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# Space group Clebsch-Gordan coefficients: II. Computer generated special solutions of the multiplicity problem by Dirl's method

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**Abstract.** In paper I of this series, special solutions of the multiplicity problem were established for wavevector selection rules (WVSR) of types I and II occurring in the reduction of Kronecker products of space group unirreps. In this paper, a computer program based on Dirl's method is described which has been used to show that special solutions of the multiplicity problem exist for all WVSR of type III in the reduction of Kronecker products of Miller and Love matrix unirreps in all 230 (single and double) space groups.

## 1. Introduction

In this paper, which is the second of three papers on space group Clebsch-Gordan (CG) coefficients, we consider special solutions of the multiplicity problem for wavevector selection rules (WVSR) of type III occurring in the reduction of Kronecker products of space group unirreps. In the first paper (Davies 1986, hereafter referred to as DI) special solutions of the multiplicity problem were established for all WVSR of types I and II. Here we describe a computer program, using the method of Dirl (1979), which has been used to show that special solutions of the multiplicity problem exist for all WVSR of type III in the reduction of Miller and Love (1967) (hereafter referred to as ML) matrix unirreps in all 230 (single and double) space groups. In the following, we use the same notation and definitions as in DI. Equations in DI are referenced by the prefix 'I' followed by the equation number.

## 2. Special solutions of the multiplicity problem for WVSR of type III by Dirl's method

For a WVSR (I.7) of type III, there is no simple criterion, like (I.22), for the existence of a special solution of the multiplicity problem. A WVSR of type III is distinguished from those of type I or type II by the fact that the triple intersection group $\mathrm{P}^{\boldsymbol{q},\boldsymbol{q}';\boldsymbol{q}_0}_{\bar{\sigma},\bar{\sigma}'}$ is non-trivial (see (I.13)-(I.16)). However, Dirl (1979) has given a method to search for special solutions of the multiplicity problem in the case of non-trivial triple intersection groups. We reproduce the essential steps of his method here in order to describe more conveniently the algorithm on which our computer program is based. As in (I.22), we prefer to express all appropriate equations in terms of the allowed matrix unirreps $\Gamma^{(\kappa,\boldsymbol{q})}$ of the little groups $\mathrm{G}^{\boldsymbol{q}}$, $\boldsymbol{q} \in \Delta\mathrm{BZ}$, instead of the projective matrix unirreps $R^{\kappa}$ of the little co-groups $\mathrm{P}^{\boldsymbol{q}}$ ($\simeq \mathrm{G}^{\boldsymbol{q}}/\mathrm{T}$). This is done because the $\Gamma^{(\kappa,\boldsymbol{q})}$, rather than $R^{\kappa}$, are tabulated in ML and in Cracknell *et al* (1979) (hereafter referred to as CDML). The use of $\Gamma^{(\kappa,q)}$ also has the advantage that terms involving the factor systems do not appear explicitly in the equations which helps to reveal their structure.

Recall that the CG matrix (I.11) is built up column by column. For given component multiplicity (see (I.9))

$$m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}>0 \tag{1}$$

the task is to find special column indices $(\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v)$ of the Kronecker product $\Lambda^{(\kappa,q)}\otimes\Lambda^{(\kappa',q')}$ so that the multiplicity index

$$w=(\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v) \qquad v=1,2,\ldots,m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} \tag{I.12}$$

when a 'special solution of the multiplicity problem' has been found. The special column indices above are chosen in such a way that all the elements of the CG matrix (I.11) in the columns labelled by $(\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0)$ can be computed using a single explicit formula in terms of only the allowed matrix unirreps $\Gamma^{(\kappa,q)}$, $\Gamma^{(\kappa',q')}$, $\Gamma^{(\kappa_0,q_0)}$. The steps for choosing these special column indices are as follows (Dirl 1979).

(*a*) Starting with $(\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0)$, and assuming $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}>0$, construct the triple intersection group

$$\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}=(\bar{\sigma}\mathrm{P}^{q}\bar{\sigma}^{-1})\cap(\bar{\sigma}'\mathrm{P}^{q'}\bar{\sigma}'^{-1})\cap\mathrm{P}^{q_0}. \tag{2}$$

(*b*) Decompose $\mathrm{P}^{q_0}$ into left cosets with respect to the subgroup $\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}$ and select left coset representatives $v_j\in\mathrm{P}^{q_0}:\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}$.

