CHAIN ADAPTATION OF SPACE GROUP REPRESENTATIONS AND INDUCED SPACE GROUP CLEBSCH-GORDAN MATRICES

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Specific subgroup chain adaptations of representations and corresponding CG-matrices are discussed. Simple applicable analytic formulas are derived which allow one to express supergroup CG-matrices in terms of subgroup CG-matrices. The results are applied to space groups.

CHAIN ADAPTED IRREPS: Let $\mathcal{G}$ be a group and $\mathcal{H}$ a subgroup of $\mathcal{G}$. We denote $\mathcal{G}$-irreps by $\mathbf{G}^\gamma = \{\mathbf{G}^\gamma(g) : g \in \mathcal{G}\}$ where $\gamma \in A(\mathcal{G})$ (= index set of $\mathcal{G}$-irrep labels) and $\mathcal{H}$-irreps by $\mathbf{H}^\mu = \{\mathbf{H}^\mu(h) : h \in \mathcal{H}\}$ where $\mu \in A(\mathcal{H})$ (= index set of $\mathcal{H}$-irrep labels) respectively. An arbitrary $\mathcal{G}$-irrep $\mathbf{G}^\gamma$ subduced onto $\mathcal{H}$ in general becomes *reducible* but does not automatically decompose into a direct sum of $\mathcal{H}$-irreps $\mathbf{H}^\mu$; $\mu \in A(\mathcal{H})$. Thus in general we have

$$\mathbf{Z}^{\gamma\dagger}\mathbf{G}^\gamma(h)\mathbf{Z}^\gamma = \sum_\mu \oplus\, m(\gamma|\mu)\, \mathbf{H}^\mu(h) \tag{1}$$

with some non-trivial unitary matrix $\mathbf{Z}^\gamma$. The symbol $m(\gamma|\mu)$ denotes the frequency of $\mathbf{H}^\mu$ in $\mathbf{G}^\gamma$. By definition every $\mathcal{G}$-irrep $\mathbf{G}^\gamma$ is called $\mathcal{G} \downarrow \mathcal{H}$*-chain adapted* if the unitary matrix $\mathbf{Z}^\gamma$ commutes with every $\mathbf{G}^\gamma(h); h \in \mathcal{H}$. Note that this property is not automatically satisfied for arbitrary $\mathcal{G}$-irreps. It is commonly accepted that, when talking about chain adapted $\mathcal{G}$-irreps, it is implicitly assumed that *every* $\mathcal{G}$-irrep is chain adapted with respect to the *same* subgroup $\mathcal{H}$. Thus to chain adapt *inequivalent* $\mathcal{G}$-irreps with respect to *different* subgroups of $\mathcal{G}$ is possible but cannot be of practical utility as for instance the *orthogonality relations* of subgroup-irreps are not usable.

Two conceptually different strategies are in use for constructing $\mathcal{G} \downarrow \mathcal{H}$-adapted $\mathcal{G}$-irreps. For the first case one starts from given $\mathcal{G}$-irreps and $\mathcal{H}$-irreps and tries to compute suitable $\mathbf{Z}$-matrices satisfying (1). This can be achieved by various methods, for instance the so-called *projection method*[1)2)3)] or by the so-called *eigenfunction method*[4)]. However both methods are inappropriate for yielding systematic results since in both approaches the *multiplicity problem* is resolved by Schmidt's procedure. Only the so-called *auxiliary group approach*[5)6)7)8)] allows one to solve the problem more systematically.

An alternative way to construct $\mathcal{G} \downarrow \mathcal{H}$-adapted $\mathcal{G}$-irreps is based on the *"induction method"* where $\mathcal{G}$-irreps are determined out of given $\mathcal{H}$-irreps. However to achieve this in a systematic manner one has to assume in addition that $\mathcal{H} = \mathcal{N}$ is a *normal* subgroup of $\mathcal{G}$, since otherwise there does not exist, at least to our knowledge, a systematic procedure to gain chain adapted irreps. If $\mathcal{N} \triangleleft \mathcal{G}$ holds then a well-known method[9)2)3)], is straightforwardly applicable to achieve $\mathcal{G}$-irreps that are automatically $\mathcal{G} \downarrow \mathcal{N}$-chain adapted. The *induction method* is in many cases much more appropriate than the first method as the computational work is much smaller compared to the first one. Moreover the latter method is in many respects more systematic as for instance the ambiguities caused by Schmidt's procedure are avoided.

