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Space group Clebsch–Gordan coefficients: I. Special solutions of the multiplicity problem and Dirl's criterion

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Abstract. The wavevector selection rules (WVSR) occurring in the reduction of Kronecker products of space group unirreps are classified, for convenience, into three types. For WVSR of type I, Dirl has shown that special solutions of the multiplicity problem always exist. For WVSR of type II, Dirl has given a simple criterion for the existence of special solutions of the multiplicity problem and in this paper it is shown that, for all 230 (single and double) space groups, the Miller and Love matrix unirreps satisfy this criterion. WVSR of type III will be considered in a subsequent paper.

1. Introduction

The construction of selection rules governing many important quantum mechanical interactions in crystals (e.g. infrared absorption, Raman scattering, electron scattering, etc) is facilitated by the knowledge of the multiplicities (also called Clebsch-Gordan (CG) series coefficients or reduction coefficients) in the reduction of the Kronecker products or symmetrised Kronecker powers of unitary irreducible representations (unirreps) of crystallographic space groups (Winston and Halford 1949, Elliott and Loudon 1960, Lax and Hopfield 1961, Bradley and Cracknell 1972, Birman 1974a, Dirl 1979b, Cornwell 1984). Space group unirreps have a convenient realisation as induced representations from small (or allowed) unirreps of a little group (or group of the $\boldsymbol{q}$ vector). The mathematical problem of the reduction of the Kronecker products of these induced representations of space groups within the framework of little group theory was solved by Bradley (1966) using a theorem of Mackey (1951, 1952). The related problem of reducing the symmetrised and antisymmetrised Kronecker squares was solved by Bradley and Davies (1970). Later this work was extended by Gard (1973a, b) to solve the general problem of the reduction of symmetrised Kronecker powers entirely within the little group framework. On the other hand, several authors have tackled these problems without using the full power of little group theory (Birman 1962, Streitwolf 1969, Doni and Pastori Parravicini 1973, Lewis 1973, Dirl 1979b).

The present author, in collaboration with A P Cracknell, developed computer programs, using little group methods, for the systematic calculation of multiplicities in the reduction of Kronecker products and symmetrised Kronecker powers of unirreps of all 230 (single and double) space groups (Cracknell *et al* 1979) (hereafter referred to as CDML), Cracknell and Davies 1979, Davies and Cracknell 1979, 1980a, b). The Miller and Love (1967) (hereafter referred to as ML) computer generated tables of space group unirreps, on magnetic tape, formed the bulk of the input data to our programs. The ML tables were declared 'out of print' by Pruett Press and so these tables were reprinted (with some modifications) in CDML.

Following the calculation of multiplicities, the next stage is the calculation of CG coefficients. Physical applications of these include two-photon absorption matrix elements, scattering tensors for multipole-dipole resonance Raman scattering, higher order moment expansions in infrared absorption, etc (Birman 1974a, b, Birman and Berenson 1974, Birman *et al* 1976). Whereas the multiplicities are independent of the basis functions, the CG coefficients are, of course, basis dependent. However, the value of any physical observable, which can be expressed in terms of the CG coefficients, is invariant under a change of basis (Birman *et al* 1976). In the past few years much attention has been devoted to the theoretical problem of calculating CG coefficients (Litvin and Zak 1968, Gard 1973c, Birman 1974a, Sakata 1974, Berenson and Birman 1975, van den Broek and Cornwell 1978, Dirl 1979a, c, 1981, 1982, Chen *et al* 1983) and some hand calculations have been done on a few space groups (Berenson *et al* 1975, Suffczyński and Kunert 1978, Dirl 1979d, Kunert and Suffczyński 1980, Kunert 1983).

Dirl (1979a, c, 1981, 1982) exploits the fact that the columns of the CG matrix may be seen as symmetry adapted vectors which may then be constructed by projection operator techniques. This elegant method correctly deals with the 'multiplicity problem' which arises from the fact that space groups are not simply reducible. A remarkable feature of this method is the possibility of identifying the multiplicity index with special column indices of the Kronecker product. When this can be done, a 'special solution of the multiplicity problem' has been found and then all the elements of the corresponding columns of the CG matrix can be computed using a single explicit formula. An interesting example of this in the non-symmorphic body-centred cubic space group Ia3d has been briefly reported (Davies and Dirl 1984).

