Computer programs for the reduction of Kronecker products
and symmetrized Kronecker powers of space group irreducible representations.

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The reduction of the Kronecker product of the irreducible representations
\( (\Gamma_k^p + G) \) and \( (\Gamma_k^q + G) \) of a space group \( G \) into its irreducible components
\( (\Gamma_k^r + G) \) is determined by the values of the Clebsch-Gordan (C-G) series coefficients \( C_{pq, r}^{k_i, k_j, k_z} \) in the expression

\[
(\Gamma_k^p + G) \otimes (\Gamma_k^q + G) = \sum_{k_r, r} C_{pq, r}^{k_i, k_j, k_z} (\Gamma_k^r + G),
\]

where \( (\Gamma_k^p + G) \) is a (single or double valued) irreducible representation of \( G \)
induced from the small (or allowed) representation \( \Gamma_k^p \) of the little group \( G_k^l \), etc. and \( k_i, k_j, k_z \) are restricted to lie in the representation domain \( \phi \) of \( G \).

At last year's Colloquium in Tübingen we reported on the Wave Vector Selection Rule (WVS) and Kronecker Product (KP) programs we have developed to evaluate the coefficients in equation (1) for any choice of vectors \( k_i \) and \( k_j \) in \( \phi \) for any of the 230 space groups \([1,2]\). At that time our programs had run successfully
for more than 150 groups and since then we have completed the remainder and the results are in the press \([3]\).

The Kronecker \( n^{th} \) power of an induced representation has been shown by Gard
\([4]\) to be capable of reduction in terms of the symmetric group of degree \( n \), so
that within each symmetry class, the reduction is expressed as a sum of induced representations. This is the generalization of the work of Mackey \([5]\) and Bradley
and Davies \([6]\) for the case \( n = 2 \) to which we shall confine ourselves in the
following.

The calculation to be performed is the evaluation of the coefficients \( C(\pm) \)
in the expansion of the symmetrized and antisymmetrized Kronecker square respectively:

\[
[(\Gamma_k^p + G) \otimes (\Gamma_k^p + G)] = \sum_{\ell, r} C(\pm) (\Gamma_k^\ell + G),
\]

\[
[(\Gamma_k^p + G) \otimes (\Gamma_k^p + G)] = \sum_{\ell, r} C(+)(\Gamma_k^\ell + G),
\]

(2)
The coefficients in equation (1) when \( k_i = k_j \) and \( p = q \) are related to those in equations (2) and (3) by

\[
C_{p,p,r} = C^{(+)} + C^{(-)}
\]

(4)

The first stage in the calculation is to evaluate the WVSRs for the Kronecker square which determine the values of \( k_r \in \mathfrak{g} \) which may appear on the right hand sides of equations (1) - (3). Each WVSR

\[
R_{\lambda} k_i + R_{\mu} k_i = k_r
\]

(5)

is determined by the pair \((R_\lambda, R_\mu)\) where \(\{R_\lambda | \chi_\lambda\}\) and \(\{R_\mu | \chi_\mu\}\) form a very restricted subset of the left coset representatives of \(G^*\) with respect to \(G\) [7]. Furthermore, the set of WVSRs is in one-to-one correspondence with the set of double cosets \(G^*:G^*\) of \(G\):

\[
G = \sum_{\nu} G^* \{R_\nu | \chi_\nu\} G^* \quad k_i
\]

(6)

where

\[
R_\nu = R^{-1}_{\nu} R_{\lambda},
\]

(7)

and \((R_\lambda, R_\mu)\) defines the WVSR in equation (5). Thus, each WVSR may be labelled self-inverse or non-self-inverse according as the corresponding double coset is self-inverse or non-self-inverse respectively. It is convenient to classify the WVSRs as belonging to type 0, 1 or 2 according as the corresponding double coset is self-inverse and identical to \(G^*\), self-inverse but not identical to \(G^*\) or non-self-inverse, respectively. It can then be shown from Bradley and Davies [6] that the coefficients in equations (2) and (3) are given by

\[
C^{(\pm)} = \sum_{\lambda, \mu} D^{\pm}(\lambda, \mu ; p, r) \delta(R_\lambda k_i + R_\mu k_i - k_r)
\]

(8)

where

\[
\delta(k) = \begin{cases} 1 & \text{if } k \text{ is a reciprocal lattice vector} \\ 0 & \text{otherwise} \end{cases}
\]

(9)

and \(D^{\pm}(\lambda, \mu ; p, r)\) is defined as follows.

**WVSR TYPE 0**

\[
D^{\pm}(\lambda, \mu ; p, r) = \frac{|T|}{N_{\lambda \mu}} \sum_{\nu} \chi_{\lambda}^{2} \left(\{S|\tilde{y}\}\right) e_{N_{\lambda \mu}}^{T} \chi_{\lambda p}^{2} \left(\{S|\tilde{y}\}\right) \chi_{r}^{2} \left(\{S|\tilde{y}\}\right)
\]

(10)