

SELECTION RULES FOR MAGNETIC GROUPS  
APPLICATION TO TYPE II SHUBNIKOV SPACE GROUPS

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A general method for calculating subduction matrices for corepresentations of a magnetic group is discussed and the results are then specified to compute with them Clebsch-Gordan matrices for type II Shubnikov space groups.

## I. Preliminaries

Let  $G = \{H, sH\}$  be a coset decomposition of a finite magnetic ("antiunitary") group  $G$  with respect to the normal ("unitary") subgroup  $H$ . Unitary corepresentations of  $G$  are matrix representations satisfying <sup>1,2</sup>

$$B^*(s^{-1}hs) = B(s)^+ B(h) B(s) \quad \text{for all } h \in H \quad (I.1)$$

$$B(s) B^*(s) = B(s^2) \quad \text{with } s^2 \in H \quad (I.2)$$

$$B(s) B^*(h) = B(sh) \quad \text{for all } h \in H \quad (I.3),$$

where  $B(h); h \in H$  forms an ordinary vector representation of  $H$ . (Projective corepresentations will not be discussed for the sake of simplicity). We call two unitary corepresentations  $B(g); g \in G$  and  $B'(g); g \in G$  as equivalent, if and only if there exists a unitary matrix  $W$  with the property

$$W^+ B(g) W^G = B'(g) \quad \text{for all } g \in G \quad (I.4)$$

where the superscript  $g \in sH$  implies complex conjugation of  $W$ , whereas  $g \in H$  that  $W$  remains unchanged.

Concerning the unitary irreducible corepresentations (counirreps) of  $G$  one distinguishes three different types, which read in standard form as follows.

type I:  $D^\alpha(h) = D^\alpha(h) \quad (I.5)$

$$D^\alpha(s) = U^\alpha; \quad U^\alpha U^{\alpha*} = D^\alpha(s^2) \quad (I.6)$$

$$D^\alpha(s^{-1}hs)^* = U^{\alpha+} D^\alpha(h) U^\alpha \quad (I.7)$$

type II:  $D^\beta(h) = \begin{vmatrix} D^\beta(h) & 0 \\ 0 & D^\beta(h) \end{vmatrix} \quad (I.8)$

$$D^\beta(s) = \begin{vmatrix} 0 & U^\beta \\ -U^\beta & 0 \end{vmatrix}; \quad U^\beta U^{\beta*} = -D^\beta(s^2) \quad (I.9)$$

$$D^\beta(s^{-1}hs)^* = U^{\beta+} D^\beta(h) U^\beta \quad (I.10)$$

type III:  $D^\gamma(h) = \begin{vmatrix} D^\gamma(h) & 0 \\ 0 & D^\gamma(s^{-1}hs)^* \end{vmatrix}; \quad D^\gamma(s^{-1}hs)^* = Z^{\gamma+} D^{\bar{\gamma}}(h) Z^\gamma \quad (I.11)$

$$D^\gamma(s) = \begin{vmatrix} 0 & D^\gamma(s^2) \\ 1_Y & 0 \end{vmatrix} \quad (I.12)$$

Thereby the symbols  $D^i(g); g \in G$  denote counirreps of  $G$ ,  $D^i(h); h \in H$  the corresponding  $n_\mu$ -dimensional vector unirreps of  $H$  and  $\mu$  equivalence classes.

## II. Subduction matrices for corepresentations

Starting from a N-dimensional reducible corepresentation  $\mathbf{B}(g)$ ;  $g \in G$ , we call a unitary matrix  $W$  a "subduction matrix", if

$$W^\dagger \mathbf{B}(g) W = \sum_{\mu} \oplus M_{\mu} \mathbf{D}^{\mu}(g) \quad \text{for all } g \in G \quad (\text{II.1})$$

is satisfied, at which the quantity  $M_{\mu}$  ("multiplicity") indicates how many times the counirrep  $\mathbf{D}^{\mu}$  is contained in  $\mathbf{B}$ . (In this connection we remark that the name subduction matrix originates therefrom that in general  $\mathbf{B}$  forms a representation of a larger group  $M$  which contain  $G$  as subgroup).

Now the problem is to determine a unitary matrix  $W$  as systematic as possible, which satisfies (II.1). A first step towards a solution of this problem is done by re-writing (II.1) in the following manner.

$$\mathbf{B}(g) \{\tilde{W}_p^{\mu W}\}^G = \sum_q \mathbf{D}_{qp}^{\mu}(g) \tilde{W}_q^{\mu W} \quad (\text{II.2})$$

This implies that we consider the columns  $\tilde{W}_p^{\mu W}$  ( $\{\tilde{W}_p^{\mu W}\}_k = W_{k;\mu W p}$  where  $k = 1, 2, \dots, N$  and  $\mu \in A_G$ ;  $w = 1, 2, \dots, M_{\mu}$ ;  $p = 1, 2, \dots, N_{\mu}$ ) of  $W$  as  $G$ -adapted vectors of a N-dimensional Euclidean space  $V$ . For obvious reasons we divide the procedure of determining  $W$  into two steps. First we compute a subduction matrix  $S$  which decompose  $\mathbf{B}(h)$ ;  $h \in H$  into a direct sum of its irreducible constituents (with respect to  $H$ ) and secondly we use (parts of) this matrix  $S$  in order to compute  $W$ .

