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LETTER TO THE EDITOR

The auxiliary group approach to the reduction of Kronecker products

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Abstract. Bijective mappings of matrix representations are used to derive generating relations for Clebsch–Gordon coefficients and to reduce the multiplicity problem.

We start with an auxiliary group Q^{REP} consisting of transformations which map unitary matrix representations (reps) of a given group G onto reps of the same dimension, especially irreducible ones (irreps) onto irreps. This group has been introduced by Dirl *et al* (1986) systematising and generalising similar ideas of other authors (e.g. Butler and Ford 1979). Three kinds of transformations are considered.

(i) *Associations*, which are multiplications with one-dimensional irreps D^J, i.e. $D(g)\to D^J(g)D(g)$.

(ii) *Automorphisms*, which are substitutions $D(g)\to D(\beta^{-1}(g))$ where $g\to\beta(g)$ is an automorphism of G.

(iii) *Complex conjugation*: $D(g)\to D(g)^*$.

The orbits of Q^{rep} define a partition of equivalence classes of irreps (irrep labels K) into disjoint sets (q-classes). It is possible to generate representatives for each of these equivalence classes by applying suitable transformations q on one specific irrep of a q-class (standard irreps). That is, if K' is in the same q-class as K, then

$$qD^K(g)=U^{K'K}(q)^\dagger D^{K'}(g)U^{K'K}(q) \tag{1}$$

for some $q\in Q^{\mathrm{rep}}$. If D^K is the first standard irrep and $K'\not\sim K$ then relation (1) can be used to define the standard irrep $D^{K'}$ by fixing q and choosing $U^{K'K}$ as unit matrix. For a general transformation $q\in Q^{\mathrm{rep}}$ the matrix $U^{K'K}(q)$ in (1) may be written as a product of a few specific matrices $U^{K'K}(q')$. Each of these matrices is fixed by the transformation q' up to a phase factor.

For Kronecker products we consider the transformations $D^K\otimes D^L\to(q_1D^K)\otimes(q_2D^L)$. Setting $D^{KL}(g)=D^K(g)\otimes D^L(g)$ and $U^{K'L',KL}(q_1,q_2)=U^{K'K}(q_1)\otimes U^{L'L}(q_2)$ one obtains from (1)

$$(q_1,q_2)D^{KL}(g)=U^{K'L',KL}(q_1,q_2)^\dagger D^{K'L'}(g)U^{K'L',KL}(q_1,q_2). \tag{2}$$

For the reduction of Kronecker products we define a second auxiliary group $\boldsymbol{Q}$ which is generated by the pairs (q_1,q_2) of associations $q_{1,2}$ and by the transformations (q,q) where q is an arbitrary automorphism or the complex conjugation. The structure of

Q is

$$Q = (\text{ASS} \times \text{ASS}) \circledS (\text{AUT} \times \text{CON}) \tag{3}$$

where $\circledS$ denotes a semi-direct and $\times$ a direct product. The direct product group ASS × ASS consists of the Abelian groups ASS. The symbol AUT denotes the group of automorphisms and CON contains the identity and the operation of complex conjugation.

There exists a natural homomorphism of Q onto Q^{rep} which maps a pair (q_1, q_2) of associations onto the association $q_{12} = q_1 q_2 = q_2 q_1$, and the elements $(q_1, q_2) = (q, q) \in Q$ onto the elements $q_{12} = q \in Q^{\text{rep}}$, if q is an automorphism or the complex conjugation. In detail we have

$$D^{J_1}(g) \otimes D^{J_2}(g) = D^{J_{12}}(g) \tag{4}$$

where $(q_1, q_2) \in \text{ASS} \times \text{ASS}$ is assigned to the LHS and its homomorphic image q_{12} to the RHS of (4). Relation (4) allows one to choose the corresponding Clebsch-Gordan coefficients as Kronecker deltas.

Clebsch-Gordan coefficients are elements of the rectangular matrices $S^{KL,M}$ (CG blocks) which satisfy, for a given triple K, L, M of irreps,

$$D^{KL}(g) S^{KL,M} = S^{KL,M} D^M(g). \tag{5}$$

The transformations of the reps may be related to transformations of the CG blocks by transforming both sides of (5) by the following operations: (i) multiplication with a one-dimensional irrep, (ii) substitution $g \to \beta^{-1}(g)$, (iii) complex conjugation. Now if $q_{12} \in Q^{\text{rep}}$ is the image of $(q_1, q_2) \in Q$ and if qS is defined by

$$qS = \begin{cases} S^* & \text{if } q \text{ contains the complex conjugation} \\ S & \text{otherwise} \end{cases} \tag{6}$$

then it follows from (1), (2), (5) and (6) that the blocks

$$T(q_1, q_2) S^{KL,M} = U^{K'L',KL}(q_1, q_2)(q_{12} S^{KL,M}) U^{M'M}(q_{12})^\dagger \tag{7}$$

satisfy (5) for the triple K', L', M'. This fact may be exploited to reduce the calculation of CG blocks by the following steps which require only the knowledge of the matrices $U^{PP}(q)$ for the representatives of the q-classes.

Step 1. If $K' \neq K$ and/or $L' \neq L$, D^K and D^L are class representatives, $D^{K'}$ and $D^{L'}$ are standard irreps, and $D^{K'L'} = (q_1, q_2)\ D^{KL}$ for some $(q_1, q_2) \in Q$, then the blocks $S^{K'L',M'}$ can be defined as $T(q_1, q_2) S^{KL,M}$ (generating relations).