(*c*) Generate $|\mathrm{P}^{q_0}:\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|$ pairs of fixed left coset representatives $\bar{\sigma}_j$, $\bar{\sigma}'_j$ of $\mathrm{P}^{q}$, $\mathrm{P}^{q'}$ respectively, in P:

$$\bar{\sigma}_j=v_j\bar{\sigma}z_j^{-1}\in\mathrm{P}:\mathrm{P}^{q} \qquad \text{where } z_j\in\mathrm{P}^{q} \tag{3a}$$

$$\bar{\sigma}'_j=v_j\bar{\sigma}'z_j'^{-1}\in\mathrm{P}:\mathrm{P}^{q'} \qquad \text{where } z'_j\in\mathrm{P}^{q'}. \tag{3b}$$

The $z_j$, $z'_j$ in (3) are uniquely determined by the requirement that $\bar{\sigma}_j$, $\bar{\sigma}'_j$ must be elements of the sets of previously chosen fixed left coset representatives $\mathrm{P}:\mathrm{P}^{q}$, $\mathrm{P}:\mathrm{P}^{q'}$ respectively.

(*d*) For each of the pairs $\bar{\sigma}_j$, $\bar{\sigma}'_j$ in (3), define the column vectors $\boldsymbol{B}^{(\kappa,q)(\kappa',q');(\kappa_0,q_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0}$, $c=1,2,\ldots,n_\kappa$, $c'=1,2,\ldots,n_{\kappa'}$, (giving a total of $n_\kappa n_{\kappa'}|\mathrm{P}^{q_0}:\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|$ vectors) by

$$\begin{aligned}\{\boldsymbol{B}^{(\kappa,q)(\kappa',q');(\kappa_0,q_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0}\}_{\bar{\tau}d,\bar{\tau}'d'}\\ =\delta_{q(\bar{\tau})+q'(\bar{\tau}'),q_0+Q[q(\bar{\tau})+q'(\bar{\tau}')]}\frac{n_{\kappa_0}}{|\mathrm{P}^{q_0}|}\sum_{\beta\in\mathrm{P}^{q_0}}\Delta^{q}(\bar{\tau},\beta\bar{\sigma}_j)\\ \times\Delta^{q'}(\bar{\tau}',\beta\bar{\sigma}'_j)\Delta^{q_0}(\bar{e},\beta\bar{e})\Gamma^{(\kappa,q)}_{dc}[(\bar{\tau}|\boldsymbol{\tau}(\bar{\tau}))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}_j|\boldsymbol{\tau}(\bar{\sigma}_j))]\\ \times\Gamma^{(\kappa',q')}_{d'c'}[(\bar{\tau}'|\boldsymbol{\tau}(\bar{\tau}'))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}'_j|\boldsymbol{\tau}(\bar{\sigma}'_j))]\Gamma^{(\kappa_0,q_0)*}_{a_0a_0}[(\beta|\boldsymbol{\tau}(\beta))]\end{aligned} \tag{4}$$

where $\Delta^{q}(\gamma,\gamma')=\delta_{\gamma\mathrm{P}^{q},\gamma'\mathrm{P}^{q}}$ for all $\gamma,\gamma'\in\mathrm{P}$, $a_0$ is a fixed integer in the range $1\leqslant a_0\leqslant n_{\kappa_0}$, $\bar{e}$ is the identity element of P, $\bar{\tau}\in\mathrm{P}:\mathrm{P}^{q}$, $d=1,2,\ldots,n_\kappa$, $\bar{\tau}'\in\mathrm{P}:\mathrm{P}^{q'}$, $d'=1,2,\ldots,n_{\kappa'}$.

(*e*) The square of the norm of a column vector (4) is equal to its 'diagonal' element:

$$\begin{aligned}\|\boldsymbol{B}^{(\kappa,q)(\kappa',q');(\kappa_0,q_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0}\|^2\\ =\frac{n_{\kappa_0}}{|\mathrm{P}^{q_0}|}\sum_{\beta\in\mathrm{P}^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}}\Gamma^{(\kappa,q)}_{cc}[(\bar{\sigma}_j|\boldsymbol{\tau}(\bar{\sigma}_j))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}_j|\boldsymbol{\tau}(\bar{\sigma}_j))]\\ \times\Gamma^{(\kappa',q')}_{c'c'}[(\bar{\sigma}'_j|\boldsymbol{\tau}(\bar{\sigma}'_j))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}'_j|\boldsymbol{\tau}(\bar{\sigma}'_j))]\Gamma^{(\kappa_0,q_0)*}_{a_0a_0}[(\beta|\boldsymbol{\tau}(\beta))].\end{aligned} \tag{5}$$