### II.a. Subduction matrices for ordinary representations

Let us start from

$$S^\dagger \mathbf{B}(h) S = \sum_{\mu} \oplus m_{\mu} \mathbf{D}^{\mu}(h) \quad \text{for all } h \in H \quad (\text{II.3})$$

$$\mathbf{B}(h) \tilde{S}_a^{\mu V} = \sum_b \mathbf{D}_{ba}^{\mu}(h) \tilde{S}_b^{\mu V} \quad v = 1, 2, \dots, m_{\mu}; b = 1, 2, \dots, n_{\mu} \quad (\text{II.4})$$

by considering the columns of  $S$  as  $H$ -adapted vectors of  $V$ , at which the multiplicities  $m_{\mu}$  have to be computed by means of the usual character formula. When calculating subduction matrices it is known, that the main difficulties arise from the problem how to fix the "multiplicity index"  $v$ , if  $m_{\mu}$  is greater than one. But Eqs.(II.4) together with the unitarity of  $S$  suggest how the multiplicity index  $v$  can be determined. Namely by utilizing the usual projection techniques.

For this purpose we introduce a N-dimensional matrix representation of the group algebra A(H). The corresponding "units"

$$\mathbf{E}_{ab}^{\mu} = n_{\mu} |H|^{-1} \sum_h D_{ab}^{\mu*}(h) \mathbf{B}(h) \quad (\text{II.5})$$

satisfying well known rules are because of

$$\mathbf{E}_{ab}^{\mu} \mathbf{S}_c^{\mu'v} = \delta_{\mu\mu'} \delta_{bc} \mathbf{S}_a^{\mu'v} \quad (\text{II.6})$$

especially suited to simplify the computation of S, since now we can apply the usual projection techniques. In doing so we start for fixed  $\mu$  and appropriated chosen index a from the subspace

$$V_a^{\mu} = \mathbf{E}_{aa}^{\mu} V; \quad \dim V_a^{\mu} = m_{\mu} \quad (\text{II.7})$$

Obviously any orthonormal basis

$$\{\tilde{Z}_a^{\mu v}\}_p = Z_{p;\mu v a} \quad ; \quad v = 1, 2, \dots m_{\mu} \quad (\text{II.8})$$

of  $V_a^{\mu}$  represents already a part of the columns of S. In this connection we have to note that the arbitrariness of choosing a basis of  $V_a^{\mu}$  reflects the difficulties concerning "phase conventions" etc. Apart from this the remaining columns of S (which belong to  $\mu$ ) must be computed by

$$\tilde{Z}_b^{\mu v} = \mathbf{E}_{ba}^{\mu} \tilde{Z}_a^{\mu v} \quad ; \quad v = 1, 2, \dots m_{\mu}; b = 1, 2, \dots n_{\mu} \quad (\text{II.9}),$$

otherwise the defining equation (II.4) (or (II.3)) cannot be satisfied.

Hence it follows that the only problem of this method consists of determining for each subspace  $V_a^{\mu}$  (a = fixed for a given  $\mu$ ) an orthonormal basis. This can be done in any way by Schmidt's procedure. But instead of applying this procedure immediately, we consider in more detail the  $m_{\mu}$ -dimensional subspace  $V_a^{\mu}$ . In order to obtain a basis of  $V_a^{\mu}$ , it suffices to apply the corresponding projection matrix  $\mathbf{E}_{aa}^{\mu}$  to each element of the orthonormalized basis  $\tilde{\mathbf{B}}_q$ ;  $q = 1, 2, \dots N$  ( $\{\tilde{\mathbf{B}}_q\}_p = \delta_{pq}$ ) of V.

$$\tilde{\mathbf{B}}_a^{\mu q} = \mathbf{E}_{aa}^{\mu} \tilde{\mathbf{B}}_q \quad ; \quad \{\tilde{\mathbf{B}}_a^{\mu q}\}_p = n_{\mu} |H|^{-1} \sum_h D_{aa}^{\mu*}(h) \mathbf{B}_{pq}(h) \quad (\text{II.10})$$

Our approach of computing subduction matrices is now as follows: In case we can find  $m_{\mu}$  vectors  $\tilde{\mathbf{B}}_a^{\mu v}$ ;  $v = 1, 2, \dots m_{\mu}$  satisfying

$$\|\tilde{\mathbf{B}}_a^{\mu q_v}\|^2 = \langle \tilde{\mathbf{B}}_a^{\mu q_v}, \mathbf{E}_{aa}^{\mu} \tilde{\mathbf{B}}_{q_v} \rangle = n_{\mu} |H|^{-1} \sum_h D_{aa}^{\mu*}(h) \mathbf{B}_{q_v q_v}(h) > 0 \quad (\text{II.11})$$

$$\begin{aligned} \langle \tilde{B}_a^{\mu q_V}, \tilde{B}_a^{\mu q_V'} \rangle &= \langle \tilde{B}_{q_V}, E_{aa}^{\mu} \tilde{B}_{q_V'} \rangle = \\ &= n_{\mu} |H|^{-1} \sum_h D_{aa}^{\mu*}(h) B_{q_V q_V'}(h) = 0 \iff q_V \neq q_V', \end{aligned} \quad (II.12)$$

the following vectors with their components

$$\{\tilde{S}_a^{\mu v}\}_p = \|\tilde{B}_a^{\mu q_V}\|^{-1} \langle \tilde{B}_p, E_{aa}^{\mu} \tilde{B}_{q_V} \rangle = \|\tilde{B}_a^{\mu q_V}\|^{-1} n_{\mu} |H|^{-1} \sum_h D_{aa}^{\mu*}(h) B_{pq_V}(h) \quad (II.13)$$

