3]}$ contains $(L^2 \uparrow G)$. If $D^k = L^2$, then $\Gamma^{[3]}$ contains $(L^2 \uparrow G)$, $\Gamma^{[2,1]}$ contains $2(L^3 \uparrow G)$ and $\Gamma^{[1^3]}$ contains $(L^1 \uparrow G)$. If $D^k = L^3$, then $\Gamma^{[3]}$ contains $2(L^1 \uparrow G) + 2(L^2 \uparrow G) + 2(L^3 \uparrow G)$, $\Gamma^{[2,1]}$ contains $4(\text{reg } L) \uparrow G + 4(L^3 \uparrow G)$ and $\Gamma^{[1^3]}$ contains $2(L^1 \uparrow G) + 2(L^2 \uparrow G)$.

Collecting together the results, we obtain:

$$(L^1)^{[3]} = 3(L^1 \uparrow G) + (L^3 \uparrow G)$$
$$(L^1)^{[2,1]} = 2(L^1 \uparrow G) + 4(L^3 \uparrow G)$$
$$(L^1)^{[1^3]} = L^2 \uparrow G$$
$$(L^2)^{[3]} = 3(L^2 \uparrow G) + (L^3 \uparrow G)$$
$$(L^2)^{[2,1]} = 2(L^2 \uparrow G) + 4(L^3 \uparrow G)$$
$$(L^2)^{[1^3]} = L^1 \uparrow G$$
$$(L^3)^{[3]} = 6(L^1 \uparrow G) + 6(L^2 \uparrow G) + 9(L^3 \uparrow G)$$
$$(L^3)^{[2,1]} = 12(L^1 \uparrow G) + 12(L^2 \uparrow G) + 30(L^3 \uparrow G)$$
$$(L^3)^{[1^3]} = 3(L^1 \uparrow G) + 3(L^2 \uparrow G) + 4(L^3 \uparrow G).$$

The motivation to obtain these results was the possible application, in the case $n = 3$, to the Landau theory of second order phase transitions in crystals. A full account of this theory may be found in Lyubarskii (1960, chapter 7) and Landau and Lifshitz (1958, chapter 14). One of the conditions that they require to be satisfied is that the totally symmetrized cube does not contain the identity representation, which we denote by A. Clearly a necessary condition for the subspace defined by equation (1.13) of I, to carry $A(G)$ is that the associated vector $\boldsymbol{q} = \boldsymbol{0}$. Hence in the above example it would only have been necessary to work out the associated vectors $\boldsymbol{q}$ to ascertain the result. More generally, $\Omega_{(\alpha)}$ carries $A(G)$ if and only if the representation $(D_{\alpha_2} \otimes D_{\alpha_1} \otimes D) \downarrow K_2$ contains $A(K_2)$, and so it is sufficient to work out the contribution from such spaces. Clearly this result generalizes to higher n.

5. Comparison with other methods

The methods for obtaining selection rules in crystals fall mainly into two types. There is the subgroup technique used by Bradley and Davies (1970), and extended in I, which is based on the theory of induced representations, and there is the full group method of Birman (1962, 1963). Davies and Lewis (1971) have calculated the Kronecker product and symmetrized square of representations of the space group $Fd3m$, corresponding to the diamond structure, using two full group methods advocated by Birman, namely, the 'direct inspection' method and the 'reduction group' method, and also by the subgroup method of Bradley (1966) and Bradley and Davies (1970). Their conclusions appear to favour the subgroup method as a general technique although in some cases 'direct inspection' is better.

Lewis (1973) has also developed a method for finding the totally symmetrized nth powers of space group representations. His is basically an inductive full group method because it relies on a formula of Littlewood (1959) to express the character of the nth symmetrized power, $\chi^{[n]}$, in terms of $\chi^{[m]}$, $m < n$, and $\chi(g^n)$. He uses subgroup techniques to analyse the components of the generalized character $g \rightarrow \chi(g^n)$, and for this he has to work out a complete set of double coset representatives, as in I, to obtain his wave-vector selection rules. The basic difference between our methods is that Lewis's is necessarily inductive at the full group level whereas ours involves symmetrizations at the subgroup level, where they are more easy to handle.

It seems to us that for space groups, in the case $n > 3$, the subgroup method is appreciably easier to use than full group methods, and indeed the only practical method available if one requires a complete decomposition into symmetry classes. For $n = 3$, since both full group and subgroup methods are available, it is a matter of taste which method is used. Certainly it seems essential that both methods should be well known, as undoubtedly attempts will be made in the future to program such decompositions for all 230 space groups, and whoever attempts this daunting task will have to compare critically the various methods available in respect of computer storage space and the number of operations involved.

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