COMPUTER PROGRAMS FOR DETERMINING WAVE VECTOR SELECTION RULES (WVSRs) FOR SPACE GROUPS

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1. Introduction

In the summer of 1975, at the Fourth Colloquium in this series and at the Crystallography Congress in Amsterdam, we outlined a project for the construction of tables giving the reductions of the Kronecker products of the irreducible representations of all the 230 classical space groups. The problem is to determine the coefficients $C^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}_{pq,r}$ in the decomposition

$$\left(\Gamma^{\underset{\sim}{k}_i}_p \uparrow \underset{\sim}{G}\right) \boxtimes \left(\Gamma^{\underset{\sim}{k}_j}_q \uparrow \underset{\sim}{G}\right) \equiv \sum_r \sum_\ell C^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}_{pq,r} \left(\Gamma^{\underset{\sim}{k}_\ell}_r \uparrow \underset{\sim}{G}\right) \qquad (1)$$

where $\left(\Gamma^{\underset{\sim}{k}_i}_p \uparrow \underset{\sim}{G}\right)$ etc. are irreducible representations of the space group $\underset{\sim}{G}$ induced from the irreducible representations $\Gamma^{\underset{\sim}{k}_i}_p$ etc. of the little groups $\underset{\sim}{G}^{\underset{\sim}{k}_i}$ etc.

This work can conveniently be divided into two parts. The first part involves the determination of wave vector selection rules (WVSRs) to identify the rather small number of wave vectors $\underset{\sim}{k}_\ell$ that are allowed to appear on the right-hand side of equation (1) for any given choice of $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$. The second part involves the use of these WVSRs, together with the character tables for the irreducible representations of a space group, to determine the coefficients $C^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}_{pq,r}$. For brief details of the theory see section 2 of Cracknell and Davies (1975).

At the time of our previous communication we had carried out this work by hand for a relatively small number of space groups. Since then we have written two big ALGOL programs, one to determine the WVSRs and the other to evaluate the coefficients $C^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}_{pq,r}$. Each program has now been tested and checked most carefully. The WVSR program has been run for all the space groups and the Kronecker products program has, so far, been run for about 150 space groups. The final tables, when they are completed, will be reproduced directly from the computer print-outs and will be published as a book by Plenum Press. In this contribution we shall consider the WVSR program and present some specimen results.

2. Representation domains and basic domains

If we include more than one wave vector from a given star when calculating $C^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}_{pq,r}$ we shall be including several equivalent representations, which might not be recognised as equivalent because they would be labelled by different vectors $\underset{\sim}{k}_\ell$ of the star. To eliminate this possibility we therefore impose the additional constraint, in addition to the restrictions imposed by double-coset decompositions, that our WVSRs are formulated in such a manner that no more than one vector $\underset{\sim}{k}_\ell$ from any given star is included. This is quite difficult to achieve in practice and has

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led us into having to make a very detailed examination of the whole question of "representation domains", see Bradley and Cracknell (1972). The detailed results are being published elsewhere (Cracknell and Davies 1977); we reproduce here an extract from these results in table 1.

3. Program structure and data preparation

For each space group a data file was constructed which contained the following information:

(i) multiplication table for the rotational parts of the space-group operations,

(ii) matrices representing the effect of these rotational operations on the reciprocal lattice vectors $\underset{\sim}{g}_1$, $\underset{\sim}{g}_2$, and $\underset{\sim}{g}_3$,

(iii) coordinates of special wave vectors,

(iv) the rotational parts of the space-group operations in the little groups $\underset{\sim}{G}^{\underset{\sim}{k}}$.

The WVSRs consist of the identification of the allowed values of $\underset{\sim}{k}_\ell$ which can appear on the right-hand side of equation (1); these are given by

$$R_\alpha \underset{\sim}{k}_i + R_\beta \underset{\sim}{k}_j \equiv \underset{\sim}{k}_\ell \qquad (2)$$

where $\{R_\alpha|\underset{\sim}{v}_\alpha\}$ and $\{R_\beta|\underset{\sim}{v}_\beta\}$ are a very restricted subset of the elements of the space group $\underset{\sim}{G}$. For each space group the WVSR program works, in turn, through all possible pairs of wave vectors $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$ (for $j \geqslant i$). For each pair of $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$, allowed values of R_α and R_β are determined using the double-coset decompositions in section 2.1 of Cracknell and Davies (1975). For any given $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$, the allowed $\underset{\sim}{k}_\ell$ are unique, except that each $\underset{\sim}{k}_\ell$ could be replaced by an equivalent wave vector or by another wave vector in its own star. To identify the $\underset{\sim}{k}_\ell$ a separate set of "SPY" conditions, which may be up to about 100 lines of ALGOL program, had to be written for each (symmorphic) space group. The WVSR program incorporates about half a dozen checks, within the double-cosets procedure and in the main program.