(*f*) Two column vectors of non-zero norm

$$\boldsymbol{B}_{\bar{e}a_0}^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}$$

and

$$\boldsymbol{B}_{\bar{e}a_0}^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_k,d;\bar{\sigma}'_k,d')}$$

are orthogonal if the scalar product, which is given by

$$\begin{aligned}\langle \boldsymbol{B}_{\bar{e}a_0}^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_k,d;\bar{\sigma}'_k,d')}, \boldsymbol{B}_{\bar{e}a_0}^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}\rangle \\ = \frac{n_{\kappa_0}}{|\mathrm{P}^{\boldsymbol{q}_0}|} \sum_{\beta\in\mathrm{P}^{\boldsymbol{q}_0}} \Delta^{\boldsymbol{q}}(\bar{\sigma}_k, \beta\bar{\sigma}_j)\Delta^{\boldsymbol{q}'}(\bar{\sigma}'_k, \beta\bar{\sigma}'_j)\Delta^{\boldsymbol{q}_0}(\bar{e}, \beta\bar{e}) \\ \times \Gamma_{dc}^{(\kappa,\boldsymbol{q})}[(\bar{\sigma}_k|\boldsymbol{\tau}(\bar{\sigma}_k))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}_j|\boldsymbol{\tau}(\bar{\sigma}_j))] \\ \times \Gamma_{d'c'}^{(\kappa',\boldsymbol{q}')}[(\bar{\sigma}'_k|\boldsymbol{\tau}(\bar{\sigma}'_k))^{-1}(\beta|\boldsymbol{\tau}(\beta))(\bar{\sigma}'_j|\boldsymbol{\tau}(\bar{\sigma}'_j))]\Gamma_{a_0a_0}^{(\kappa_0,\boldsymbol{q}_0)*}[(\beta|\boldsymbol{\tau}(\beta))] \end{aligned} \tag{6}$$

vanishes.

(*g*) The space spanned by the column vectors (4) has dimension $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$. If, by using (5) and (6), $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$ pairwise orthogonal vectors, of non-zero norm,

$$\boldsymbol{B}_{\bar{e}a_0}^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c'_v)} \qquad v = 1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$$

can be found, then the multiplicity index $w$ is identified with the special column indices:

$$w = (\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v) \qquad v = 1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)} \tag{7}$$

and we then have a 'special solution of the multiplicity problem'. When such a special solution can be found, an explicit expression exists for all elements of all the columns labelled by $(\kappa_0, (\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0)$ (Dirl 1979).

As in DI, the generalisation of steps (*a*)–(*g*) to 'double' space groups is trivial (Dirl 1981).

Dirl (1981) conjectured that the ML space group matrix unirreps might yield at least some special solutions of the multiplicity problem and we set out to investigate this using a computer program.

## 3. Program

We have written a program in ALGOL 60 for a DEC System 10 computer to calculate CG coefficients for Kronecker products of (single and double) space group unirreps and the first stage of this program is to look for special solutions of the multiplicity problem. A description of the second stage—the actual calculation of the CG coefficients themselves—is given in paper III of this series. For simplicity, the description in this section is given in terms of single groups; the extension to double groups is straightforward, as indicated at the end of § 2.

All the ML space group matrix unirreps in CDML are available on magnetic tape. The WVSR and component multiplicities for Kronecker products of all space group unirreps, involving non-trivial little co-groups $\mathrm{P}^{\boldsymbol{q}}$, $\mathrm{P}^{\boldsymbol{q}}$, which are published in Davies and Cracknell (1979) and Cracknell and Davies (1979), are also available on magnetic tape. The program has been designed to work with any of the 230 space groups. The algorithm, on which the program is based, may be briefly described as follows.

(*a*) For a given space group the following data are input.

(i) The ML allowed matrix unirreps $\Gamma^{(\kappa,\boldsymbol{q})}$ for all essentially inequivalent $\boldsymbol{q}$ vectors in the fundamental domain $\Delta$BZ.

(ii) The WVSR and component multiplicities (see (I.7) and (I.9) respectively) for all Kronecker products $\Lambda^{(\kappa,q)}\otimes\Lambda^{(\kappa',q')}$ of space group unirreps $\Lambda^{(\kappa,q)}$ and $\Lambda^{(\kappa',q')}$ having non-trivial little co-groups $P^{q}$ and $P^{q'}$ respectively.

(iii) The group multiplication table for the crystal point group P and the point group transformation matrices for the primitive lattice vectors.