In this paper (which is the first in a series of three) we classify, for convenience, the wavevector selection rules (WVSR) occurring in the reduction of Kronecker products of space group unirreps, into one of three types. For WVSR of type I, Dirl (1979c) has shown that special solutions of the multiplicity problem always exist. For WVSR of type II, Dirl (1979c) has given a simple criterion for the existence of special solutions of the multiplicity problem and here we show that, for all 230 (single and double) space groups, the ML matrix unirreps satisfy this criterion. The WVSR of type III will be considered in paper II of this series.

2. Clebsch–Gordan coefficients

In this section we establish the notation (which follows mainly that of Dirl (1977, 1979a, b, c)) for use in this paper and in the next two papers in the series.

A matrix unirrep $\Lambda^{(\kappa,\boldsymbol{q})}$ of a space group G (which contains an invariant subgroup of translations T) can be induced from an allowed matrix unirrep $\Gamma^{(\kappa,\boldsymbol{q})}$ of the little group (or group of the $\boldsymbol{q}$ vector) $G^{\boldsymbol{q}}$,

$$\Lambda^{(\kappa,\boldsymbol{q})} = \Gamma^{(\kappa,\boldsymbol{q})} \uparrow G \tag{1}$$

where $\boldsymbol{q}$ is a vector in the fundamental domain (or representation domain) Δ_{BZ} of the first Brillouin zone of G and κ labels the different allowed matrix unirreps of $G^{\boldsymbol{q}}$ (Bradley and Cracknell 1972, Altmann 1977, Dirl 1979b). (Representation domains for all 230 space groups are given in CDML.)

At this point it is important to note that, in contrast to the convention adopted by Bradley and Cracknell (1972) and Dirl (1977), we follow the convention of ML and CDML whereby the one-dimensional unirreps D^{q} of the translation group T are given by

$$D^{q}[(e|\boldsymbol{t})] = \exp(+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{t}) \tag{2}$$

for all $\boldsymbol{q} \in \Delta\mathrm{BZ}$ and $\boldsymbol{t} \in \mathrm{T}$, where the *positive* sign, and not the negative sign, occurs in the exponential term on the right-hand side of (2). As a consequence of (2), we have

$$\Gamma^{(\kappa,\boldsymbol{q})}[(\alpha|\boldsymbol{\tau}(\alpha)+\boldsymbol{t})] = \exp(+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{t})\Gamma^{(\kappa,\boldsymbol{q})}[(\alpha|\boldsymbol{\tau}(\alpha))] \tag{3}$$

where $(\alpha|\boldsymbol{\tau}(\alpha)) \in \mathrm{G}^{\boldsymbol{q}}$ and $\boldsymbol{t} \in \mathrm{T}$, which is the characteristic property of the allowed unirreps of $\mathrm{G}^{\boldsymbol{q}}$.

An allowed matrix unirrep $\Gamma^{(\kappa,\boldsymbol{q})}$ can be constructed from a projective matrix unirrep R^{κ} of the little co-group $\mathrm{P}^{\boldsymbol{q}}$ ($\simeq \mathrm{G}^{\boldsymbol{q}}/\mathrm{T}$), belonging to a certain factor system, by

$$\Gamma^{(\kappa,\boldsymbol{q})}[(\alpha|\boldsymbol{\tau}(\alpha)] = \exp(+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\tau}(\alpha))R^{\kappa}(\alpha) \tag{4}$$

where $(\alpha|\boldsymbol{\tau}(\alpha)) \in \mathrm{G}^{\boldsymbol{q}}$, $\alpha \in \mathrm{P}^{\boldsymbol{q}}$ and the same sign convention is used in (4) as in (2) and (3) (Bradley and Cracknell 1972, Altmann 1977, Dirl 1979b).