SPECIAL CHAIN ADAPTATION: To demonstrate the induction procedure we discuss the following simple situation[10]. Let $\mathcal{G}$ be the supergroup and $\mathcal{N}$ a normal subgroup of index two. To simplify the discussion we assume in addition that $\mathcal{G}$ is a semi-direct product group.

$$\mathcal{G} = \{e, g_o\} (\times \mathcal{N}; \qquad {g_o}^2 = e \tag{2}$$

This however does not present the most general situation where ${g_o}^2 = n_o \in \mathcal{N}$, $n_o \neq e$; i.e. where one cannot find coset representives which form a subgroup of $\mathcal{G}$. Even though (2) is very special it occurs very often for space groups in which we are primarily interested.

To construct $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps we assume that a complete set of $\mathcal{N}$-irreps $\mathbf{N} = \{\mathbf{N}^\nu : \nu \in A(\mathcal{N})\}$ is determined. Starting from a $n(\nu)$-dimensional $\mathcal{N}$-irrep $\mathbf{N}^\nu = \{\mathcal{N}^\nu(n) : n \in \mathcal{N}\}$ where $A(\mathcal{N})$ denotes the set of $\mathcal{N}$-irrep labels one obtains induced $\mathcal{G}$-representations by means of

$$\mathbf{D}^{\nu\uparrow G}(n) = \mathbf{N}^\nu(n) \oplus \mathbf{N}^\nu(g_o(n)); \qquad \mathbf{D}^{\nu\uparrow G}(g_o) = \begin{pmatrix} \mathbf{0} & \mathbf{E}^\nu \\ \mathbf{E}^\nu & \mathbf{0} \end{pmatrix} \tag{3}$$

The unit matrices are denoted by $\mathbf{E}^\nu$ and $g_o(n) = g_o n g_o \in \mathcal{N}$. Next one has to determine the corresponding *little group* $\mathcal{G}(\nu) = \{g \in \mathcal{G} | \mathbf{N}^\nu(gng^{-1}) \simeq \mathbf{N}^\nu(n);\ n \in \mathcal{N}\}$. As g_o defines an outer automorphism mapping $\mathcal{N}$ onto $\mathcal{N}$ it thus induces a mapping of $A(\mathcal{N})$ onto $A(\mathcal{N})$, i.e. $g_o(\nu) = \nu_o \in A(\mathcal{N})$. Accordingly we have to distinguish two different cases.

$$\text{TYPE I:} \qquad \nu_o = \nu \Longleftrightarrow \mathcal{G}(\nu) = \mathcal{G} \tag{4}$$

$$\text{TYPE II:} \qquad \nu_o \neq \nu \Longleftrightarrow \mathcal{G}(\nu) = \mathcal{N} \tag{5}$$

If (4) holds then there must exist a unitary $n(\nu)$-dimensional matrix $\mathbf{Z}^\nu(g_o)$ satisfying $\mathbf{N}^\nu(g_o(n)) = \mathbf{Z}^\nu(g_o)\mathbf{N}^\nu(n)\mathbf{Z}^\nu(g_o)$ where $\mathbf{Z}^\nu(g_o)\mathbf{Z}^\nu(g_o) = \mathbf{E}^\nu$. Note that $\mathbf{Z}^\nu(g_o)$ is unique up to an arbitrary phase factor. Following along the lines of the general induction procedure, corresponding $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps are defined by

$$\mathbf{G}^{(\nu,s)\uparrow G}(g) = (-1)^s \mathbf{Z}^\nu(g_o)\mathbf{N}^\nu(n); \qquad s = 0,1; \qquad g = g_o n \tag{6}$$

