SOFTWARE PACKAGES: Transformation Coefficients for Space Groups

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Abstract: The aim of the second contribution is to present further universal software packages for space groups. The second set of packages is called COEFF consisting of four packages: SUB, CG, SYMCG, and SYMPW. All packages allow one not only to treat every space group in *arbitrary* settings (shift of origin and/or re-orientation) but also to use space group irreps in *arbitrarily* modified forms (new representation domains and/or new little co-group irreps and/or new coset representatives). Each COEF-package yields the matrix elements of the corresponding unitary *similarity* matrices in *analytic* form.

A. Introductory Remarks: For more details concerning the definition of space groups in *standard* or in *non-standard* settings, or the computer generation of space group irreps in *standard* or in *non-standard* forms, the reader is referred to Ref.[1]. By definition, we call a space group $\mathcal{G}\{\mathcal{T},\mathcal{P};(W|\mathrm{w})\} = (W|\mathrm{w}) * \mathcal{G}\{\mathcal{T},\mathcal{P};(E|0)\} * (W|\mathrm{w})^{-1}$ a *non-standard* setting of $\mathcal{G}\{\mathcal{T},\mathcal{P};(E|0)\}$ if the element $(W|\mathrm{w}) \in \mathcal{E}(3)$ does not belong to the *Euclidean normalizer* of $\mathcal{G}$. Induced space group irreps are expressible in the form

$$\mathbb{D}^{\mathbf{k},\xi;\lambda}_{\underline{R},\underline{S}}(R|\mathrm{n}(R)+\mathrm{t}) = \Delta^{\mathbf{k}}(\underline{R},R\underline{S})\, e^{+i\lambda\underline{R}\mathbf{k}\cdot\mathbf{t}}\, \Phi^{\mathbf{k};\lambda}_{\underline{R},\underline{S}}(R)\, \mathrm{IR}^{\mathbf{k},\xi;\lambda}(\underline{R}^{-1}R\underline{S}) \tag{1}$$

and define *standard* Miller-Love space group irreps if (1) the space groups $\mathcal{G}$ are in *standard* settings, (2) the sign λ is plus one, (3) the *representation domains* $RBZ(\mathcal{T},\mathcal{P})$ are identical to those that are tabulated in Ref.[2], (4) the little co-group irreps $\mathrm{IR}^{\mathbf{k},\xi;+}$ are ML-irreps, and (5) the coset representatives $\{\underline{R}\}$ are *optimized* ones.

To transform $\mathcal{G}$-irreps in *standard* form where $\mathcal{G}$ is in *standard* setting, into *non-standard* forms and/or $\mathcal{G}$ into *non-standard* settings, the reader is again referred to Ref.[1]. To recall, all software packages, not only IRREP, create by default *single* and *double-valued* standard Miller-Love space group irreps but likewise allow one to carry out any re-setting of space groups and/or any modification of space group irreps as long as they are compatible.

B. Package — SUB: One part of our software package called SUB deals with the algebraic check of group-subgroup relations and the second part with the actual computation of tables of multiplicities and corresponding subduction matrices. On some features and computational results of package SUB we have already reported in Ref.[3].

B.1 Group-Subgroup Relations $\mathcal{G} \subset \mathcal{H}$: A complete set of certain types of group-subgroup relations is tabulated in Ref.[4] but where all groups are assumed to be in *standard* settings. To cover all possible types of group-subgroup relations we extend the scheme by admitting that groups, sub-groups, and super-groups may be simultaneously in *non-standard* settings. Let $\mathcal{G}$ be a subgroup of $\mathcal{H}$. To be more strict we assume in general

$$\mathcal{G}\{\mathcal{T}_G,\mathcal{P}_G;(V|\mathrm{v})\} \subset \mathcal{H}\{\mathcal{T}_H,\mathcal{P}_H;(E|0)\} \tag{2}$$

where $(V|\mathrm{v}) \in \mathcal{E}(3)$ that $\mathcal{H}$ is in *standard* but $\mathcal{G}$ in *non-standard* setting. Note in particular, translational group-subgroup relations $\mathcal{T}_G(V) \subset \mathcal{T}_H(E)$ where $\mathcal{T}_G(V) = (V|\mathrm{v}) * \mathcal{T}_G(E) * (V|\mathrm{v})^{-1}$

involve the possibility of considering *Bravais lattices* $\mathcal{T}_G(V)$ and $\mathcal{T}_H(E)$ that refer to different lattice constants. The option of entering *arbitrary* ratios of lattice constants of the corresponding Bravais lattices in conjunction with *arbitrary* settings of space groups opens up a wide field of applications.