are already a part of the desired columns of  $S$ , which form an orthonormal basis of  $V_a^{\mu}$  and where the remaining columns are immediately obtained by (II.9). However this approach requires that (II.12) is satisfied. Provided this is true, our method allows to identify in a systematic way the multiplicity index  $v$  in terms of special column indices  $q_V$  of  $B$ , what is called in the following "special solution of the multiplicity problem". But in general we shall find only  $m_{\mu}$  ( $m_{\mu} < m_{\mu}$ ) vectors satisfying (II.11,12) what implies that  $m_{\mu} - m_{\mu}$  vectors have to be determined by Schmidt's procedure. But even for this most complicated situation, it is reasonable to consider Eqs.(II.11,12), since their use lead to computational simplifications. In order to understand this proposition, one has to remember that there exists just  $m_{\mu}$  linear independent vectors  $\tilde{B}_a^{\mu q}$ ;  $q = 1, 2, \dots, N$  and that  $\|\tilde{B}_a^{\mu q}\|^2 = 0$  (for some  $q$ ) requires  $\{\tilde{B}_a^{\mu p}\}_q = 0$  for all  $p = 1, 2, \dots, N$ . Hence if the norm of the vectors (II.10) disappears for some  $q$  the corresponding components of the columns of the subduction matrices must be zero.

## II.b. Subduction matrices for corepresentations

Since there exists three different types of counirreps we have to consider them separately by inserting their special form (standard form) into (II.2).

Subductions of type I: According to (I.5,6) Eqs.(II.2) turn out to be

$$B(h) \tilde{W}_a^{\alpha w} = \sum_b D_{ba}^{\alpha}(h) \tilde{W}_b^{\alpha w} \quad (II.14)$$

$$B(s) \{\tilde{W}_a^{\alpha w}\}^* = \sum_b U_{ba}^{\alpha} \tilde{W}_b^{\alpha w}; \quad w = 1, 2, \dots, M_{\alpha} \text{ and } a = 1, 2, \dots, n_{\alpha} \quad (II.15)$$

where  $M_{\alpha} = m_{\alpha}$  has to be taken into account. Utilizing Schur's Lemma with respect to  $H$  we have

$$\tilde{W}_a^{\alpha w} = \sum_v B_{vw} \tilde{S}_a^{\alpha v} \quad (II.16)$$

if  $\tilde{S}_a^{\alpha V}$ ;  $v = 1, 2, \dots, m_\alpha$ ,  $a = 1, 2, \dots, n_\alpha$  is H-adapted. Consequently B must be a  $m_\alpha$ -dimensional unitary matrix. Otherwise, if knowing an orthonormal basis of  $V_a^\alpha$ , the general problem is reduced to the task of determining a  $m_\alpha$ -dimensional unitary matrix B so that (II.15) is satisfied. For this purpose we compute

$$B(s) \{ \tilde{S}_c^{\alpha V} \}^* = \sum_b U_{bc}^\alpha \sum_v F_{v,v} \tilde{S}_b^{\alpha V} \quad (II.17)$$

where F is unitary and uniquely fixed through  $\{ \tilde{S}_a^{\alpha V} \}$ .

$$F_{v,v} = \langle \tilde{S}_c^{\alpha V}, B(s) \{ \sum_b U_{cb}^\alpha \tilde{S}_b^{\alpha V} \}^* \rangle = \langle \tilde{S}_a^{\alpha V}, n_\alpha |H|^{-1} \sum_h D_{aa}^{\alpha*}(hs) B(hs) \{ \tilde{S}_a^{\alpha V} \}^* \rangle \quad (II.18).$$

Consequently it suffices to know the vectors  $\tilde{S}_a^{\alpha V}$ ;  $v = 1, 2, \dots, m_\alpha$  ( $a =$  fixed for a given  $\alpha$ ) in order to be able to compute the matrix F. Since F satisfies  $F = B B^\dagger = F^\dagger$ , respectively  $F F^* = 1_{m_\alpha}$ , it follows from (II.15)

$$F B^* = B; \quad F F^* = 1_{m_\alpha} \quad (II.19).$$

Thus any solution of (II.19) provides corresponding parts of W. Assuming that the vectors  $\tilde{S}_a^{\alpha V}$  can be fixed through a special solution of the multiplicity problem (see (II.13)) Eqs.(II.18) turn out to be

$$F_{v,v} = \| \tilde{S}_a^{\alpha q_v} \|^{-1} \| \tilde{S}_a^{\alpha q_v} \|^{-1} n_\alpha |H|^{-1} \sum_h D_{aa}^{\alpha*}(hs) B_{q_v, q_v}(hs) \quad (II.20)$$

which show that it suffices to know merely the multiplicity indices  $q_v$  in order to be able to compute the matrix elements (II.20).