The dimension of $\Lambda^{(\kappa,\boldsymbol{q})}$ is $l_{\boldsymbol{q}}n_{\kappa}$, where $l_{\boldsymbol{q}}$ $(=|\mathrm{G}:\mathrm{G}^{\boldsymbol{q}}| = |\mathrm{P}:\mathrm{P}^{\boldsymbol{q}}|, \mathrm{P} \simeq \mathrm{G}/\mathrm{T})$ is the index of $\mathrm{G}^{\boldsymbol{q}}$ in G and n_{κ} is the dimension of $\Gamma^{(\kappa,\boldsymbol{q})}$ (= dimension of R^{κ}). The matrix elements of

$$\Lambda^{(\kappa,\boldsymbol{q})}[(\beta|\boldsymbol{\tau}(\beta)+\boldsymbol{t})]$$

where $(\beta|\boldsymbol{\tau}(\beta)) \in \mathrm{G}$ and $\boldsymbol{t} \in \mathrm{T}$ are given by

$$\Lambda^{(\kappa,\boldsymbol{q})}_{\bar{\tau}d,\bar{\sigma}c}[(\beta|\boldsymbol{\tau}(\beta)+\boldsymbol{t})] = \Gamma^{(\kappa,\boldsymbol{q})}_{dc}[(\bar{\tau}|\boldsymbol{\tau}(\bar{\tau}))^{-1}(\beta|\boldsymbol{\tau}(\beta)+\boldsymbol{t})(\bar{\sigma}|\boldsymbol{\tau}(\bar{\sigma}))]\Delta^{\boldsymbol{q}}(\bar{\tau},\beta\bar{\sigma}) \tag{5}$$

where $\bar{\tau}, \bar{\sigma} \in \mathrm{P}:\mathrm{P}^{\boldsymbol{q}}$, $\Delta^{\boldsymbol{q}}(\gamma,\gamma') = \delta_{\gamma\mathrm{P}^{\boldsymbol{q}},\gamma'\mathrm{P}^{\boldsymbol{q}}}$ for all $\gamma, \gamma' \in \mathrm{P}$.

At this point it is convenient to emphasise a very important rule which must be adhered to throughout the calculation of CG coefficients for Kronecker products of space group unirreps. This rule is that *the left coset representatives of $\mathrm{P}^{\boldsymbol{q}}$ in P are chosen at the outset and from then on must remain fixed.* In Dirl (1979a, c) these left coset representatives are always underbarred, but here, for printing reasons, they are always overbarred.

The multiplicities $m_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$ in the reduction of the Kronecker product $\Lambda^{(\kappa,\boldsymbol{q})}\otimes\Lambda^{(\kappa',\boldsymbol{q}')}$ of two unirreps $\Lambda^{(\kappa,\boldsymbol{q})}$, $\Lambda^{(\kappa',\boldsymbol{q}')}$ of G into a direct sum of component unirreps $\Lambda^{(\kappa_0,\boldsymbol{q}_0)}$, are defined by

$$\Lambda^{(\kappa,\boldsymbol{q})}\otimes\Lambda^{(\kappa',\boldsymbol{q}')} \sim \sum_{\kappa_0,\boldsymbol{q}_0} \oplus\, m_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}\Lambda^{(\kappa_0,\boldsymbol{q}_0)} \tag{6}$$

where $\sim$ denotes equivalence. For given vectors $\boldsymbol{q}, \boldsymbol{q}' \in \Delta\mathrm{BZ}$, the possible vectors $\boldsymbol{q}_0 \in \Delta\mathrm{BZ}$ in the right-hand side of (6), for which non-zero multiplicities occur, are determined by wavevector selection rules (WVSR):

$$\boldsymbol{q}(\bar{\sigma}) + \boldsymbol{q}'(\bar{\sigma}') = \boldsymbol{q}_0 + \boldsymbol{Q}[\boldsymbol{q}(\bar{\sigma}) + \boldsymbol{q}'(\bar{\sigma}')] \tag{7}$$

where $\boldsymbol{Q}[\boldsymbol{q}(\bar{\sigma}) + \boldsymbol{q}'(\bar{\sigma}')]$ is a translation vector of the reciprocal lattice, and $\bar{\sigma}, \bar{\sigma}'$ are certain special left coset representatives of $\mathrm{P}^{\boldsymbol{q}}$, $\mathrm{P}^{\boldsymbol{q}'}$ respectively, with respect to P, $(\bar{\sigma} \in \mathrm{P}:\mathrm{P}^{\boldsymbol{q}}, \bar{\sigma}' \in \mathrm{P}:\mathrm{P}^{\boldsymbol{q}'})$. The restrictions on $\bar{\sigma}, \bar{\sigma}'$ are so severe that frequently, but by no means always, for given $\boldsymbol{q} \in \Delta\mathrm{BZ}$, only one WVSR (7) exists. In this connection, see § 6.1 of CDML. (The term leading wavevector selection rule (LWVSR) is sometimes used to describe (7) (Lewis 1973, Dirl 1981, 1982). Although this is a more descriptive term, we shall not use it here in order to remain consistent with the terminology used in CDML.)

