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Clebsch–Gordan coefficients for space groups

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Abstract. A practical method is given for finding Clebsch–Gordan coefficients for space groups. It is immediately applicable since the formulae derived depend only on a knowledge of the vector and projective representations of point groups which are fully tabulated elsewhere.

1. Introduction

An important application of group theory to physics is the problem of decomposing a Kronecker product of irreducible representations as a direct sum of irreducible parts. In solid state physics, the symmetry groups under consideration are space groups and a particular application would be to the theory of selection rules in crystals. This paper deals with the problem of constructing basis functions for the representations which are contained in the Kronecker product of two irreducible space group representations. This problem has also been considered by Litvin and Zak (1968), who propose a method which is basically an application of a result of Koster (1958) to the full group. We use the fact that every irreducible space group representation may be expressed as an induced representation and apply a theorem of Mackey (1952) to give a direct sum decomposition of the Kronecker product indexed by a fixed set of double coset representatives. Each direct summand is associated with a unique $\boldsymbol{k}$ vector in the first Brillouin zone and so we may decompose the induced representation of G by inducing through the little group $G^{\boldsymbol{k}}$ and reducing at this stage. Thus the method we propose for finding the Clebsch–Gordan coefficients splits naturally into three steps. We end by giving a simple example to show that this method is a practical proposition for reducing the Kronecker product of space group representations.

2. Clebsch–Gordan coefficients

Let G be a space group and let $\{\Gamma^i : i = 1, \ldots, n\}$ be a complete set of non-equivalent UIR (unitary irreducible representations) of G. The Kronecker product of two representations is equivalent to a direct sum decomposition, thus

$$\Gamma^i \otimes \Gamma^j \equiv \bigoplus_k c_{ijk} \Gamma^k \tag{2.1}$$

where the coefficients c_{ijk} are non-negative integers. Hence there exists a unitary matrix

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U such that

$$U^{-1}(\Gamma^i \otimes \Gamma^j)U = \bigoplus_k c_{ijk}\Gamma^k. \tag{2.2}$$

The matrix elements of U are called the Clebsch–Gordan coefficients. The matrix U may not be unique because in general we can find a unitary matrix V such that

$$V^{-1}\left(\bigoplus_k c_{ijk}\Gamma^k\right)V = \bigoplus_k c_{ijk}\Gamma^k. \tag{2.3}$$

Dividing V into blocks suitable for block matrix multiplication and applying Schur's lemma, we find

$$V = \bigoplus_k (V_k \otimes I_{d_k}) \tag{2.4}$$

where $d_k = \dim \Gamma^k$ and V_k is an arbitrary $c_{ijk} \times c_{ijk}$ unitary matrix. Clearly if all the c_{ijk} are either zero or one the new basis functions will be determined up to a phase factor. Otherwise the functions will only be given up to arbitrary linear combinations of the ordered sets of basis functions belonging to a given UIR.

In their book, Bradley and Cracknell (1972) have described how every UIR Γ^i of a space group $\boldsymbol{G}$ is characterized by a vector $\boldsymbol{k}$ in the representation domain of the first Brillouin zone and the label, p, of a small representation of the little group $\boldsymbol{G}^{\boldsymbol{k}}$. Indeed every representation of $\boldsymbol{G}$ can be expressed in the form $(D_p^{\boldsymbol{k}} \uparrow \boldsymbol{G})$. In what follows we shall assume that this standard form is known. In other words, the matrix form of the small representations $D_p^{\boldsymbol{k}}$ and the coset representatives of $\boldsymbol{G}^{\boldsymbol{k}}$ in $\boldsymbol{G}$ are fixed. We also need a result of Mackey (1952) which states that if C and D are representations of the subgroups $\boldsymbol{H}$ and $\boldsymbol{K}$ of $\boldsymbol{G}$ respectively, then

$$(D \uparrow \boldsymbol{G}) \otimes (C \uparrow \boldsymbol{G}) \equiv \bigoplus_\alpha [(D_\alpha \downarrow \boldsymbol{L}_\alpha) \otimes (C \downarrow \boldsymbol{L}_\alpha)] \uparrow \boldsymbol{G}, \tag{2.5}$$

where the direct sum is taken over all the double coset representatives defined by

$$\boldsymbol{G} = \bigcup_\alpha \boldsymbol{H} d_\alpha \boldsymbol{K}. \tag{2.6}$$

The group $\boldsymbol{L}_\alpha = \boldsymbol{H} \cap d_\alpha \boldsymbol{K} d_\alpha^{-1}$, and D_α is a representation of $d_\alpha \boldsymbol{K} d_\alpha^{-1}$ defined by

$$D_\alpha(d_\alpha k d_\alpha^{-1}) = D(k) \tag{2.7}$$

for all $k \in \boldsymbol{K}$.