B.2 Subductions — Complex Conjugation: The second part of package SUB deals with the actual decomposition of subduced $\mathcal{H}$-irreps into direct sums of $\mathcal{G}$-irreps. To distinguish between $\mathcal{H}$-irreps and $\mathcal{G}$-irreps we employ the notations $\mathbb{D}^{\mathbf{q},\eta;\lambda}$ for $\mathcal{H}$-irreps and $\mathbb{D}^{\mathbf{k},\xi;\lambda'}$ for $\mathcal{G}$-irreps where $h \in \mathcal{H}$ and $g \in \mathcal{G}$ respectively. Moreover $\mathcal{H}$-irrep labels are denoted by $(\mathbf{q},\eta)$ where $\mathbf{q} \in RBZ(\mathcal{T}_H, \mathcal{P}_H)$ and $\eta \in A(\mathbf{q})$; and $\mathcal{G}$-irrep labels are denoted by $(\mathbf{k},\xi)$ where $\mathbf{k} \in RBZ(\mathcal{T}_G, \mathcal{P}_G)$ and $\xi \in A(\mathbf{k})$ respectively. Finally $\lambda, \lambda' = \pm 1$ can be chosen independently.

Without going into details let us summarize the possibilities offered by the package SUB. In all the cases described here, we start from a fixed triplet $(\mathbf{q},\eta;\lambda)$ and compute for the fixed $\mathbf{q}$, not only complete tables of *multiplicities* for *all* $\eta \in A(\mathbf{q})$, but also for the given η the corresponding *similarity* transformation. Again we stress the fact that λ and λ' can be chosen independently. The results of package SUB are (1) *arbitrary subductions* for $\mathcal{G} \subset \mathcal{H}$, (2) *compatibility relations* for $\mathcal{G} = \mathcal{H}$, (3) *generalized compatibility relations* for $\mathcal{G} \subset \mathcal{H}$ by considering *limit*-representations, and (4) *complex conjugation* for $\mathcal{G} = \mathcal{H}$ respectively.

$$\begin{aligned}
\mathbf{W}^{\mathbf{q},\eta\,\dagger}_{\lambda,\lambda'}\,\mathbb{D}^{\mathbf{q},\eta;\lambda}(g)\,\mathbf{W}^{\mathbf{q},\eta}_{\lambda,\lambda'} &= \textstyle\sum_{\mathbf{k},\xi} \oplus\, m(\mathbf{q},\eta;\lambda|\mathbf{k},\xi;\lambda')\,\mathbb{D}^{\mathbf{k},\xi;\lambda'}(g)\\
\mathbf{W}^{\mathbf{k}_o,\xi\,\dagger}_{\lambda,\lambda'}\,\mathbb{L}^{\mathbf{k}_o,\xi;\lambda}(g)\,\mathbf{W}^{\mathbf{k}_o,\xi}_{\lambda,\lambda'} &= \textstyle\sum_{\mathbf{k}_o,\xi_o} \oplus\, m(\mathbf{k}_o,\xi;\lambda|\mathbf{k}_o,\xi_o;\lambda')\,\mathbb{D}^{\mathbf{k}_o,\xi_o;\lambda'}(g)\\
\mathbf{W}^{\mathbf{q}_o,\eta\,\dagger}_{\lambda,\lambda'}\,\mathbb{L}^{\mathbf{q}_o,\eta;\lambda}(g)\,\mathbf{W}^{\mathbf{q}_o,\eta}_{\lambda,\lambda'} &= \textstyle\sum_{\mathbf{k}_o,\xi_o} \oplus\, m(\mathbf{q}_o,\eta;\lambda|\mathbf{k}_o,\xi_o;\lambda')\,\mathbb{D}^{\mathbf{k}_o,\xi_o;\lambda'}(g)\\
\mathbf{W}^{\mathbf{k},\xi\,\dagger}_{\pm}\,\mathbb{D}^{\mathbf{k},\xi;+}(g)\,\mathbf{W}^{\mathbf{k},\xi}_{\pm} &= \textstyle\sum_{\mathbf{k}^*,\xi^*} \oplus\, m(\mathbf{k},\xi;+|\mathbf{k}^*,\xi^*;-)\,\mathbb{D}^{\mathbf{k}^*,\xi^*;-}(g)
\end{aligned}$$