Subductions of type II: Starting from

$$B(h) \tilde{W}_{za}^{\beta W} = \sum_b D_{ba}^\beta(h) \tilde{W}_{zb}^{\beta W}; \quad w = 1, 2, \dots, M_\beta; \quad z = 1, 2 \text{ and } a = 1, 2, \dots, n_\beta \quad (II.21)$$

$$B(s) \{ \tilde{W}_{za}^{\beta W} \}^* = (-1)^{\Delta(z+1)} \sum_b U_{ba}^\beta \tilde{W}_{z+1,b}^{\beta W}; \quad \Delta(z) = \begin{cases} 0 & \text{for } z = 1 \\ 1 & \text{for } z = 2 \end{cases} \quad (II.22)$$

where  $2M_\beta = m_\beta$  and a double index  $(z, a)$  has been introduced to enumerate row and columns of  $D^\beta(g)$ ;  $g \in G$ . Schur's Lemma with respect to H yields to

$$\tilde{W}_{za}^{\beta W} = \sum_v B_{v,za} \tilde{S}_a^{\beta V} \quad (II.23)$$

if  $\tilde{S}_a^{\beta V}$ ;  $v = 1, 2, \dots, m_\beta$ ,  $a = 1, 2, \dots, n_\beta$  is H-adapted. By similar arguments as in the foregoing case we obtain for

$$B(s) \{ \tilde{S}_c^{BV} \}^* = \sum_b U_{bc}^B \sum_v F_{v'v} \tilde{S}_b^{BV'} \quad (II.24)$$

where the  $2M_\beta$ -dimensional unitary matrix  $B$  is uniquely fixed through  $\tilde{S}_a^{BV}$ , namely

$$\begin{aligned} F_{v'v} &= \langle \tilde{S}_a^{BV'} |, n_\beta |H|^{-1} \sum_h \{ D^\beta(h) U^\beta \}_{aa}^* B(hs) \{ \tilde{S}_a^{BV} \}^* \rangle = \\ &= \| \tilde{B}_a^{BQV'} \|^{-1} \| \tilde{B}_a^{BQV} \|^{-1} n_\beta |H|^{-1} \sum_h \{ D^\beta(h) U^\beta \}_{aa}^* B_{q_v, q_v'}(hs) \end{aligned} \quad (II.25).$$

Analogously to the previous case the second line of (II.25) is only valid, if the vectors  $\tilde{S}_a^{BV}$  are given by (II.13). Furthermore we have  $F = B G^T B^T = -F^T$ , where  $G_{zw; z'w'} = (-1)^{\Delta(z)} \delta_{z, z'+1} \delta_{ww'}$ . Conversely (II.22) yields to

$$F B^* = B G^T ; \quad F F^* = -1_{2M_\beta} \quad (II.26)$$

which is in agreement with the former considerations and which has to be solved in order to obtain the corresponding parts of  $W$ .

Subductions of type III: According to (I.11,12) we have to consider

$$B(h) \tilde{W}_{1a}^{YW} = \sum_b D_{ba}^Y(h) \tilde{W}_{1b}^{YW} \quad (II.27)$$

$$B(h) \tilde{W}_{2a}^{YW} = \sum_b \{ Z^{Y\dagger} D^{\bar{Y}}(h) Z^Y \}_{ba} \tilde{W}_{2b}^{YW} \quad (II.28)$$

$$B(s) \{ \tilde{W}_{1a}^{YW} \}^* = \tilde{W}_{2a}^{YW} \quad (II.29)$$

$$B(s) \{ \tilde{W}_{2a}^{YW} \}^* = \sum_b D_{ba}^Y(s^2) \tilde{W}_{1b}^{YW} \quad (II.30),$$

where  $M_Y = m_Y = m_{\bar{Y}}$  and a double index  $(z,a)$  have been introduced. Obviously

$$\tilde{W}_{1a}^{YW} = \sum_v B_{vw} \tilde{S}_a^{YV} \quad \text{and} \quad \tilde{W}_{2a}^{YW} = \sum_v C_{vw} \tilde{S}_a^{\bar{Y}V} \quad (II.31)$$

presupposed  $\{ \tilde{S}_a^{YV} \}$  and  $\{ \tilde{S}_a^{\bar{Y}V} \}$  are  $H$ -adapted. On the other hand we obtain for

$$B(s) \{ \tilde{S}_a^{YV} \}^* = \sum_v F_{v'v} \tilde{S}_a^{\bar{Y}V'} \quad (II.32)$$

where the unitary matrix  $F$  is uniquely fixed through  $\{ \tilde{S}_a^{YV} \}$  and  $\{ \tilde{S}_a^{\bar{Y}V} \}$ .

$$\begin{aligned} F_{v'v} &= \langle \tilde{S}_a^{\bar{Y}V'} |, n_Y |H|^{-1} \sum_h \{ Z^{Y\dagger} D^{\bar{Y}}(h) Z^Y \}_{aa}^* B(hs) \{ \tilde{S}_a^{YV} \}^* \rangle = \\ &= \| \tilde{B}_a^{\bar{Y}QV'} \|^{-1} \| \tilde{B}_a^{YQV} \|^{-1} n_Y |H|^{-1} \sum_h \{ Z^{Y\dagger} D^{\bar{Y}}(h) Z^Y \}_{aa}^* B_{q_v, q_v'}(hs) \end{aligned} \quad (II.33)$$

The second line of (II.33) is only valid, if special solutions of the corresponding multiplicity problems can be found. Apart from this special situation we obtain as consequence of (II.29,30)

$$F B^* = C \quad ; \quad F F^{\dagger} = 1_{M_Y} \quad (II.34)$$

which can be solved directly. We choose as possible solution

$$B = 1_{M_Y} \iff C = F \quad (II.35)$$

by which the corresponding columns of  $W$  are immediately obtained.

Concluding this Section we recall that the crucial point of this method is to consider the columns of  $W$  as  $H$ -adapted vectors, but which have to satisfy additional transformation properties originating from a special representative of the "antiunitary" group elements. This lead us to the main result that it suffices to know only parts of  $S$  in order to be able to determine the corresponding parts of  $W$ , respectively to utilize (II.9) in order to obtain the whole subduction matrix  $W$ . (In this connection we remark that other approaches of computing Clebsch-Gordan coefficients for corepresentations are described within the papers which are listed in Ref.3).