4. Results

The WVSR program has now been tested and run successfully for all the space groups so that we have a complete set of WVSRs for all the classical space groups. These WVSRs are stored in files on magnetic tape; each file contains all the $\underset{\sim}{k}_i$, $\underset{\sim}{k}_j$, $\underset{\sim}{k}_\ell$, R_α and R_β. From these files we can construct, with a small ALGOL program, a triangular table of the WVSRs for any given space group. An example is given in table 2. A similar table can be constructed, very quickly, for any other space group from our WVSR result files. For many space groups the WVSR table is considerably larger than the example in table 2. If any worker would like to have the WVSRs for a particular space group in the period before our book of tables is published, we shall be pleased to supply a copy.

References

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Table 1. Special wave vectors for I23 (197) and $I2_13$ (199).

Label		Coordinates	Label		Coordinates	Label		Coordinates
GM (Γ)	1	$0,0,0$	P	7	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	C_{2a}:P	16	$-\frac{1}{4},-\frac{1}{4},\frac{3}{4}$
DT (Δ)	2	$\alpha,-\alpha,\alpha$	D	8	$\alpha,\alpha,\frac{1}{2}-\alpha$	C_{2a}:D	17	$-\alpha,-\alpha,\frac{1}{2}+\alpha$
LD (Λ)	3	α,α,α	F	9	$\frac{1}{2}-\alpha,3\alpha-\frac{1}{2},\frac{1}{2}-\alpha$	C_{2a}:F	18	$-\frac{1}{2}+\alpha,\frac{1}{2}-3\alpha,\frac{1}{2}+\alpha$
H	5	$\frac{1}{2},-\frac{1}{2},\frac{1}{2}$						
N	6	$0,0,\frac{1}{2}$	C_{2a}:LD	15	$-\alpha,-\alpha,3\alpha$	GP	19	α,β,γ

Note: The special points, lines, and planes are labelled in the notation of Miller and Love (1967), extended (for the planes of symmetry) by Davies and Cracknell (1976).

Table 2. WVSRs for I23 (197) and $I2_13$ (199).

K \ M	1	2	3	5	6	7	8	9	15	16	17	18
1	1 1 1	1 1 2	1 1 3	1 1 5	1 1 6	1 1 7	1 1 8	1 1 9	1 1 15	1 1 16	1 1 17	1 1 18
2		1 1 2 2 1 2 1 5 19 5 1 19	1 1 19 10 1 19	2 1 2	9 1 8 10 1 17 2 1 19 7 1 19	10 1 8	9 1 8 10 1 8 2 1 19 7 1 19	2 1 19 10 1 19	5 1 19 9 1 19	9 1 17	9 1 17 10 1 17 2 1 19 7 1 19	7 1 19 9 1 19
3			1 1 3 3 1 19	3 1 18	2 1 19 4 1 19	3 1 9	3 1 19 4 1 19	3 1 9 2 1 19	4 1 15 1 1 19	4 1 15	2 1 19 4 1 19	3 1 18 4 1 19
5				1 1 1	1 2 6	1 1 16	1 2 17	1 2 15	1 2 9	1 1 7	1 2 8	1 3 3
6					1 1 1 1 2 5 5 11 6 9 6 6	5 1 2	5 5 2 5 6 2 5 11 19 9 6 19	2 3 19 2 4 19	1 3 19 1 4 19	6 1 2	6 5 2 6 6 2 6 9 19 11 5 19	2 2 19 2 4 19
7						1 1 5	1 5 2	1 1 18	1 4 3	1 1 1	1 5 2	1 2 15
8							5 5 2 5 6 2 5 11 19 9 6 19	2 3 19 2 4 19	1 3 19 1 4 19	6 1 2	6 5 2 6 6 2 6 9 19 11 5 19	2 2 19 2 4 19
9								2 2 15 1 2 19	1 2 9 3 2 19	3 1 3	3 2 19 4 2 19	3 3 3 2 3 19
15									1 1 15 2 1 19	2 1 18	2 1 19 4 1 19	2 1 18 3 1 19
16										1 1 5	1 6 2	1 1 9
17											6 5 2 6 6 2 6 9 19 11 5 19	2 2 19 2 4 19
18												3 3 3 1 3 19

Note: K represents $\underset{\sim}{k}_i$ and M represents $\underset{\sim}{k}_j$. Each entry is in the form $R_\alpha\ R_\beta\ \underset{\sim}{k}_\ell$ where R_α and R_β are coded according to Miller and Love (1967) and $\underset{\sim}{k}_\ell$ is coded according to table 1.