This theorem has immediate application to our problem if $\boldsymbol{H}$ and $\boldsymbol{K}$ are the little groups corresponding to the representations C and D. For convenience we use general notation but it should not be forgotten that $\boldsymbol{G}$ is a space group.

We have already assumed the existence of standard sets of left coset representatives, so take

$$\boldsymbol{G} = \bigcup_\tau p_\tau \boldsymbol{K} = \bigcup_\sigma p_\sigma \boldsymbol{H}. \tag{2.8}$$

However, the double coset representatives need not be fixed beforehand and the resulting Clebsch–Gordan coefficients will depend on the particular set chosen. Suppose we take

$$\boldsymbol{G} = \bigcup_\alpha \boldsymbol{H} d^\alpha \boldsymbol{K}. \tag{2.9}$$

From equations (2.8) and (2.9), each $p_\tau = h^\alpha_\tau d_\alpha k_\tau$ where $h^\alpha_\tau \in \boldsymbol{H}, k_\tau \in \boldsymbol{K}$. It can be shown that

$$\boldsymbol{H} = \bigcup_\tau h^\alpha_\tau \boldsymbol{L}_\alpha \tag{2.10}$$

is a decomposition of $\boldsymbol{H}$ into distinct left cosets.

Let the UIR D have basis set $\{\phi_i : i = 1, \dots, d\}$ and the UIR C have basis set $\{\psi_j : j = 1, \dots, f\}$, then a basis for the Kronecker product $(D \uparrow \boldsymbol{G}) \otimes (C \uparrow \boldsymbol{G})$ is $\{(p_\tau \phi_i, p_\sigma \psi_j):$ for all $i, j, \tau, \sigma\}$. We are using the definition of an induced representation given by Bradley (1966). A carrier space for the representation $[(D_\alpha \downarrow \boldsymbol{L}_\alpha) \otimes (C \downarrow \boldsymbol{L}_\alpha)] \uparrow \boldsymbol{G}$ in the direct sum decomposition (2.5) is

$$\Omega_\alpha = \sum_{\sigma, \tau, i, j} p_\sigma h^\alpha_\tau (d_\alpha \phi_i, \psi_j) \tag{2.11}$$

where the summation sign on the right-hand side means the set of all linear combinations of the functions $p_\sigma h^\alpha_\tau (d_\alpha \phi_i, \psi_j)$. The next lemma shows that Ω_α is independent of the particular choice of double coset representative.

Lemma (2.1). If $\boldsymbol{H} d_\alpha \boldsymbol{K} = \boldsymbol{H} d_\beta \boldsymbol{K}$ then $\Omega_\alpha = \Omega_\beta$.

Proof. Let $d_\beta = h d_\alpha k$, where $h \in \boldsymbol{H}$, $k \in \boldsymbol{K}$, then it can be shown that $\boldsymbol{L}_\beta = h \boldsymbol{L}_\alpha h^{-1}$. Now

$$\boldsymbol{H} = \bigcup_\tau h^\alpha_\tau \boldsymbol{L}_\alpha = \bigcup_\tau h^\alpha_\tau h^{-1} \boldsymbol{L}_\beta$$

hence

$$\Omega_\beta = \sum p_\sigma h^\alpha_\tau h^{-1} (d_\beta \phi_i, \psi_j) = \sum p_\sigma h^\alpha_\tau (d_\alpha k \phi_i, h^{-1} \psi_j).$$

But the space generated by the basis set $\{\phi_i\}$ is invariant under the action of $k \in \boldsymbol{K}$ and the space generated by the basis set $\{\psi_i\}$ is invariant under the action of $h^{-1} \in \boldsymbol{H}$. Hence $\Omega_\alpha = \Omega_\beta$.

Before proceeding, we must consider the representations more closely. If $D^{\boldsymbol{k}}_p$ is a UIR of $\boldsymbol{K} = \boldsymbol{G}^{\boldsymbol{k}}$ which subduces a multiple of the representation $\exp(-i\boldsymbol{k} \cdot \boldsymbol{t})$ on $\boldsymbol{T}$, then it can be written

$$D^{\boldsymbol{k}}_p(\{R|\boldsymbol{v}\}) = \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{v})\, \Lambda^{\boldsymbol{k}}_p(\{R|\boldsymbol{v}\}) \tag{2.12}$$