If (5) holds then (3) already defines $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps. By definition $\mathcal{G}$-irreps are called *standardized* $\mathcal{G} \downarrow \mathcal{N}$-chain adapted if

$$\mathbf{G}^{\nu\uparrow G}_{a,b}(n) = \delta_{a,b}\mathbf{N}^{\nu(a)}(n); \qquad \mathbf{G}^{\nu\uparrow G}_{a,b}(g_o) = \delta_{a,b+1}\mathbf{E}^\nu; \qquad a,b = 0,1 \tag{7}$$

holds where $\nu(0) = \nu$ and $\nu(1) = \nu_o$ respectively. Still there is one point worth mentioning. Let us assume that the $\mathcal{N}$-irreps have been fixed from the outset. Then if ν is of *type II* one has to be aware that in general $\mathbf{N}^\nu(g_o(n))$ and $\mathbf{N}^{\nu_o}(n)$ are only *equivalent* $\mathcal{N}$-irreps. This implies that $\mathbf{N}^\nu(g_o(n)) = \mathbf{V}^\nu \mathbf{N}^{\nu_o}(n)\mathbf{V}^{\nu\dagger}$ with some non-trivial $\mathbf{V}^\nu$. Thus in order to relate (6) with (3) one needs the similarity matrix $\mathbf{V}^{\nu\uparrow G} = \mathbf{E}^\nu \oplus \mathbf{V}^\nu$. This suggests the redefinition of *type II* $\mathcal{N}$-irreps by setting $\mathbf{V}^\nu = \mathbf{E}^\nu$. Moreover to arrive at a *complete* set of $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps and to avoid redundancies one has to determine the *representation domain* $\Delta A(\mathcal{N})$. This subset of $A(\mathcal{N})$ consists of all *type I* $\mathcal{N}$-irrep labels

ν and of one element of each *type II orbit* $\{\nu, \nu_o\}$ respectively. Finally to have a more concise notation we set $(\nu, s) \uparrow \mathcal{G} = \nu s$ and $\nu \uparrow \mathcal{G} = \star\nu$ for type I and type II *induced* $\mathcal{G}$-irrep labels respectively.

SUBGROUP PROPERTIES OF STANDARD SPACE GROUP IRREPS: It is well known that any irrep of a given space group $\mathcal{G}$ containing a translation group $\mathcal{T}$ as normal subgroup must be equivalent to $\mathcal{G} \downarrow \mathcal{T}$-chain adapted $\mathcal{G}$-irreps[2)11)]. The latter are called *standard* and are of the form

$$\mathbf{G}^K_{\underline{R},\underline{S}}[(R|\mathbf{v}(R)+\mathbf{t})] = \Delta^{\mathbf{k}}(\underline{R}, R\underline{S})\mathbf{R}^K[(\underline{R}|\mathbf{v}(\underline{R}))^{-1}(R|\mathbf{v}(R)+\mathbf{t})(\underline{S}|\mathbf{v}(\underline{S}))] \qquad (8)$$

where a partly matrix notation is used. In detail, *standard* $\mathcal{G}$-irrep labels are abbreviated by $K = (\mathbf{k}, \lambda) \uparrow \mathcal{G}$ where $\mathbf{k} \in \Delta BZ(\mathcal{G})$ (= *"representation domain"* of the Brillouin zone $BZ(\mathcal{G})$) and $\lambda \in A(\mathbf{k})$ is a $\mathcal{P}(\mathbf{k})$-irrep label. Moreover $\mathbf{R}^K$ is a *small* irrep of the *little group* $\mathcal{G}(\mathbf{k}) \subseteq \mathcal{G}$.

$$\mathbf{R}^K[(R|\mathbf{v}(R)+\mathbf{t})] = e^{-i\mathbf{k}\cdot\mathbf{t}}\mathbf{D}^\lambda(R); \quad (R|\mathbf{v}(R)+\mathbf{t}) \in \mathcal{G}(\mathbf{k}) \qquad (9)$$