### III. CG-matrices for corepresentations

Since Clebsch-Gordan matrices (CG-matrices) are a special case of subduction matrices (the supergroup is the direct product group  $G \times G$  and the subgroup the Kronecker product  $G[\times]G \approx G$ ), it is obvious due to our approach to consider at first the simpler task of determining (parts of) CG-matrices for ordinary representations of  $H$ . For this purpose the formulas of Sec.II.a. have to be transferred correspondingly by replacing  $B(h)$  through the Kronecker product  $D^{\mu\mu'}(h) = D^{\mu}(h) \otimes D^{\mu'}(h)$  being composed of vector unirreps of  $H$ , whose dimensions are  $n_{\mu}$  and  $n_{\mu'}$ , respectively. Consequently the single index  $p$  ( $p = 1, 2, \dots, N$ ) has to be replaced by the double index  $p, r$  ( $p = 1, 2, \dots, n_{\mu}$ ;  $r = 1, 2, \dots, n_{\mu'}$ ). Nevertheless the formulas and results of Sec.II.a. remain valid and in case we can find a "special solution of the multiplicity problem" the former index  $q_v$  is now a double index  $q_v, s_v$ ;  $v = 1, 2, \dots, m_{\mu\mu'}; \mu_0$ . (For a detailed discussion the reader is referred to Ref.4).

Now let us turn to the task of determining CG-matrices for  $G$ . Accordingly we have to replace  $B(g)$  through the Kronecker product  $D^{\mu\mu'}(g) = D^{\mu}(g) \otimes D^{\mu'}(g)$  which is composed of counirreps. Remembering that  $D^{\mu\mu'}(h)$  is already a direct sum of Kronecker products  $D^{\mu\mu'}(h)$ , if at least one of the two constituents of  $D^{\mu\mu'}(g)$  is of type II or III, the first step must be to compute parts of CG-matrices decomposing  $D^{\mu\mu'}(h)$  into direct sums. This can be done by means of the method described in Sec.II.a. Provided parts of convenient CG-matrices for  $H$  have been calculated we have to find only solutions  $B$  of (II.19) and (II.26) for the six possible combinations of  $D^{\mu\mu'}(g)$ ;  $\mu, \mu' = I, II, III$ , since (II.34) has already been solved quite generally through (II.35). Now we can imagine that depending on the six different types of Kronecker products of  $G$ , the structure of the corresponding matrices  $F$  (see (II.18), (II.25) and (II.33)) are quite different, since they split up into well-defined submatrices. Consequently the solutions of the corresponding defining equations (II.19), (II.26) and (II.34) are also quite different. Nevertheless we are able to solve these equations without reference to a special magnetic group, presupposed convenient CG-matrices for  $H$  are known. This problem has been extensively discussed in Ref.5.

In order to gain more insight into this problem let us discuss briefly and without any proof two examples.

(I  $\otimes$  I)-CG-matrices: Because of

$$D^{\alpha\alpha'}(h) = D^{\alpha\alpha'}(h) \quad (III.1)$$

it suffices to know (parts of) that CG-matrix  $M$  which decompose  $D^{\alpha\alpha'}(h)$  into a direct sum of its irreducible constituents. Hence CG-coefficients of type  $\mu_0$  ( $\mu_0 = I, II, III$ ) for  $G$  are obtained from (II.16, 23, 31), if solutions of (II.19, 26, 34) are found. The

corresponding matrices  $F$  have to be computed with (II.18,25,33).

(I  $\otimes$  III)-CG-matrices: Because of

$$D^{\alpha\gamma}(h) = D^{\alpha\gamma}(h) \oplus D^{\alpha\bar{\gamma}}(h) \quad (\text{III.2})$$

we have to determine (parts of) that CG-matrices  $M$  and  $N$  by which a decomposition of  $D^{\alpha\gamma}(h)$  and  $D^{\alpha\bar{\gamma}}(h)$  into a direct sum is achieved. CG-coefficients of type I for  $G$  are obtained in principle in the same manner as before, but where the following modifications have to be carried out: Due to the block structure of  $D^{\alpha\gamma}(h)$  we have

$$S_a^{\alpha_0^V} \leftrightarrow \tilde{Q}_a^{\alpha_0^V Z}; \{ \tilde{Q}_a^{\alpha_0^V 1} \}_{i;j} = \delta_{z'1} \{ \tilde{M}_a^{\alpha_0^V} \}_{ij}; \{ \tilde{Q}_a^{\alpha_0^V 2} \}_{i;j} = \delta_{z'2} \{ \tilde{N}_a^{\alpha_0^V} \}_{ij} \quad (\text{III.3})$$

Inserting these special vectors into (II.18) we obtain

$$F_{V'V} \leftrightarrow F_{Z'V';ZV} = \langle \tilde{Q}_a^{\alpha_0^V Z'} , D^{\alpha\gamma}(s) \{ \sum_b U_{ab}^{\alpha_0} \tilde{Q}_b^{\alpha_0^V Z} \}^* \rangle \quad (\text{III.4})$$

$$F = \begin{bmatrix} 0 & F^{\alpha_0} \\ \bar{F}^{\alpha_0} & 0 \end{bmatrix}; F^{\alpha_0 T} = \bar{F}^{\alpha_0}; F^{\alpha_0} \bar{F}^{\alpha_0*} = 1_m \quad (\text{III.5})$$

$$F_{V'V}^{\alpha_0} = \langle \tilde{M}_a^{\alpha_0^V Z'} , U^{\alpha} \otimes D^{\gamma}(s^2) \{ \sum_b U_{ab}^{\alpha_0} \tilde{N}_b^{\alpha_0^V} \}^* \rangle \quad (\text{III.6})$$

from what immediately the following solution of (II.19) can be found.