The last facility especially can be used not only to verify, for arbitrary *single* and *double-valued* space group irreps, their *reality* and *degeneracy* due to Kramer's degeneracy, but also to construct explicitly co-irreps, in full generality, for all Shubnikov space groups of type II.

B.3 Automorphisms — Subductions — Complex Conjugation: For maximum versatility of package SUB the user can also invoke the option of considering *automorphisms* acting on $\mathcal{H}$ exclusively. The most general *automorphisms* are elements of the *Affine Group* $\mathcal{A}(3)$. Let $a = (Z|\mathbf{z})$ be an *automorphism* of $\mathcal{H}$, i.e. $a(\mathcal{H}) = (Z|\mathbf{z}) * \mathcal{H} * (Z|\mathbf{z})^{-1} = \mathcal{H}$ which means that $\mathcal{H}$ is mapped onto itself. Now let $\mathcal{G} \subset \mathcal{H}$ be a group-subgroup relation, it remains valid on replacing $\mathcal{H}$ by $a(\mathcal{H})$. This entails $\mathcal{G} \subset a(\mathcal{H}) \Longleftrightarrow a^{-1}(\mathcal{G}) \subset \mathcal{H}$ which reveals the subtle point that one has to distinguish between the cases $a^{-1}(\mathcal{G}) = \mathcal{G}$ and $a^{-1}(\mathcal{G}) \neq \mathcal{G}$ respectively. Starting from a given $\mathcal{H}$-irrep, say $\mathbb{D}^{\mathbf{q},\eta;\lambda}$, subduction to $\mathcal{G}$-representations means

$$\mathbb{D}^{\mathbf{q},\eta;\lambda}(a(h)) \downarrow \mathcal{G} = \begin{cases} \mathbb{D}^{\mathbf{q},\eta;\lambda}(a(g)) & \Longleftrightarrow a^{-1}(\mathcal{G}) = \mathcal{G} \\ \mathbb{D}^{\mathbf{q},\eta;\lambda}(a(h)) \downarrow \mathcal{G} & \Longleftrightarrow a^{-1}(\mathcal{G}) \neq \mathcal{G} \end{cases} \tag{3}$$

Thus when carrying out (3) one can do it either directly or split the procedure into two steps: (1) $\mathbb{D}^{\mathbf{q},\eta;\lambda}(a(h)) \sim \mathbb{D}^{a(\mathbf{q}),a(\eta);\lambda}(h)$ and (2) $\mathbb{D}^{a(\mathbf{q}),a(\eta);\lambda}(h) \downarrow \mathcal{G}$ where $a(\mathbf{q},\eta) = (a(\mathbf{q}), a(\eta))$ are the images of the $\mathcal{H}$-irreps labels $(\mathbf{q},\eta)$ under the *automorphisms* a respectively.

Again without going into details let us summarize the possibilities offered by the package SUB. In all the cases described here, we start from a fixed triplet $(\mathbf{q},\eta;\lambda)$ determining a $\mathcal{H}$-irrep and compute for the fixed $\mathbf{q}$ not only complete tables of *multiplicities* for *all* $\eta \in A(\mathbf{q})$, but also for the given η the corresponding *similarity* transformation. The results of SUB are (1) *automorphism mappings* for $\mathcal{G} = \mathcal{H}$, (2) *automorphism mappings* for $\mathcal{G} \subset \mathcal{H}$, (3) *automorphisms* combined with *compatibility relations* for $\mathcal{G} = \mathcal{H}$, (4) *automorphisms* combined with *generalized compatibility relations* for $\mathcal{G} \subset \mathcal{H}$, and (5) *automorphisms* combined with *complex conjugation* for $\mathcal{G} = \mathcal{H}$.