Observe that $\mathbf{D}^\lambda(R); R \in \mathcal{P}(\mathbf{k})$ are *projective* irreps of $\mathcal{P}(\mathbf{k})$ where $\mathcal{P}(\mathbf{k}) \simeq \mathcal{G}(\mathbf{k})/\mathcal{T}$. Their *factor systems* are determined by $F^K(R,S) = exp\{-i\mathbf{k}\cdot\mathbf{t}(R,S)\}; R, S \in \mathcal{P}(\mathbf{k})$ where $\mathbf{t}(R,S) = \mathbf{v}(R) + R\mathbf{v}(S) - \mathbf{v}(RS) \in \mathcal{T}$. If $\mathcal{G}$ is *symmorphic* then the factor system reduces to unity but turns out to be non-trivial for *non-symmorphic* space groups. Finally the generalized δ-function $\Delta^{\mathbf{k}}(\underline{R}, R\underline{S}) = \delta_{\underline{R}\mathcal{P}(\mathbf{k}),R\underline{S}\mathcal{P}(\mathbf{k})}$ determines the generalized permutational structure of *standard* $\mathcal{G}$-irreps, where the *coset representatives* $\underline{R}, \underline{S} \in \underline{\mathcal{P}}(\mathbf{k})$ which decompose $\mathcal{P} \simeq \mathcal{G}/\mathcal{T}$ with respect to $\mathcal{P}(\mathbf{k})$ are fixed by conventions. As has been discussed in many places[12)13)14)] *standard* $\mathcal{G}$-irreps are uniquely determined if and only if (i) the representation domain $\Delta BZ(\mathcal{G})$, (ii) the little co-group irreps $\mathbf{D}^\lambda$, and (iii) the set $\underline{\mathcal{P}}(\mathbf{k})$ of coset representatives are *fixed* simultaneously by imposing further conventions as none of the three entities is unique. Recently various proposals[12)14)15)16)] have been made how for choosing the *representation domains* $\Delta BZ(\mathcal{G})$ to unify them. Clearly $\mathcal{P}(\mathbf{k})$-irreps are not unique if their dimensions are greater than one. In some approaches standardized Miller-Love-matrices[13)14)] are used but in other approaches chain adapted $\mathcal{P}(\mathbf{k})$-irreps are constructed via the so-called *eigenfunction method*[4)].

This raises immediately the question whether *standard* $\mathcal{G}$-irreps are chain adapted with respect to $\mathcal{G}(\mathbf{k})$. Clearly this cannot be the case in general. Only if $\mathcal{P}(\mathbf{k})$ is a *normal* subgroup of $\mathcal{P}$ then $\mathbf{G}^K$ decomposes into a direct sum of *small* irreps. Thus chain adaptation of $\mathcal{P}(\mathbf{k})$-irreps does not lead in general to $\mathcal{G} \downarrow \mathcal{G}(\mathbf{k})$-chain adapted $\mathcal{G}$-irreps. To argue that this specific type of $\mathcal{G}$-irreps[4)] is especially suited for describing so-called *compatibility relations*[17)] is incorrect. This is because compatibility relations for $\mathcal{G}$-irreps subducing $\mathcal{G}(\mathbf{k})$-irreps differ essentially from the corresponding compatibility relations for $\mathcal{P}(\mathbf{k})$-irreps due to their reciprocity[18)]. Since $\mathcal{G}$-irreps subducing $\mathcal{G}(\mathbf{k})$-irreps may become reducible if and only if $\mathcal{G}(\mathbf{k}') \supset \mathcal{G}(\mathbf{k})$ holds. Whereas $\mathcal{P}(\mathbf{k})$-irreps may become reducible if $\mathcal{P}(\mathbf{k}') \subset \mathcal{P}(\mathbf{k})$ is valid.

ALTERNATIVE SPACE GROUP IRREPS: By virtue of our definitions *alternative* space group irreps[12)] are specific chain adapted space group irreps. Their properties and applications to physical applications have been discussed in [12]. It is worth repeating that *analytic* formulas are derived for the corresponding $\mathbf{Z}^\nu$- and $\mathbf{V}^\nu$-matrices respectively. This allows one to carry out successively chain adaptations for composite chains like

$Fm3m(2a) \triangleleft Pm3m(a) \triangleleft Im3m(a)$ or $P23(a) \triangleleft P432(a) \triangleleft Pm3m(a) \triangleleft Im3m(a)$. These composite subgroup chains refer to different Bravais lattices and except for the first chain to different point groups as well. This is of course a much wider class of chain adaptations in comparison to Chen's approach. Note that the subgroup chains are not restricted to symmorhic space groups exclusively. For instance $Pm3n(a) \triangleleft Im3m(a)$ combines a symmorphic with a non-symmorphic space group.