$$B = \frac{1}{\sqrt{2}} \begin{bmatrix} 1_m & 1_m \\ -i\bar{F}^{\alpha_0} & \bar{F}^{\alpha_0} \end{bmatrix} \quad (\text{III.7})$$

Summarizing the main points of this example, we see that the former index  $v$  is replaced by the double index  $z,v$  which take also the role of the multiplicity index  $w$  of the whole problem. The index  $v$  originates now from the corresponding CG-matrices  $M$  and  $N$ . Consequently we have found a general solution of (II.19) without reference to a special magnetic group  $G$ .

(I  $\otimes$  III:II)-CG-coefficients are obtained in a similar way (see Ref.5). Finally (I  $\otimes$  III:III)-CG-coefficients follow from (II.31) by inserting (II.35) and taking into account, that  $F$  has as row and column indices double indices  $z,v$  where  $v$  originates from  $M$  and  $N$ .

Concluding this section we mention that in case both constituents  $D^{\mu}(g)$  and  $D^{\mu'}(g)$  of  $D^{\mu\mu'}(g)$  are of type II or III, the matrices  $F$  are enumerated by triplet in dices  $(z,z',v)$  which originate from the special block structure of  $D^{\mu\mu'}(g)$  (see Ref.5).

#### IV. CG-matrices for type II Shubnikov space groups

Let  $G = \{H, \theta H\} = \{E, \theta\} \times H$  be a type II Shubnikov space group, where  $\theta$  represents the time reversal operation and  $H$  an ordinary space group. The multiplication law of  $G$  reads as

$$(R|\vec{\tau}(R) + \vec{\tau}|\theta^k)(S|\vec{\tau}(S) + \vec{\tau}'|\theta^n) = (RS|\vec{\tau}(RS) + \vec{\tau}(R,S) + \vec{\tau} + R\vec{\tau}'|\theta^{k+n}) \quad (IV.1)$$

$$\vec{\tau}(R,S) = \vec{\tau}(R) + R\vec{\tau}(S) - \vec{\tau}(RS); \quad R, S \in P \approx H/T \quad (IV.2)$$

where  $T$  denotes the translation and  $P$  the point group of the crystal,  $\vec{\tau}$  primitive and  $\vec{\tau}(R)$  nonprimitive lattice translations and  $R$  either an abstract element of  $P$  or a faithful matrix representation of the corresponding group element. Due to our approach the first step will be the computation (of parts) of convenient CG-matrices for the normal subgroup  $H$ .

##### IV.a. CG-matrices for $H$

In order to be able to transfer the general formulas of Sec.II.a. to space group representations, we recall briefly the form of their vector unirreps<sup>6</sup>

$$D_{\underline{Ra}; \underline{Sb}}^{\underline{\mu}}(R|\vec{\tau}(R) + \vec{\tau}) = \Delta_{\vec{q}}^{\vec{\tau}}(\underline{R}, \underline{RS}) e^{-i\vec{q}(\underline{R}) \cdot \vec{\tau}} B_{\underline{R}, \underline{S}}^{\vec{q}}(R) \mathcal{R}_{ab}^{\kappa}(\underline{R}^{-1} \underline{RS})$$

$$\begin{aligned} \mu &\leftrightarrow (\kappa, \vec{q}) + H; \quad \vec{q} \in \Delta BZ, \quad \kappa \in A_{P(\vec{q})} \\ a, b &= 1, 2, \dots, n_{\kappa}; \quad \underline{R}, \underline{S} \in P: P(\vec{q}) \end{aligned} \quad (IV.3)$$

$$P(\vec{q}) = \{R \in P \mid R\vec{q} = \vec{q} + \vec{Q}(\vec{q})\} \subseteq P \quad (IV.4)$$

$$\Delta_{\vec{q}}^{\vec{\tau}}(R, S) = \delta_{RP(\vec{q}), SP(\vec{q})} \quad (IV.5)$$

$$B_{\underline{R}, \underline{S}}^{\vec{q}}(R) = \exp(-i\vec{q}(\underline{R}) \cdot (\vec{\tau}(R) + R\vec{\tau}(\underline{S}) - \vec{\tau}(\underline{R}))) \quad (IV.6)$$

Thereby  $\Delta BZ$  denotes the fundamental (representation) domain of the corresponding Brillouin zone,  $P(\vec{q}) \approx H(\vec{q})/T$  the little cogroup,  $\vec{Q}(\vec{q})$  reciprocal lattice vectors;  $\underline{R}, \underline{S} \in P: P(\vec{q})$  left coset representatives and  $\mathcal{R}^{\kappa}(R); R \in P(\vec{q})$   $n_{\kappa}$ -dimensional projective unirreps of  $P(\vec{q})$  which belong to the factor system  $S_{\vec{q}}^{\kappa}(R, S) = \exp(-i\vec{q} \cdot (R - 1)\vec{\tau}(S))$ .