$$\mathbf{W}^{a(\mathbf{k},\xi)\dagger}_{\lambda,\lambda'}\,\mathbb{D}^{\mathbf{k},\xi;\lambda}(a(g))\,\mathbf{W}^{a(\mathbf{k},\xi)}_{\lambda,\lambda'} = \textstyle\sum_{\mathbf{k}',\xi'} \oplus\, m(a(\mathbf{k}),a(\xi);\lambda|\mathbf{k}',\xi';\lambda')\,\mathbb{D}^{\mathbf{k}',\xi';\lambda'}(g)$$

$$\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{q},\eta)\dagger}\,\{\mathbb{D}^{\mathbf{q},\eta;\lambda}(a(h))\downarrow\mathcal{G}\}\,\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{q},\eta)} = \textstyle\sum_{\mathbf{k}',\xi'}\oplus\, m(a(\mathbf{q}),a(\eta);\lambda|\mathbf{k},\xi);\lambda')\,\mathbb{D}^{\mathbf{k},\xi;\lambda'}(g)$$

$$\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{k}_o,\xi)\dagger}\,\mathbb{L}^{\mathbf{k}_o,\xi;\lambda}(a(g))\,\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{k}_o,\xi)} = \textstyle\sum_{\mathbf{k}_o',\xi_o'}\oplus\, m(a(\mathbf{k}_o),a(\xi);\lambda|\mathbf{k}_o{}',\xi_o';\lambda')\,\mathbb{D}^{\mathbf{k}_o',\xi_o';\lambda'}(g)$$

$$\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{q}_o,\eta)\dagger}\,\{\mathbb{L}^{\mathbf{q}_o,\eta;\lambda}(a(h))\downarrow\mathcal{G}\}\,\mathbf{W}_{\lambda,\lambda'}^{a(\mathbf{q}_o,\eta)} = \textstyle\sum_{\mathbf{k}_o,\xi_o}\oplus\, m(a(\mathbf{q}_o),a(\eta);\lambda|\mathbf{k}_o,\xi_o;\lambda')\,\mathbb{D}^{\mathbf{k}_o,\xi_o;\lambda'}(g)$$

$$\mathbf{W}_{\pm}^{a(\mathbf{k},\xi)\dagger}\,\mathbb{D}^{\mathbf{k},\xi;+}(a(g))\,\mathbf{W}_{\pm}^{a(\mathbf{k},\xi)} = \textstyle\sum_{\mathbf{k}',\xi'}\oplus\, m(a(\mathbf{k}^*),a(\xi^*);+|\mathbf{k}',\xi';-)\,\mathbb{D}^{\mathbf{k}',\xi';-}(g)$$

For instance the last facility allows one to construct for every *Shubnikov space group* of type III and of type IV corresponding co-irreps. To sketch the procedure, let $\mathcal{G}$ be a subgroup of index two of the space group $\mathcal{H}$, and $\mathcal{H}(\mathcal{G}) = \mathcal{G} + h_o * \mathcal{G}$ a coset decomposition. To arrive at a Shubnikov space group of type III or of type IV, symbolically written as $\mathcal{M}\{\mathcal{H}(\mathcal{G})\} = \mathcal{G} + (c;h_o)*\mathcal{G}$, one considers the extensions $h \longmapsto (c;h)$ for all $h \in \mathcal{H}\setminus\mathcal{G}$ and requires in addition $(c;h_o)^2 = (e;\bar{E}|0)*(e;h_o^2)$ where $\bar{E}$ denotes the non-trivial element of the centre of $\mathcal{SU}(2)$. Applying package SUB to this particular situation one arrives at

$$\begin{array}{llcl}
\text{type I:} & \mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\ \{\mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\}^* & = & +\ \mathbb{D}^{\mathbf{k},\xi}(\bar{E}|0)\ \mathbb{D}^{\mathbf{k},\xi}(h_o^2) \\
\text{type II:} & \mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\ \{\mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\}^* & = & -\ \mathbb{D}^{\mathbf{k},\xi}(\bar{E}|0)\ \mathbb{D}^{\mathbf{k},\xi}(h_o^2) \\
\text{type III:} & \mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\ \{\mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)\}^\dagger & = & +\ \mathbb{D}^{\mathbf{k},\xi}(E|0)
\end{array}$$

which allows one not only to check directly *reality* and *degeneracy* of *single* and of *double-valued* space group irreps but also to construct explicitly co-irreps of Shubnikov space groups of any type due to the knowledge of the *similarity* matrices $\mathbf{W}^{\mathbf{k},\xi;\pm}(c;h_o)$ respectively.