Equivalent versions of the formula for multiplicity in (6) have been given by Bradley (1966), Lewis (1973) and Dirl (1979b). The WVSR and multiplicities for all Kronecker products involving non-trivial little co-groups P^{q}, $P^{q'}$ have been computer generated for all 230 (single and double) space groups (Davies and Cracknell 1979, Cracknell and Davies 1979).

In the calculation of CG coefficients it is crucial to distinguish between different WVSR (7) having identical vectors $q_0 \in \Delta BZ$, and to emphasise this point, we extend slightly the notation of Dirl (1979b). For given q, q'; q_0, each WVSR (7) may be labelled by a pair of left coset representatives $(\bar{\sigma}, \bar{\sigma}')$ and the set of such pairs is denoted by $P(q, q'; q_0)$. We denote by $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$, which we call a 'component multiplicity', the contribution to the multiplicity $m_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$ from the WVSR labelled by $(\bar{\sigma}, \bar{\sigma}')$. Equation III.83 of Dirl (1979b) then reads

$$m_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} = \sum_{(\bar{\sigma},\bar{\sigma}')\in P(q,q';q_0)} m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} \tag{8}$$

where

$$m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} = \frac{1}{|P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}|} \sum_{x\in P^{q,q';q_0}_{\sigma,\sigma'}} B^{q_0^*}_{\bar{e},\bar{e}}(x) B^{q}_{\bar{\sigma},\bar{\sigma}}(x) B^{q'}_{\bar{\sigma}',\bar{\sigma}'}(x)$$
$$\times X^{\kappa}(\bar{\sigma}^{-1}x\bar{\sigma}) X^{\kappa'}(\bar{\sigma}'^{-1}x\bar{\sigma}') X^{\kappa_0^*}(x). \tag{9}$$

Equations (7), (8) and (9) are equivalent to equations (6.33), (6.31) and (6.32), respectively, of CDML.

The unitary CG matrix $C^{(\kappa,q)(\kappa',q')}$ is defined by

$$(C^{(\kappa,q)(\kappa',q')})^{+}(\Lambda^{(\kappa,q)}[g]\otimes\Lambda^{(\kappa',q')}[g])C^{(\kappa,q)(\kappa',q')}$$
$$= \sum_{\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0} \oplus\, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} \Lambda^{(\kappa_0,q_0)}[g] \tag{10}$$

for all $g \in G$, where + denotes the adjoint. The dimension of $C^{(\kappa,q)(\kappa',q')}$ is $(l_q n_\kappa)\times(l_{q'} n_{\kappa'})$ and the CG coefficients are the elements of this matrix:

$$C^{(\kappa,q)(\kappa',q')}_{\bar{\tau}d,\bar{\tau}'d';(\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0)w\bar{\sigma}_0 j} \tag{11}$$

where the rows are indexed lexicographically by $\bar{\tau}d$, $\bar{\tau}'d'$ such that $\bar{\tau}\in P:P^{q}$, $d=1, 2,\ldots,n_\kappa$, $\bar{\tau}'\in P:P^{q'}$, $d'=1, 2,\ldots,n_{\kappa'}$; and the columns are indexed by $(\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0)w\bar{\sigma}_0 j$ for those $(\kappa_0,(\bar{\sigma},\bar{\sigma}')q_0)$ such that in (10)

$$m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)} > 0 \qquad w = 1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,q)(\kappa',q');(\kappa_0,q_0)}$$

$\bar{\sigma}_0 \in P:P^{q_0}$, $j=1,2,\ldots,n_{\kappa_0}$. The index w is called a 'component multiplicity index', and in the following, when we refer to 'multiplicity index', we mean 'component multiplicity index'.