To gain more insight into the present procedure when applied to chain adapted space group irreps we sketch one example[19)20)]. The present example deals with *"translationsgleiche"* space groups. Examples concerning *"klassengleiche"* space groups have already been presented[12)]. We consider $\mathcal{G} = Pm3m(a)$ and $\mathcal{N} = P432(a)$ and choose the following coset decomposition $Pm3m(a) = \{(E|\mathbf{O}),(\sigma_z|\mathbf{O})\}(\times P432(a)$. Note that the corresponding point groups are $\mathcal{P}(\mathcal{N}) = \mathcal{O}$ and $\mathcal{P}(\mathcal{G}) = \mathcal{O}_h$ respectively. Starting from the *standard* $\mathcal{N}$-irrep label set $A(\mathcal{N}) = \{(\mathbf{k}_N, \lambda_N) : \mathbf{k}_N \in \Delta BZ(\mathcal{N}); \lambda_N \in A(\mathbf{k}_N)\}$ one readily proves that the *representation domain* $\Delta A(\mathcal{N}, \mathcal{G})$ involves the set $\Delta BZ(\mathcal{N}, \mathcal{G}) = \Delta BZ(\mathcal{G})$. Thus chain adaptation leads not surprisingly to the reduction of $\Delta BZ(\mathcal{N})$ to $\Delta BZ(\mathcal{G})$. In order to distinguish *standard* $\mathcal{G}$-irrep labels from *standard* $\mathcal{N}$-irrep labels we provide them with subscripts $(\mathbf{k}_G, \lambda_G)$ and $(\mathbf{k}_N, \lambda_N)$ respectively. To give an example later showing the multiplicity splitting we recall from [20] that $(\mathbf{\Lambda}_N, 2_N)$ and $(\mathbf{\Lambda}_N, 3_N)$ are of type II satisfying $g_o((\mathbf{\Lambda}_N, 2_N)) = (\mathbf{\Lambda}_N, 3_N)$ where $g_o = (\sigma_z|\mathbf{O})$. One readily proves $(\mathbf{\Lambda}_N, 2_N) \uparrow \mathcal{G} = (\mathbf{\Lambda}_N, 3_N) \uparrow \mathcal{G} = (\mathbf{\Lambda}_G, 3_G)$.

INDUCED CHAIN ADAPTED CG-MATRICES: The objective of this part is to sketch how the induction procedure for $\mathcal{G}$-irreps can be extended to construct *induced* CG-matrices. For the sake of simplicity we assume that (2) holds. Moreover we assume that $\mathcal{N}$-CG-matrices for Kronecker products (KPs) of $\mathcal{N}$-irreps are known. The goal is to express CG-matrices decomposing KPs of $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps in terms of $\mathcal{N}$-CG-matrices. For convenience we treat the general case without referring to particular groups. $\mathcal{N}$-CG-blocks denoted by $\mathbf{C}_N^{\cdot;\cdot}$ have to satisfy

$$\mathbf{N}^{\nu,\nu'}(n)\mathbf{C}_N^{\nu;\nu'|\nu'',w} = \mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{N}^{\nu''}(n) \tag{10}$$

They are rectangular submatrices of the corresponding CG-matrix $\mathbf{C}_N^{\nu,\nu'}$. The $\mathcal{N}$-KP $\mathbf{N}^{\nu} \otimes \mathbf{N}^{\nu'}$ is abbreviated by $\mathbf{N}^{\nu,\nu'}$. The multiplicity index varies from 1 to $m(\nu;\nu'|\nu'')$. Since two types of $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-irreps exist we have to distinguish between three different forms of possible $\mathcal{G}$-KPs. The KPs may be composed of type I-irreps, or of type II-irreps exclusively or of combinations of both. In every case type I- and/or type II-irreps may occur in the corresponding decompositions.