where $\Lambda^{\boldsymbol{k}}_p$ is a projective representation of the point group isomorphic to the little co-group $\bar{\boldsymbol{G}}^{\boldsymbol{k}}$. Let $d_\alpha = \{S|\boldsymbol{w}\}$, then for all $\{R|\boldsymbol{v}\} \in \boldsymbol{L}_\alpha$ it can be shown that

$$(D^{\boldsymbol{k}_1}_{p_1;\alpha} \otimes D^{\boldsymbol{k}_2}_{p_2})(\{R|\boldsymbol{v}\}) = \exp[-\mathrm{i}(S\boldsymbol{k}_1 + \boldsymbol{k}_2) \cdot \boldsymbol{v}] \Lambda^{\boldsymbol{k}_1}_{p_1;\alpha}(R) \otimes \Lambda^{\boldsymbol{k}_2}_{p_2}(R) \tag{2.13}$$

where

$$D^{\boldsymbol{k}}_{p;\alpha}(\{R|\boldsymbol{v}\}) = \exp(-\mathrm{i}S\boldsymbol{k} \cdot \boldsymbol{v}) \Lambda^{\boldsymbol{k}}_{p;\alpha}(R) \tag{2.14}$$

and

$$\Lambda^{\boldsymbol{k}}_{p;\alpha}(R) = \exp[-\mathrm{i}S\boldsymbol{k} \cdot (R\boldsymbol{w} - \boldsymbol{w})]\, \Lambda^{\boldsymbol{k}}_p(S^{-1}RS). \tag{2.15}$$

Let $\boldsymbol{k} = S\boldsymbol{k}_1 + \boldsymbol{k}_2$, then since $\{R|\boldsymbol{v}\} \in \boldsymbol{L}_\alpha$ we have $R\boldsymbol{k} \sim \boldsymbol{k}$ and it follows that $\boldsymbol{L}_\alpha \subset \boldsymbol{G}^{\boldsymbol{k}}$. Thus the block labelled by α is associated with the wavevector $\boldsymbol{k}$ which may or may not lie in the representation domain. In the latter case there exists an element P in the point group such that $P\boldsymbol{k}$ lies in the representation domain. The representation induced from $\boldsymbol{G}^{P\boldsymbol{k}}$ is identical with the representation induced from $\boldsymbol{G}^{\boldsymbol{k}}$ if we conjugate both the standard representations of $\boldsymbol{G}^{P\boldsymbol{k}}$ and the standard coset representatives of $\boldsymbol{G}^{P\boldsymbol{k}}$ in $\boldsymbol{G}$ with the same element $\{P|\boldsymbol{u}\} \in \boldsymbol{G}$, where $\boldsymbol{u}$ is either the vector or a non-primitive translation.

The method we employ is to induce up to $\boldsymbol{G}$ through $\boldsymbol{G}^k$ and reduce the representation at the $\boldsymbol{G}^k$ stage. This means that the coset representatives of $\boldsymbol{L}_\alpha$ in $\boldsymbol{G}$ must be chosen more carefully. We take

$$\boldsymbol{G}^k = \bigcup_\nu q_\nu^\alpha \boldsymbol{L}_\alpha \tag{2.16}$$

where $\{q_\nu^\alpha\}$ is the required subset of $\{p_\sigma h_\tau^\alpha\}$ and take a standard set, as described above, for $\boldsymbol{G}^k$ in $\boldsymbol{G}$. From the theory of induced representations, a change of coset representatives leads to a unitarily equivalent representation.

The first step is to calculate the unitary matrix U_1 which achieves the partial reduction, namely

$$(U_1)^{-1}[(D \uparrow \boldsymbol{G}) \otimes (C \uparrow \boldsymbol{G})]U_1 = \bigoplus_\alpha \{[(D_\alpha \downarrow \boldsymbol{L}_\alpha) \otimes (C \downarrow \boldsymbol{L}_\alpha)] \uparrow \boldsymbol{G}^k\} \uparrow \boldsymbol{G}. \tag{2.17}$$

Since

$$p_\omega q_\nu^\alpha(d_\alpha \phi_i, \psi_j) = \sum_{l,m} (p_\tau \phi_l, p_\sigma \psi_m) D(p_\tau^{-1} p_\omega q_\nu^\alpha d_\alpha)_{li} C(p_\sigma^{-1} p_\omega q_\nu^\alpha)_{mj} \tag{2.18}$$

where $p_\tau^{-1} p_\omega q_\nu^\alpha d_\alpha \in \boldsymbol{K}$, $p_\sigma^{-1} p_\omega q_\nu^\alpha \in \boldsymbol{H}$ and $\{p_\omega\}$ is the standard set of left coset representatives for $\boldsymbol{G}^k$ in $\boldsymbol{G}$, we have

$$U_1(\tau\sigma lm, \alpha\omega\nu ij) = D(p_\tau^{-1} p_\omega q_\nu^\alpha d_\alpha)_{li} C(p_\sigma^{-1} p_\omega q_\nu^\alpha)_{mj}. \tag{2.19}$$