The main difficulty in calculating CG coefficients for space groups arises from component multiplicities greater than unity and not necessarily from multiplicities greater than unity since the latter, from (8), can arise from a sum of unit component multiplicities. The first example of this was found by Bradley (1966) and other examples may be found in Davies and Cracknell (1979) and Cracknell and Davies (1979) using table 6.1 in CDML.

The CG matrix (11) is built up column by column and an important part of this procedure is to identify the different values of the multiplicity index w with different special column indices of the Kronecker product $\Lambda^{(\kappa,q)}\otimes\Lambda^{(\kappa',q')}$. In other words, for given $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)} > 0$, the task is to find special column indices $(\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v)$, so that

$$w = (\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v) \qquad v = 1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}. \tag{12}$$

When this can be done, then a 'special solution of the (component) multiplicity problem' has been found and then all the elements of the CG matrix in the columns labelled by $(\kappa_0, (\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0)$ can be computed using a single explicit formula in terms of only the allowed matrix unirreps $\Gamma^{(\kappa,\boldsymbol{q})}$, $\Gamma^{(\kappa',\boldsymbol{q}')}$, $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$ (Dirl 1979c). In the next section we discuss the circumstances in which such special solutions can be found.

3. Special solutions of the multiplicity problem and Dirl's criterion

For convenience, we classify the WVSR (7) that can occur in the reduction of a given Kronecker product $\Lambda^{(\kappa,\boldsymbol{q})} \otimes \Lambda^{(\kappa',\boldsymbol{q}')}$ into one of the following three types. The triple intersection group $P^{\boldsymbol{q},\boldsymbol{q}';\boldsymbol{q}_0}_{\bar{\sigma},\bar{\sigma}'}$ is defined by

$$P^{\boldsymbol{q},\boldsymbol{q}';\boldsymbol{q}_0}_{\bar{\sigma},\bar{\sigma}'} = (\bar{\sigma} P^{\boldsymbol{q}} \bar{\sigma}^{-1}) \cap (\bar{\sigma}' P^{\boldsymbol{q}'} \bar{\sigma}'^{-1}) \cap P^{\boldsymbol{q}_0} \tag{13}$$

and $\{e\}$ denotes the trivial group.

Type I

$$P^{\boldsymbol{q}_0} = \{e\}. \tag{14}$$

Type II

$$P^{\boldsymbol{q}_0} \neq \{e\} \qquad \text{and} \qquad P^{\boldsymbol{q},\boldsymbol{q}';\boldsymbol{q}_0}_{\bar{\sigma},\bar{\sigma}'} = \{e\}. \tag{15}$$

Type III

$$P^{\boldsymbol{q},\boldsymbol{q}';\boldsymbol{q}_0}_{\bar{\sigma},\bar{\sigma}'} \neq \{e\}. \tag{16}$$

Type I WVSR correspond to cases A.1, B.1, C.1 of Dirl (1979c). Type II WVSR correspond to cases A.2, B.2, C.2a of Dirl (1979c). Type III WVSR correspond to case C.2 of Dirl (1979c), but excluding subcase C.2a.

Dirl (1979c) has shown that special solutions of the multiplicity problem always exist for WVSR of type I.

The existence of special solutions for type II WVSR depends on the projective matrix unirreps R^{κ_0} of $P^{\boldsymbol{q}_0}$. If R^{κ_0} is such that n_{κ_0} group elements $x_i \in P^{\boldsymbol{q}_0}$, $i = 1, 2, \ldots, n_{\kappa_0}$, can be found such that, for some fixed integer a_0 in the range $1 \leq a_0 \leq n_{\kappa_0}$,

$$R^{\kappa_0^*}_{a_0 a_0}(x_i x_j^{-1}) = \delta_{ij} \tag{17}$$

for all $i, j = 1, 2, \ldots, n_{\kappa_0}$, then Dirl (1979c) has shown that a special solution of the multiplicity problem exists. We refer to (17) as 'Dirl's criterion'.

Special solutions of the multiplcity problem for WVSR of type III will be considered in paper II of this series.