Type I $\otimes$ Type I – KP: One readily derives for the $\mathcal{G}$-multiplicities

$$m(\nu s;\nu' s'|\nu'' s'') = \delta_{s+s',s''}\, m(\nu;\nu'|\nu'') \tag{11}$$

$$m(\nu s;\nu' s'|\star\nu'') = m(\nu;\nu'|\nu'') = m(\nu;\nu'|\nu_o'') \tag{12}$$

$$\mathbf{C}_G^{\nu s;\nu' s'|\nu'' s'',w} = \delta_{s+s',s''}\,\mathbf{C}_N^{\nu;\nu'|\nu'',w} \tag{13}$$

$$\mathbf{C}_G^{\nu s;\nu' s'|\star\nu'',w} = \left[\mathbf{C}_N^{\nu;\nu'|\nu'',w}, (-1)^{s+s'}\mathbf{Z}^{\nu\nu'}(g_o)^{\dagger}\mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{V}^{\nu''}\right] \tag{14}$$

The corresponding $\mathcal{G}$-CG-blocks are obtained by applying Schur's Lemma where the range of variation of the *multiplicity index* w is due to (11) and (12) respectively.

Type I ⊗ Type II – KP: In every such case one arrives at

$$m(\nu s; \star\nu'|\nu'' s'') = m(\nu; \nu'|\nu'') = m(\nu; \nu_o'|\nu'') \tag{15}$$

$$m(\nu s; \star\nu'|\star\nu'') = m(\nu; \nu'|\nu'') + m(\nu; \nu_o'|\nu'') \tag{16}$$

$$\mathbf{C}_G^{\nu s;\star\nu'|\nu'' s'',w} = \frac{1}{\sqrt{2}} \begin{bmatrix} (-1)^{s+s''}\mathbf{C}_N^{\nu;\nu'|\nu'',w} \\ [\mathbf{Z}^{\nu}(g_o)\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{Z}^{\nu''}(g_o) \end{bmatrix} \tag{17}$$

$$\mathbf{C}_{G,1}^{\nu s;\star\nu'|\star\nu'',w} = \begin{bmatrix} \mathbf{C}_N^{\nu;\nu'|\nu'',w} & \mathbf{O} \\ \mathbf{O} & (-1)^s[\mathbf{Z}^{\nu}(g_o)\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{V}^{\nu''} \end{bmatrix} \tag{18}$$

$$\mathbf{C}_{G,2}^{\nu s;\star\nu'|\star\nu'',w} = \begin{bmatrix} \mathbf{O} & (-1)^s[\mathbf{Z}^{\nu}(g_o)\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu_o'|\nu'',w}\mathbf{V}^{\nu''} \\ \mathbf{C}_N^{\nu;\nu_o'|\nu'',w} & \mathbf{O} \end{bmatrix} \tag{19}$$

where the range of variation of w for the various $\mathcal{G}$-CG-blocks is due to the corresponding $\mathcal{N}$-multiplicities occurring in (15) and (16) respectively. Hence in this method the multiplicity problem for $\mathcal{G}$ is traced back to that for $\mathcal{N}$ which implies that we automatically gain in addition a *natural* separation of the multiplicity problem.

Type II ⊗ Type II – KP: Finally in every such case one derives

$$m(\star\nu; \star\nu'|\nu'' s'') = m(\nu; \nu'|\nu'') + m(\nu; \nu_o'|\nu'') \tag{20}$$

$$\begin{aligned} m(\star\nu; \star\nu'|\star\nu'') &= m(\nu; \nu'|\nu'') + m(\nu; \nu_o'|\nu'') \\ &\quad + m(\nu_o; \nu'|\nu'') + m(\nu_o; \nu_o'|\nu'') \end{aligned} \tag{21}$$

$$\mathbf{C}_{G,1}^{\star\nu;\star\nu'|\nu'' s'',w} = \frac{1}{\sqrt{2}} \begin{bmatrix} (-1)^{s''}\mathbf{C}_N^{\nu;\nu'|\nu'',w} \\ \mathbf{O} \\ \mathbf{O} \\ [\mathbf{V}^{\nu}\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{Z}^{\nu''}(g_o) \end{bmatrix} \tag{22}$$