Step 2. If $K' = K$ and $L' = L$ and $M' \neq M$, then the matrices $U^{M'M}$ relate blocks belonging to different standard irreps D^M contained in D^{KL}, i.e. $S^{KL,M'}$ may be generated from $S^{KL,M}$.

Step 3. For fixed K, L, M the transformations (7) act only on the multiplicity index. The blocks $S^{KL,M/1}, \ldots S^{KL,M/m}$ belonging to the m-fold direct sum of D^M can then be chosen to transform according to projective irreducible co-representations of subgroups of Q. This gives further generating relations and reduces the multiplicity problem (even resolves it sometimes).

Step 4. If $K = L$ then there exists a permutation matrix X of order two which commutes with D^{KK}. In this case the transformation $S^{KK,M} \to X S^{KK,M}$ may be combined with those of the auxiliary group to define symmetrised CG coefficients for

Kronecker squares. Accordingly the extended auxiliary group reads

$$\boldsymbol{Q}' = (\text{ASS} \times \text{ASS}) \circledS (\text{AUT} \times \text{CON} \times \text{PERM}) \tag{8}$$

where PERM is of order two.

To illustrate the scheme sketched above we consider the double space group P23 and its irreps *Zk*, where *Z* denotes the special points of the Brillouin zone and $k = 1, 2, \ldots$, labels the irreps of the corresponding little co-groups. Here $Z = G$(amma), *R*, *X*, *M* and we have 24 P23 irreps: $G1$–$G7$, $R1$–$R7$, $X1$–$X5$, $M1$–$M5$. They decompose into six *q*-classes $/G1/, /G4/, /G5/, /X1/, /X2/, /X5/$; the corresponding matrix dimensions are 1, 3, 2, 3, 3, 6 (Cracknell *et al* 1979).

Step 1 reduces the calculation of CG matrices from 300 (=24.25/2) to 23. These belong to the six trivial products $G1 \otimes G1$, $G1 \otimes G4$, $G1 \otimes G5$, $G1 \otimes X1$, $G1 \otimes X2$, $G1 \otimes X5$, and the following non-trivial Kronecker products (Davies and Cracknell 1979):

$$\begin{aligned}
&G4 \otimes G4 \simeq \underline{G1 \oplus G2 \oplus G3} \oplus \underline{\underline{2}}\ G4\\
&G4 \otimes G5 \simeq \underline{G5 \oplus G6 \oplus G7}\\
&G4 \otimes X1 \simeq \underline{X2 \oplus X3} \oplus X4\\
&G4 \otimes X2 \simeq \underline{X1 \oplus X4} \oplus X3\\
&G4 \otimes X5 \simeq (\underline{\underline{2}} \oplus \underline{\underline{1}})X5\\
&G5 \otimes G5 \simeq G1 \oplus G4\\
&G5 \otimes X1 \simeq X5\\
&G5 \otimes X2 \simeq X5\\
&G5 \otimes X5 \simeq \underline{X1 \oplus X4} \oplus \underline{X2 \oplus X3}\\
&X1 \otimes X1 \simeq \underline{G1 \otimes G2 \otimes G3} \oplus \underline{\underline{2}}\ M1\\
&X1 \otimes X4 \simeq G4 \oplus \underline{M3 \oplus M4}\\
&X2 \otimes X2 \simeq \underline{G1 \oplus G2 \oplus G3} \oplus \underline{\underline{2}}\ M3\\
&X2 \otimes X3 \simeq G4 \oplus \underline{M1 \oplus M2}\\
&X1 \otimes X2 \simeq G4 \oplus M2 \oplus M4\\
&X1 \otimes X5 \simeq \underline{G5 \oplus G6 \oplus G7} \oplus \underline{\underline{2}}\ M5\\
&X2 \otimes X5 \simeq \underline{G5 \oplus G6 \oplus G7} \oplus \underline{\underline{2}}\ M5\\
&X5 \otimes X5 \simeq \underline{G1 \oplus G2 \oplus G3} \oplus (\underline{\underline{2}} \oplus \underline{\underline{1}})\ G4 \oplus (\underline{\underline{1}} \oplus \underline{\underline{1}})(\underline{M1 \oplus M2} \oplus \underline{M3 \oplus M4}).
\end{aligned}$$

In this table the implications of step 2 are shown by underlining certain direct sums of inequivalent irreps. The meaning of these lines is that $\boldsymbol{S}^{G4,G4;G2}$ and $\boldsymbol{S}^{G4,G4;G3}$ may be generated from $\boldsymbol{S}^{G4,G4;G1}$, etc.

The result of step 3 and of step 4 are indicated by the double underbars. (For the symmetrised squares see Davies and Cracknell (1980).) For instance $(\underline{\underline{2}} \oplus \underline{\underline{1}})$ means that the three irreps $X5$ contained in $G4 \otimes X5$ transform according to two- and one-dimensional irreducible co-reps, respectively.

In this example all multiplicities can be explained in terms of irreducible projective co-reps of subgroups of the auxiliary group Q. Moreover, steps 2–4 reduce the calculation of CG coefficients for the above listed products by almost 50%. It is especially this reduction and that of step 1 which suggest the consideration of this method in the calculation and tabulation of extensive Kronecker product tables.

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