Returning to type II WVSR, it is convenient to express (17) in terms of the allowed matrix unirrep $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$ rather than the projective matrix unirrep R^{κ_0}. Using (4), it is straightforward to show that

$$R^{\kappa_0^*}_{a_0 a_0}(x_i x_j^{-1}) = \exp[i\boldsymbol{q}_0 \cdot (\boldsymbol{t}_{ij} + \boldsymbol{\tau}(x_i x_j^{-1}))] \\ \times \sum_{b=1}^{n_{\kappa_0}} \Gamma^{(\kappa_0,\boldsymbol{q}_0)^*}_{a_0 b}[(x_i | \boldsymbol{\tau}(x_i))] \Gamma^{(\kappa_0^*,\boldsymbol{q}_0)}_{a_0 b}[(x_j | \boldsymbol{\tau}(x_j))] \tag{18}$$

where

$$t_{ij} = \tau(x_i) - x_i x_j \tau(x_j) - \tau(x_i x_j^{-1}) \tag{19}$$

and $t_{ij} \in \mathrm{T}$.

Now

$$\tau(e) = \mathbf{0} \tag{20}$$

and so (20) in (19) implies

$$t_{ii} = \mathbf{0}. \tag{21}$$

Using (18)-(21) in (17), Dirl's criterion can now be expressed in terms of the allowed matrix unirrep $\Gamma^{(\kappa_0, q_0)}$ as follows.

If $\Gamma^{(\kappa_0,q_0)}$ is such that n_{κ_0} group elements $(x_i | \tau(x_i)) \in \mathrm{G}^{q_0}$, $i = 1, 2, \ldots, n_{\kappa_0}$, can be found such that, for some fixed integer a_0 in the range $1 \leq a_0 \leq n_{\kappa_0}$,

$$\sum_{b=1}^{n_{\kappa_0}} \Gamma_{a_0 b}^{(\kappa_0,q_0)*}[(x_i | \tau(x_i))]\Gamma_{a_0 b}^{(\kappa_0,q_0)}[(x_j | \tau(x_j))] = \delta_{ij} \tag{22}$$

for all $i, j = 1, 2, \ldots, n_{\kappa_0}$, then a special solution of the multiplicity problem exists.

The left-hand side of (22) is in the form of a scalar product of the a_0th row vector of the matrix representing $(x_i | \tau(x_i))$, with the a_0th row vector of the matrix representing $(x_j | \tau(x_j))$. Thus (22) requires that these vectors be orthonormal. We now see that Dirl's criterion is satisfied if, from amongst the allowed matrices $\Gamma^{(\kappa_0,q_0)}$, n_{κ_0} matrices can be found such that for fixed integer a_0 in the range $1 \leq a_0 \leq n_{\kappa_0}$, the a_0th rows are pairwise orthogonal. (The unitarity of the matrices $\Gamma^{(\kappa_0,q_0)}$ guarantees that the rows are of unit norm.) If, further, the n_{κ_0} unitary matrices $\Gamma^{(\kappa_0,q_0)}[(x_i | \tau(x_i))]$, $i = 1, 2, \ldots, n_{\kappa_0}$, satisfying (22), for some integer a_0, are also *monomial* matrices (i.e. with exactly one non-zero element in each row and column) then these matrices will satisfy (22) for *all* values of the integer a_0 in the range $1 \leq a_0 \leq n_{\kappa_0}$.

Up to this point we have only considered 'single' space groups. Dirl (1981) has shown that the results in Dirl (1979b, c) for 'single' space groups G generalise naturally to 'double' space groups G*. For double space groups, the trivial group in (14)-(16) is replaced by the group $\mathrm{Z}^* = \{e, \bar{e}\}$, where e is the identity and $\bar{e}$ is the rotation through 2π. Equation (22) remains unchanged, where $\Gamma^{(\kappa_0,q_0)}$ now denotes an allowed matrix unirrep of the double group $\mathrm{G}^{q_0^*}$. With these minor changes, the classification of WVSR into three types and the corresponding statements concerning special solutions of the multiplicity problem, remain true for double space groups.

4. Miller and Love standard matrices

We show below that, for all 230 (single and double) space groups, the ML allowed matrix unirreps $\Gamma^{(\kappa_0,q_0)}$, as extended by CDML, satisfy Dirl's criterion (22) for all $q_0 \in \Delta\mathrm{BZ}$.