$$\mathbf{C}_{G,2}^{\star\nu;\star\nu'|\nu'' s'',w} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{O} \\ (-1)^{s''}\mathbf{C}_N^{\nu;\nu_o'|\nu'',w} \\ [\mathbf{V}^{\nu}\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu_o'|\nu'',w}\mathbf{Z}^{\nu''}(g_o) \\ \mathbf{O} \end{bmatrix} \tag{23}$$

$$\mathbf{C}_{G,1}^{\star\nu;\star\nu'|\star\nu'',w} = \begin{bmatrix} \mathbf{C}_N^{\nu;\nu'|\nu'',w} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & [\mathbf{V}^{\nu}\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu;\nu'|\nu'',w}\mathbf{V}^{\nu''} \end{bmatrix} \tag{24}$$

$$\mathbf{C}_{G,2}^{\star\nu;\star\nu'|\star\nu'',w} = \begin{bmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{C}_N^{\nu;\nu_o'|\nu'',w} & \mathbf{O} \\ \mathbf{O} & [\mathbf{V}^{\nu}\otimes\mathbf{V}^{\nu_o'}]^{\dagger}\mathbf{C}_N^{\nu;\nu_o'|\nu'',w}\mathbf{V}^{\nu''} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \tag{25}$$

$$\mathbf{C}_{G,3}^{\star\nu;\star\nu'|\star\nu'',w} = \begin{bmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{O} & [\mathbf{V}^{\nu_o}\otimes\mathbf{V}^{\nu'}]^{\dagger}\mathbf{C}_N^{\nu_o;\nu'|\nu'',w}\mathbf{V}^{\nu''} \\ \mathbf{C}_N^{\nu_o;\nu'|\nu'',w} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \tag{26}$$

$$\mathbf{C}_{G,4}^{*\nu;*\nu'|*\nu'',w} = \begin{bmatrix} \mathbf{O} & [\mathbf{V}^{\nu_o} \otimes \mathbf{V}^{\nu_o'}]^{\dagger} \mathbf{C}_N^{\nu_o;\nu_o'|\nu'',w} \mathbf{V}^{\nu''} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{C}_N^{\nu_o;\nu_o'|\nu'',w} & \mathbf{O} \end{bmatrix} \tag{27}$$

where the corresponding $\mathcal{G}$-CG-blocks are automatically two- and fourfold split in accordance with the mutliplicity separation. Note that the range of w is due to the corresponding $\mathcal{N}$-multiplicities occurring in (20) and (21) respectively. To summarize in all three cases one merely needs to know a subset of $\mathcal{N}$-CG-blocks and the corresponding similarity transformations $\mathbf{Z}^{\nu}$ and $\mathbf{V}^{\nu}$ respectively to arrive at $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-CG-matrices. The merits of the present approach are obvious. Firstly the matrices $\mathbf{Z}^{\nu}$ and $\mathbf{V}^{\nu}$ are *unique* up to phase factors. Secondly we achieve automatically a separation of the multiplicity problem as it is traced back to that of the subgroup $\mathcal{N}$. Finally it can be easily applied to any composite chain because it is remarkably simple. Thirdly $\mathcal{G}$-CG-blocks are analytically expressable in terms of $\mathcal{N}$-CG-blocks. The reader is referred to [21] where the symmetries of the $\mathcal{N}$-multiplicities with respect to the outer automorphism $g_o \in \mathcal{G}$ have been derived.

APPLICATION TO CHAIN ADAPTED SPACE GROUP CG-MATRICES: The application of the present approach to space group chains like $Pm3m(a) \triangleleft Im3m(a)$ or $P432(a) \triangleleft Pm3m(a)$ or $Fm3m(a) \triangleleft Pm3m(a)$ is straightforward. A series of illustrative examples concerning the above subgroup chains are extensively discussed in [19], [20].