C. Package — CG: The software package called CG deals with (i) the analysis of so-called *Wave Vector Selection Rules,* (ii) the computation of *multiplicities* for Kronecker product decompositions, and (iii) with the actual computation of *Clebsch-Gordan* matrices. The basic ideas have already been published elsewhere (for further references consult eg. Ref.[3]).

By definition, Clebsch-Gordan matrices are unitary matrices that reduce *Kronecker products* of $\mathcal{G}$-irreps $\mathbb{D}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'}(g) = \mathbb{D}^{\mathbf{k},\xi;\lambda}(g)\otimes\mathbb{D}^{\mathbf{k}',\xi';\lambda'}(g)$ into direct sums of their *irreducible* constituents. They are called *standard* CG-matrices if $\mathcal{G}$ is in *standard* setting and if the $\mathcal{G}$-irreps are in *standard* form respectively.

$$\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'\dagger}\,\mathbb{D}_{\lambda;\lambda'}^{\mathbf{k},\xi|\mathbf{k}',\xi'}(g)\,\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'} = \textstyle\sum_{\mathbf{k}'',\xi''}\oplus\, m(\mathbf{k},\xi;\lambda|\mathbf{k}',\xi';\lambda'||\mathbf{k}'',\xi'';\lambda'')\,\mathbb{D}^{\mathbf{k}'',\xi'';\lambda''}(g) \qquad (4)$$

Note CG-matrices are denoted by $\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'}$, their non-zero entries are located at positions that are determined by so-called *Wave Vector Selection Rules* (WVSRs). By definition, *Leading* WVSRs (LWVSRs) are WVSRs of the type $\underline{S}\mathbf{k}+\underline{S}'\mathbf{k}' = \mathbf{k}''+\mathbf{g}$ where it is assumed that $\mathbf{k},\mathbf{k}',\mathbf{k}'' \in RBZ(\mathcal{G})$ respectively. Note that depending on the chosen k-vectors $\mathbf{k}$ and $\mathbf{k}'$, more than one LWVSR may exist which implies a *natural* splitting of the multiplicities.

$$m(\mathbf{k},\xi;\lambda|\mathbf{k}',\xi';\lambda'||\mathbf{k}'',\xi'';\lambda'') = \textstyle\sum_{(\underline{S},\underline{S}')}\, m(\underline{S}\mathbf{k},\xi;\lambda|\underline{S}'\mathbf{k}',\xi';\lambda'||\mathbf{k}'',\xi'';\lambda'')$$

Note that the sum runs over all pairs of admissible coset representatives $(\underline{S},\underline{S}')$ that define LWVSRs. This splitting is extensively used in package CG to compute CG-matrices.

To achieve the most compact representation of CG-matrices we apply a rearrangement procedure which consists of rearranging rows and columns of CG-matrices in a specific manner. The basic ideas of this rearrangement procedure are described in Ref.[5]. The rearrangement procedure, symbolically written as $\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'} \longmapsto \mathbf{A}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'}$, leads to new unitary matrices that decompose into a direct sum of *unitary* sub-matrices (Sub-CG-matrices). To summarize

$$\mathbf{A}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'} = \textstyle\sum_{\mathbf{k}''}\sum_{(\underline{S},\underline{S}')}\sum_{\underline{R}''}\ \oplus\ \mathbf{B}(\underline{R}'')\ \mathbf{A}_{\lambda\lambda'\lambda''}^{\underline{S}\mathbf{k},\xi|\underline{S}'\mathbf{k}',\xi'}(\mathbf{k}'',\underline{E}'') \qquad (5)$$

where the matrices $\mathbf{A}_{\lambda\lambda'\lambda''}^{\underline{S}\mathbf{k},\xi|\underline{S}'\mathbf{k}',\xi'}(\mathbf{k}'',\underline{E}'')$ are called Leading Sub-CG-matrices. The unitary matrices $\mathbf{B}(\underline{R}'')$ are *monomial* for the vast majority of possible cases.