Obviously, all $\Gamma^{(\kappa_0,q_0)}$, for which $n_{\kappa_0} = 1$, automatically satisfy (22), and this includes the special case when $\mathrm{P}^{q_0^*} = \mathrm{Z}^*$, i.e. when q_0 is a 'general point' for which the WVSR (7) is of type I. All $\Gamma^{(\kappa_0,q_0)}$ for all 'special points', i.e. for which $\mathrm{P}^{q_0^*} \supset \mathrm{Z}^*$, are tabulated for all 230 (single and double) space groups in CDML. Thus, if all of these $\Gamma^{(\kappa_0,q_0)}$ satisfy (22), then special solutions of the multiplicity problem will exist for all WVSR of type II.

In CDML, for given $(\kappa_0, \boldsymbol{q}_0)$, only 'augmenting matrices' $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}[(a\,|\,\boldsymbol{\tau}(a))]$ are tabulated, where $\{(a\,|\,\boldsymbol{\tau}(a))\}$ is a special subset of $G^{\boldsymbol{q}_0^*}:T$, and $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}[(\alpha\,|\,\boldsymbol{\tau}(\alpha)+\boldsymbol{t})]$, for any $(\alpha\,|\,\boldsymbol{\tau}(\alpha)+\boldsymbol{t}) \in G^{\boldsymbol{q}_0^*}$, may be generated from the tabulated set of augmenting matrices by using (3) and matrix multiplication.

Furthermore, for any given $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$, of dimension n_{κ_0} $(=d)$, any augmenting matrix is given by

$$\Gamma^{(\kappa_0,\boldsymbol{q}_0)}[(a\,|\,\boldsymbol{\tau}(a))] = \varepsilon_a^{(\kappa_0,\boldsymbol{q}_0)} S_a^d \tag{23}$$

where

$$|\varepsilon_a^{(\kappa_0,\boldsymbol{q}_0)}| = 1 \tag{24}$$

and S_a^d is one of a *small set of standard unitary matrices* $\{S_i^d\}$ of dimension d.

Given $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$, suppose that U^i is a (unitary) matrix generated from the set of augmenting standard matrices, then (3), (23) and (24) imply that there exists $(x_i\,|\,\boldsymbol{\tau}(x_i)) \in G^{\boldsymbol{q}_0^*}$ such that

$$\Gamma^{(\kappa_0,\boldsymbol{q}_0)}[(x_i\,|\,\boldsymbol{\tau}(x_i))] = \omega_i^{(\kappa_0,\boldsymbol{q}_0)} U^i \tag{25}$$

where

$$|\omega_i^{(\kappa_0,\boldsymbol{q}_0)}| = 1. \tag{26}$$

Suppose further that n_{κ_0} monomial unitary matrices U^i, $i = 1, 2, \ldots, n_{\kappa_0}$ can be found such that, for all $a_0 = 1, 2, \ldots, n_{\kappa_0}$,

$$\sum_{b=1}^{n_{\kappa_0}} U^{i*}_{a_0 b}\, U^{j}_{a_0 b} = \delta_{ij} \tag{27}$$

for all $i, j = 1, 2, \ldots, n_{\kappa_0}$, then (25)-(27) imply that Dirl's criterion (22) is satisfied so that a special solution of the multiplicity problem exists for any value of the integer a_0, $1 \leqslant a \leqslant n_{\kappa_0}$.

An ALGOL computer program was written to examine the augmenting standard matrices tabulated for each $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$ for all 230 (single and double) space groups. The tabulations of CDML on magnetic tape formed the input data to the program. (Note: the complete set of standard matrices of ML, which are required for the tabulation of representations *and co-representations*, were reprinted in table 5.1 of CDML. Not all the standard matrices in table 5.1 of CDML are actually used in the tabulation of representations. For example, all the eight-dimensional matrices only occur for co-representations. Only one-, two-, three-, four- and six-dimensional standard matrices occur in the tabulation of representations.)