Inserting (IV.3) into (II.10), where  $B(h) \rightarrow D^{\mu\mu'}(R|\vec{\tau}(R) + \vec{\tau})$  with  $\mu \leftrightarrow (\kappa, \vec{q}) + H$  and  $\mu' \leftrightarrow (\kappa', \vec{q}') + H$ , we consider  $\mu_0 \leftrightarrow (\kappa_0, \vec{q}_0) + H$  by choosing appropriately the index  $a$  as

$\underline{R} = e$  and  $a = \text{fixed}$ . A simple calculation yields for

$$\begin{aligned} \langle \vec{B}_{\underline{S}, d; \underline{S}', d'}^{\mu_0}, \vec{E}_{ea, ea}^{\mu_0} \vec{B}_{\underline{R}, c; \underline{R}', c'}^{\mu_0} \rangle &= \langle \vec{B}_{ea}^{\mu_0}(\underline{S}, d; \underline{S}', d'), \vec{B}_{ea}^{\mu_0}(\underline{R}, c; \underline{R}', c') \rangle = \\ &= \delta_{\vec{q}(\underline{S}) + \vec{q}'(\underline{S}'), \vec{q}_0 + \vec{q}|\vec{q}(\underline{S}) + \vec{q}'(\underline{S}')|} \times \\ &\quad n_{\kappa_0} |P(\vec{q}_0)|^{-1} \sum_{\underline{R} \in P(\vec{q}_0)} \Delta_{\vec{q}(\underline{S}, \underline{R})}^{\vec{q}} \Delta_{\vec{q}'(\underline{S}', \underline{R}\underline{R}')}' \times \\ &\quad \vec{B}_{e, e}^{\vec{q}_0 *}(R) \vec{B}_{\underline{S}, \underline{R}}^{\vec{q}}(R) \vec{B}_{\underline{S}', \underline{R}'}^{\vec{q}'}(R) \mathbf{R}_{aa}^{\kappa_0}(R) * \mathbf{P}_{dc}^{\kappa_0}(\underline{S}^{-1} \underline{R}\underline{R}') \mathbf{R}_{d'c'}^{\kappa_0}(\underline{S}'^{-1} \underline{R}\underline{R}') \end{aligned}$$

$$\underline{R}, \underline{S} \in P: P(\vec{q}) ; \quad \underline{R}', \underline{S}' \in P: P(\vec{q}') \quad (\text{IV.7})$$

where the orthogonality relations for the unirreps of the translation group  $T$  have been already taken into account. Obviously Eqs.(IV.7) contain all informations to look for "special solutions of the multiplicity problem". In case we can find  $m_{\mu\mu'; \mu_0}$  orthogonal vectors, the corresponding column indices of  $D^{\mu\mu'}(R|\vec{\tau}(R) + \vec{\epsilon})$  can be chosen as multiplicity index

$$v \leftrightarrow (\underline{R}_v, c_v; \underline{R}'_v, c'_v) ; \quad v = 1, 2, \dots, m_{\mu\mu'; \mu_0} \quad (\text{IV.8})$$

and the corresponding CG-coefficients follow from (II.13). Inspecting (IV.7) for all possible cases which may occur, we obtain simple defining equations for  $v$ , because of the "wave vector selection rules" and the last two lines of (IV.7). In this connection we remark that we succeeded in solving these equations quite generally (for nearly all cases) without reference to a special space group  $H$  (see Refs.6,7,8).

#### IV.b. CG-matrices for type II Shubnikov space groups

Since  $G$  is a direct product group, it suffices to determine unitary matrices  $U^{\mu}$  ( $\mu \leftrightarrow (\kappa, \vec{q}) \uparrow H$ ) which satisfy

$$D^{\mu}(R|\vec{\tau}(R) + \vec{\epsilon})^* = U^{\mu\dagger} D^{\bar{\mu}}(R|\vec{\tau}(R) + \vec{\epsilon}) U^{\mu} \quad (\text{IV.9})$$

in order to write down the corresponding counirreps for the time reversal operation.

type I:  $D^{\mu}(e) = U^{\mu} ; \quad U^{\mu} U^{\mu *} = + 1_{\mu} \quad (\text{IV.10})$

$$\text{type II:} \quad D^\mu(\theta) = \begin{vmatrix} 0 & U^\mu \\ -U^\mu & 0 \end{vmatrix}; \quad U^\mu U^{\mu*} = -1_\mu \quad (\text{IV.11})$$

$$\text{type III:} \quad D^\mu(\theta) = \begin{vmatrix} 0 & 1_\mu \\ 1_\mu & 0 \end{vmatrix} \quad (\text{IV.12})$$

Presupposed the inversion I as point group operation belongs to P, closed expressions for  $U^\mu$  can be derived (see Refs.9,10,11). Apart from this we are now in the position to compute by means of the general formulas of the foregoing sections the unitary matrices which link CG-coefficients for H with those for G, since the solutions of (II.19,26,34) can be written down explicitly. Furthermore since the multiplicity problem for space groups is solved for nearly all cases in the sense of the former considerations, we are able to give simple formulas, which have to be inspected in order to obtain CG-matrices for G (see Ref.12).

#### IV.c. CG-matrices for Pn3'n

Let us write down some results concerning Pn3'n in order to get an impression how the proposed method works. Thereby we shall list F and the corresponding solution B.