Again without going into details let us summarize the possibilities offered by the package CG. In all the cases described here, we start from two fixed triplets, say $(\mathbf{k},\xi;\lambda)$ and $(\mathbf{k}',\xi';\lambda')$, and compute for the fixed $\mathbf{k}$ and $\mathbf{k}'$, not only complete tables of *multiplicities*, but also for the given ξ and ξ' the corresponding CG-matrices. The package CG allows one to compute (1) *generic* CG-matrices (given by (4) if none of the resulting $\mathbf{k}''$ coincides with *limit*-vectors of $RBZ(\mathcal{G})$), (2) *non-generic* CG-matrices (at least one $\mathbf{k}''$ coincides with a *limit*-vector), and (3) *limit* CG-matrices (at least one constituent of the Kronecker product is a *limit*-representation of $\mathcal{G}$), for *arbitrary* settings of $\mathcal{G}$ and *arbitrary* forms of $\mathcal{G}$-irreps.

$$\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'\,\dagger}\,\mathbb{D}_{\lambda;\lambda'}^{\mathbf{k},\xi|\mathbf{k}',\xi'}(g)\,\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k},\xi|\mathbf{k}',\xi'} = \textstyle\sum_{\mathbf{k}''_o,\xi''_o}\oplus\, m(\mathbf{k},\xi;\lambda|\mathbf{k}',\xi';\lambda'||\mathbf{k}''_o,\xi''_o;\lambda'')\,\mathbb{D}^{\mathbf{k}''_o,\xi''_o;\lambda''}(g)$$

$$\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k}_o,\xi|\mathbf{k}'_o,\xi'\,\dagger}\,\mathbb{L}_{\lambda;\lambda'}^{\mathbf{k}_o,\xi|\mathbf{k}'_o,\xi'}(g)\,\mathbf{C}_{\lambda\lambda'\lambda''}^{\mathbf{k}_o,\xi|\mathbf{k}'_o,\xi'} = \textstyle\sum_{\mathbf{k}'',\xi''}\oplus\, m(\mathbf{k}_o,\xi;\lambda|\mathbf{k}'_o,\xi';\lambda'||\mathbf{k}'',\xi'';\lambda'')\,\mathbb{D}^{\mathbf{k}'',\xi'';\lambda''}(g)$$

REMARKS: Thus the program can be run for Kronecker products of *reducible* $\mathcal{G}$-representations. Corresponding results have been discussed in Ref.[6]. The package SYMCG offers analogous options for decomposing *symmetrized* Kronecker powers of space group representations.

D. Package — SYMPW: The software package called SYMPW allows one to construct systematically so-called *Symmetrized Plane Waves* (SPWs). These states transform according to space group irreps and are linear combinations of *plane waves.*

To sketch the procedure, one starts from a given *plane wave*, say $\Phi^{\mathbf{k},\mathbf{g}}$ where $\mathbf{k} \in RBZ(\mathcal{G})$ and $\mathbf{g} \in \mathcal{T}_{rec}$, and constructs by a two-step procedure SPWs. The first step consists of generating such linear combinations of the PW $\Phi^{\mathbf{k},\mathbf{g}}$ that transform according to *allowed* $\mathcal{G}(\mathbf{k})$-irreps. The second step consists of applying the induction procedure to the latter states to generate SPWs. The procedure written symbolically

$$\Phi^{\mathbf{k},\mathbf{g}}(\mathbf{x}) \longmapsto \Phi_a^{(\mathbf{k}|\mathbf{g};\xi,w)}(\mathbf{x}) \longmapsto \Phi_{\underline{R},a}^{(\mathbf{k}|\mathbf{g};\xi,w)}(\mathbf{x})$$

corresponds precisely to the induction procedure $\{\{\mathrm{D}^{\mathbf{k}} = \mathcal{T} - \mathrm{irrep}\} \uparrow \mathcal{G}(\mathbf{k})\} \uparrow \mathcal{G}$ of $\mathcal{G}$-irreps. To summarize, for uniqueness of the SPWs, one has not only to restrict the k-vectors to $RBZ(\mathcal{G})$, but also to take from each g-*star* with respect to $\mathcal{P}(\mathbf{k})$ only one element, as otherwise ambiguities would occur.

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