The remarkable fact is that for every $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$ in all 230 (single and double) space groups, it is possible to generate from the augmenting standard matrices for $\Gamma^{(\kappa_0,\boldsymbol{q}_0)}$, n_{κ_0} monomial unitary matrices U^i, $i = 1, 2, \ldots, n_{\kappa_0}$, which satisfy (27) and therefore Dirl's criterion (22). This is demonstrated as follows. Apart from the trivial case $n_{\kappa_0} = 1$, each set of augmenting standard matrices is such that one special matrix A (for $n_{\kappa_0} = 2, 3$) or two special matrices A and B (for $n_{\kappa_0} = 4, 6$) can be found from which the set $\{U^i\}$, $i = 1, 2, \ldots, n_{\kappa_0}$, can be generated to satisfy (27). Let S_i^d denote the ith standard matrix of dimension d in table 5.1 of CDML. Let $E = S_1^d$, $d = 1, 2, 3, 4, 6$, where E denotes the identity matrix. Consider the cases $n_{\kappa_0} = 1, 2, 3, 4, 6$ in turn.

$n_{\kappa_0} = 1$

$$U^1 = E.$$

$n_{\kappa_0} = 2$

$$U^1 = E \qquad U^2 = A \tag{28}$$

where

$$A = S_i^2 \qquad i \in \{2, 3, 7, 12\}. \tag{29}$$

General form:

$$A = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix} \qquad |\alpha| = |\beta| = 1.$$

$n_{\kappa_0} = 3$

$$U^1 = E \qquad U^2 = A^{-1} \qquad U^3 = A \tag{30}$$

where

$$A = S_i^3 \qquad i \in \{4, 9\}. \tag{31}$$

General form:

$$A = \begin{pmatrix} 0 & 0 & \pm 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

$n_{\kappa_0} = 4$

$$U^1 = E \qquad U^2 = A \qquad U^3 = B \qquad U^4 = AB \tag{32}$$

where either

$$\begin{aligned} & A = S_i^4 \qquad i \in \{3, 8, 9, 11, 12, 24, 27, 46\} \\ \text{or} \quad & A = (S_{32}^4)(S_{33}^4) \end{aligned} \tag{33}$$

and

$$B = S_j^4 \qquad j \in \{5, 13, 17, 54, 73\}. \tag{34}$$

General forms:

$$A = \begin{pmatrix} 0 & \alpha & 0 & 0 \\ \beta & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma \\ 0 & 0 & \delta & 0 \end{pmatrix} \qquad |\alpha| = |\beta| = |\gamma| = |\delta| = 1$$

$$B = \begin{pmatrix} 0 & 0 & a & 0 \\ 0 & 0 & 0 & b \\ c & 0 & 0 & 0 \\ 0 & d & 0 & 0 \end{pmatrix} \qquad |a| = |b| = |c| = |d| = 1$$

$$AB = \begin{pmatrix} 0 & 0 & 0 & \alpha b \\ 0 & 0 & \beta a & 0 \\ 0 & \gamma d & 0 & 0 \\ \delta c & 0 & 0 & 0 \end{pmatrix}.$$

$n_{\kappa_0} = 6$

$$U^1 = E \qquad U^2 = A^{-1} \qquad U^3 = A$$
$$U^4 = B \qquad U^5 = ABA^{-1} \qquad U^6 = AB \tag{35}$$

where

$$A = S^6_{10} \tag{36}$$

and

$$B = S^6_7. \tag{37}$$

$$A = \begin{pmatrix} X & 0 \\ 0 & X^{\mathrm{T}} \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & -E \\ E & 0 \end{pmatrix} \qquad E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$AB = \begin{pmatrix} 0 & -X \\ X^{\mathrm{T}} & 0 \end{pmatrix} \qquad ABA^{-1} = \begin{pmatrix} 0 & -X^{\mathrm{T}} \\ X & 0 \end{pmatrix}.$$

For each $\Gamma^{(\kappa_0, q_0)}$ in all 230 (single and double) space groups, the program checked the existence of the special matrices A and B, given by (29), (31), (33), (34), (36) and (37) in the set of augmenting standard matrices. This was also double-checked by hand!

5. Conclusion

In this paper we report 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 satisfy Dirl's criterion (22) and so provide special solutions of the multiplicity problem for all wavevector selection rules of type II occurring in any Kronecker product of space group unirreps.

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