Example 1: (I ⊗ I: I)-CG-coefficients: This example is characterized through  $\mu \leftrightarrow (0, \vec{q}) + H$  ( $\vec{q} = \pi(x, y, z) \in \Delta BZ$ ) and  $\mu' \leftrightarrow (0, \vec{q}') + H$  ( $\vec{q}' = \pi(1-x, 1-z, 1-y) \in \Delta BZ$ ), respectively  $\mu_0 \leftrightarrow (\kappa_0, \vec{q}_0) + H$  ( $\vec{q}_0 = \pi(1, 1, 1)$  and  $\kappa_0 = (0) + \sigma_h$ ), where the special symbols for  $\kappa$  are explained in Ref.13. Since a special solution of the multiplicity problem is known ( $v \leftrightarrow (x_v; x_v \sigma_{df})$ ;  $v = 1, 2, \dots, 6$  with  $x_v \in \sigma_h$ , where superfluous indices are omitted) we have to inspect a simple formula in order to obtain F.

$$F^{\mu_0}(\mu \mu') = \begin{vmatrix} 0 & 0 & \omega & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega & 0 & 0 \\ \omega & 0 & 0 & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \omega' \\ 0 & 0 & 0 & 0 & \omega' & 0 \end{vmatrix} \quad \begin{aligned} \omega &= e^{2i\vec{q}' \cdot \vec{\tau}(I)} \\ \omega' &= \exp(i\vec{q} \cdot \vec{\tau}_1 + i\vec{q}' \cdot (\sigma_{df}) \cdot (\vec{\tau}_2 + \vec{\tau}_3)) \\ \{\vec{\tau}_j\}_k &= \delta_{jk} \end{aligned} \quad (\text{IV.13})$$

$$B = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & 0 & -i & 0 & 0 & 0 \\ 0 & 1 & 0 & -i & 0 & 0 \\ \omega & 0 & -i\omega & 0 & 0 & 0 \\ 0 & \omega & 0 & -i\omega & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -i \\ 0 & 0 & 0 & 0 & \omega' & -i\omega' \end{vmatrix} \quad (\text{IV.14})$$

A comparison of  $\dim M = \dim W = 2304$  with  $\dim B = 6$  demonstrates the utility of the present method, since the computation of (IV.13) is very simple. The columns of the

CG-matrix M for Pn3n have not been written down, but are easily obtained from (IV.7) by inserting the special values for the multiplicity index (see Ref.13).

Example 2: (I  $\otimes$  III:I)-CG-coefficients: This example is characterized through  $\mu \leftrightarrow (0, \vec{q}) + H$  ( $\vec{q} = \pi(x, y, z)$ ) and  $\mu' \leftrightarrow (\kappa', \vec{q}') + H$  ( $\vec{q}' = \pi(0, 1, 0)$  and  $\kappa' = (0, 5) + P(\vec{q}')$ ), respectively  $\mu_0 \leftrightarrow (0, \vec{q}_0) + H$  ( $\vec{q}_0 = \pi(y, 1-z, x) = \vec{q}(S_{63}^+ + \vec{q}')$ ). A special solution of the multiplicity problem is given by  $v \leftrightarrow (S_{63}^+; e, v)$ ;  $v = 1, 2$  ( $v$  on the right hand side represents the column index of  $R^{\kappa'}$ ). A simple calculation yields

$$F = \begin{vmatrix} 0 & 0 & \xi & 0 \\ 0 & 0 & 0 & -\xi \\ \xi & 0 & 0 & 0 \\ 0 & -\xi & 0 & 0 \end{vmatrix} \quad \xi = \exp(i\vec{q} \cdot (\vec{\xi}_1 + \vec{\xi}_2)) \quad (IV.15)$$

$$B = \frac{1}{\sqrt{2}} \begin{vmatrix} i & 0 & 1 & 0 \\ 0 & i & 0 & 1 \\ -i\xi & 0 & \xi & 0 \\ 0 & i\xi & 0 & -\xi \end{vmatrix} \quad (IV.16)$$

Comparing the dimensions of  $\dim B = 4$  with  $\dim M = \dim N = 288 = 1/2 \dim W$ , we realize once more the utility of this approach, since also for this case the computation of F is very simple. Like in the previous case columns of the convenient CG-matrices M and N for Pn3n are not listed (see Ref.13). The only demerit of Pn3'n is that type II representations are not realized.

## References

- 1 C.J. Bradley, A.P. Cracknell, The Mathematical Theory of Symmetry in Solids (Clarendon, Oxford, 1972)
- 2 L. Jansen, M. Boon, Theory of Finite Groups, Applications in Physics (North-Holland, Amsterdam, 1967)
- 3 A. Aviran, J. Zak, J.Math.Phys.9,2138(1968)  
A. Aviran, D.B. Litvin, J.Math.Phys.14,1491(1973)  
P. Rudra, J.Math.Phys.15,2031(1974)  
J.N. Kotzev, Sov.Phys.Christallogr.19,286(1974)  
P. Gard and N.B. Backhouse, J.Phys. A8, 450(1975).  
P.M. van den Broek, J.Math.Phys.20,2028(1979)
- 4 R. Dirl, J.Math.Phys.20,659(1979)
- 5 R. Dirl, "Clebsch-Gordan coefficients for corepresentations: A  $\otimes$  B" J.Math.Phys.(in press)
- 6 R. Dirl, J.Math.Phys.20,664(1979)
- 7 R. Dirl, J.Math.Phys.20,671(1979)
- 8 R. Dirl, J.Math.Phys.20,679(1979)
- 9 R. Dirl, J.Math.Phys.20,1566(1979)
- 10 R. Dirl, J.Math.Phys.20,1570(1979)
- 11 R. Dirl, J.Math.Phys.20,1575(1979)
- 12 R. Dirl, "Selection rules for type II Shubnikov space groups" J.Math.Phys.(in press)
- 13 R. Dirl, "Selection rules for Pn3'n" J.Math.Phys.(in press)