To gain some insight into this procedure let us briefly sketch an example which is given earlier. To follow our approach we only have to consider the following $\mathcal{N}$-KPs which are written in symbolical form.

$$(\mathbf{\Lambda}_N, 2_N) \otimes (\mathbf{\Lambda}'_N, 3_N) \simeq (\mathbf{\Lambda}''_N, 1_N) \oplus (\mathbf{\Lambda}'''_N, 2_N) \oplus (\mathbf{q}'_N, 1_N) \oplus (\mathbf{q}''_N, 1_N) \tag{28}$$

$$(\mathbf{\Lambda}_N, 2_N) \otimes g_o((\mathbf{\Lambda}'_N, 3_N)) \simeq (\mathbf{\Lambda}''_N, 3_N) \oplus (\mathbf{\Lambda}'''_N, 1_N) \oplus (\mathbf{q}'_N, 1_N) \oplus (\mathbf{q}''_N, 1_N) \tag{29}$$

General points of $\Delta BZ(\mathcal{N})$ are denoted by $\mathbf{q}_N$. Note that $\mathbf{q}'_N \in \Delta BZ(\mathcal{N})$ specifies to $\mathbf{C}_G \in \Delta BZ(\mathcal{G})$ and $\mathbf{q}''_N \in \Delta BZ(\mathcal{N})$ to $\mathbf{J}_G \in \Delta BZ(\mathcal{G})$ respectively. On the other hand the corresponding $\mathcal{G}$-KP reads

$$\begin{aligned} &(\mathbf{\Lambda}_G, 3_G) \otimes (\mathbf{\Lambda}'_G, 3_G) \simeq \\ &(\mathbf{\Lambda}''_G, 1_G) \oplus (\mathbf{\Lambda}''_G, 2_G) \oplus (\mathbf{\Lambda}''_G, 3_G) \oplus (\mathbf{\Lambda}'''_G, 1_G) \oplus (\mathbf{\Lambda}'''_G, 2_G) \oplus (\mathbf{\Lambda}'''_G, 3_G) \\ &(\oplus 2)\{(\mathbf{C}_G, 1_G) \oplus (\mathbf{C}_G, 2_G)\}(\oplus 2)\{(\mathbf{J}_G, 1_G) \oplus (\mathbf{J}_G, 2_G)\} \end{aligned} \tag{30}$$

where four $\mathcal{G}$-irreps occur twice. Proceeding as usual one has to solve the multiplicity problem by some conventions. However by applying our approach one readily finds for $(\mathbf{k}''_N, \lambda''_N) = (\mathbf{q}'_N, 1_N)$ which is of type I that (20) is realized. Both frequencies are one, i.e. $m(\nu;\nu'|\nu'') = m(\nu;\nu_o'|\nu'') = 1$, where $\nu = (\mathbf{\Lambda}_N, 2_N)$, $\nu' = (\mathbf{\Lambda}'_N, 3_N)$ and $\nu'' = (\mathbf{q}'_N, 1_N)$. This leads automatically to a multiplicity separation for $((\mathbf{q}'_N, 1_N), s) \uparrow \mathcal{G}$ since these two *alternative* $\mathcal{G}$-irrep labels coincide with $(\mathbf{C}_G, 1_G)$ and $(\mathbf{C}_G, 2_G)$ respectively.

GENERAL CHAIN ADAPTATIONS: Of course the present approach for constructing $\mathcal{G} \downarrow \mathcal{N}$-chain adapted $\mathcal{G}$-CG-matrices where $\mathcal{N}$ is of index two in $\mathcal{G}$ can be easily generalized. Let $\mathcal{G}$ be a supergroup and $\mathcal{N}$ a normal subgroup whose index with respect to $\mathcal{G}$ is finite.

Then one can derive similar expressions for $\mathcal{G}$-CG-blocks in terms of $\mathcal{N}$-CG-blocks. The latter approach allows one to express directly $Pm3m$-CG-blocks in terms of $P23$-CG-blocks without the intermediate step of determining the $P423$-CG-blocks as required by our original approach.

In summary our philosophy is to start from a fixed set of *standardized* space group CG-matrices in *canonical* form[22)23)24)] and to provide a software package running on IBM PCs to compute not only *standardized* CG-matrices and displaying them in *canonical* form but also to carry out any chain adaptation by pressing just a few keys at the keyboard. The versatility of our approach is that every chain adaptation can be carried out straightforwardly as *analytic* formulas have been derived that correlate the various subgroup CG-matrices with the corresponding supergroup CG-matrices.

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