(*b*) Choose and *fix*, *once and for all*, the left coset representatives $\bar{\tau}\in P:P^{q}$ for all essentially inequivalent $\boldsymbol{q}$ vectors in ΔBZ.

(*c*) (i) Select, in turn, a Kronecker product $\Lambda^{(\kappa,q)}\otimes\Lambda^{(\kappa',q')}$ in (*a*) (ii) above.

(ii) Select, in turn, a WVSR (see (I.7)) for that Kronecker product and generate the $|P^{q_0}:P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|$ pairs of fixed left coset $\bar{\sigma}_j$, $\bar{\sigma}'_j$ given by (3).

(iii) Select, in turn, a non-zero component multiplicity $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$ for that WVSR. Fix $a_0$ $(1\leqslant a_0\leqslant n_{\kappa_0})$ and by using (5) and (6), select from the $n_\kappa n_{\kappa'}|P^{q_0}:P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|$ column vectors

$$B^{(\kappa,q)(\kappa',q);(\kappa_0,q_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0}\qquad j=1,2,\ldots,|P^{q_0}:P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|,\ c=1,2,\ldots,n_\kappa,\ c'=1,2,\ldots,n_{\kappa'},$$

a maximal set of non-zero, pairwise orthogonal, vectors, which may be indexed by $(\bar{\sigma}_v, c_v;\bar{\sigma}'_v, c'_v)$, $v=1,2,\ldots,\bar{m}^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$. If

$$\bar{m}^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}=m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$$

then a *special solution of the multiplicity problem* has been found and the multiplicity index $w$ may be identified with these special column indices of the Kronecker product:

$$w=(\bar{\sigma}_v, c_v;\bar{\sigma}'_v, c'_v)\qquad v=1,2,\ldots,m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}.$$

If

$$\bar{m}^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}<m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$$

then a Gram–Schmidt orthogonalisation procedure is required as described by Dirl (1979).

If

$$\bar{m}^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}>m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$$

then a failure has occurred due to an error in the program or the data.

## 4. Results

The program was run for all 230 (single and double) space groups for all Kronecker products $\Lambda^{(\kappa,q)}\otimes\Lambda^{(\kappa',q')}$ involving non-trivial little co-groups $P^{q}$ and $P^{q'}$ and which are published by Davies and Cracknell (1979) and Cracknell and Davies (1979).

*For every value of the component multiplicity* $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$ *a special solution of the multiplicity problem was found.*

The value of $a_0$ in (4)–(6) was fixed at unity and it was not even found necessary to alter this value. This splendid result means that the calculation and tabulation of the CG matrices is considerably simplified. Dirl (1981) conjectured that the ML matrix unirreps could yield at least some special solutions of the multiplicity problem. The fact that the above computer program found special solutions *in every case* came as a complete surprise. It would seem that there is latent structure in the ML matrix unirreps to account for this. The nature of this structure, if it exists, is unknown to this author at present.

It is interesting to note that there is considerable overlap between the set of WVSR considered in DI and those considered here. In DI special solutions of the multiplicity problem were established for *all* WVSR of types I and II. In Davies and Cracknell (1979) and Cracknell and Davies (1979), *all* WVSR of type III are tabulated. But also, there are many WVSR of types I and II (see § C of Dirl (1979) and (I.14)-(I.16) of DI), and so the results of DI are consistent with the results reported here using the computer program.

The running of the program for all 230 (single and double) space groups was carried out on the DEC System 10 computer at the University College of North Wales, Bangor during the months September to December 1982. Typical run times were 10 min for $P2_13$ (198) and 3 h for $Pm3m$ (221). The total run time for all groups was approximately 75 h.

The example to be found in paper III of this series will serve two purposes. Firstly, it will illustrate the solving of the multiplicity problem with which we are concerned in this paper. Secondly, it will illustrate the complete construction of the CG matrix for which the solution of the multiplicity problem is the first stage.

## 5. Conclusion

We have shown, by computer, that for all 230 (single and double) space groups, the Miller and Love (1967) (induced) matrix unirreps, as extended by Cracknell *et al* (1979), possess the remarkable property that they provide special solutions of the multiplicity problem for all wavevector selection rules of type III occurring in any Kronecker product of space group unirreps. Using the special solutions of the multiplicity problem established here and in paper I, it will be shown in paper III that *all* elements of a Clebsch-Gordan (CG) matrix for the reduction of *any* Kronecker product of space group unirreps can be computed using a single explicit formula in terms of only the Miller and Love allowed matrix unirreps of the little groups occurring in the Kronecker product and its CG series decomposition.

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