Now we may restrict attention to the projective representations $(\Lambda_{p_1;\alpha}^{k_1} \otimes \Lambda_{p_2}^{k_2})$ given by equation (2.13). In general this will be reducible, so there exists a unitary matrix U_2 such that

$$(U_2)^{-1}(\Lambda_{p_1;\alpha}^{k_1} \otimes \Lambda_{p_2}^{k_2})U_2 = \bigoplus_\gamma a_\gamma W_\gamma^k \tag{2.20}$$

then

$$U_2 = U_2(\alpha\omega\nu ij, \alpha\omega\nu\gamma i_r) \tag{2.21}$$

where $r = 1, \ldots, a_\gamma$ and i_r denotes the ith basis vector of the rth representation W_γ^k. To obtain the required decomposition, it remains for us to reduce each $(W_\gamma^k \uparrow \bar{\boldsymbol{G}}^k)$. Let U_3 be the unitary matrix such that

$$(U_3)^{-1}(W_\gamma^k \uparrow \bar{\boldsymbol{G}}^k)U_3 = \bigoplus b_q \Lambda_q^k \tag{2.22}$$

then

$$U_3 = U_3(\alpha\omega\nu\gamma i_r, \alpha\omega\nu'\gamma q j_s) \tag{2.23}$$

where $s = 1, \ldots, b_q$ and j_s denotes the jth basis vector of the sth representation Λ_q^k. Since the coset representatives $\{p_\omega\}$ were chosen to be in standard form, the required matrix is

$$U = U_1\left(\bigoplus_{\alpha,\omega,\nu} U_2(\alpha\omega\nu)\right)\left(\bigoplus_{\alpha,\omega,\gamma} U_3(\alpha\omega\gamma)\right). \tag{2.24}$$

In general, the group $\boldsymbol{L}_\alpha$ will be small and U_2, U_3 may be found easily from a knowledge of the representations. The vector representations of the three-dimensional point groups are tabulated by Bradley and Cracknell (1972), the projective representations are tabulated by Hurley (1966) and a formula for inducing projective representations is given by Backhouse and Bradley (1970). However, in all cases the method of Koster (1958) may be used to reduce the representations. Since this method only depends on the orthogonality relations it may be extended without change to projective representations.

It is interesting to compare our method with that of Litvin and Zak (1968). Their use of Koster's method at the full group level leads to a long analysis of the properties of the matrix U in order to simplify the calculations. Using our procedure, the symmetries of the matrix are much more apparent.

3. Example

Using the notation and results of Bradley and Davies (1970), we apply our method to a pair of irreducible representations of the space group T_d^2 corresponding to the zinc-blende structure. Consider the Kronecker product

$$(X_1 \uparrow G) \otimes (L_3 \uparrow G) \equiv (L_1 \uparrow G) \oplus (L_2 \uparrow G) \oplus 2(L_3 \uparrow G). \tag{3.1}$$

The little co-groups of X, L are $\boldsymbol{D}_{2\mathrm{d}}$, $\boldsymbol{C}_{3\mathrm{v}}$, respectively, and since $\boldsymbol{C}_{3\mathrm{v}}\boldsymbol{D}_{2\mathrm{d}} = \boldsymbol{T}_{\mathrm{d}}$, there is only one double coset representative which we take to be $\{E|\boldsymbol{0}\}$. Hence

$$(X_1 \uparrow G) \otimes (L_3 \uparrow G) \equiv [(X_1 \downarrow \{E, \sigma_{de}\}) \otimes (L_3 \downarrow \{E, \sigma_{de}\})] \uparrow \boldsymbol{G} \tag{3.2}$$

with associated $\boldsymbol{k}$ vector

$$\boldsymbol{k} = (\tfrac{1}{2}, 0, \tfrac{1}{2}) + (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) = (1, \tfrac{1}{2}, 1) \sim S_{4x}^{-}\boldsymbol{k}_L. \tag{3.3}$$

The matrix U_1 is 24×24 and can be calculated from equation (2.19) if we take the standard representations to be those given by table 2.3 of Bradley and Cracknell (1972). We shall concentrate on obtaining U_2 and U_3.

Take the following as standard left coset decompositions:

$$\boldsymbol{T}_{\mathrm{d}} = E\boldsymbol{D}_{2\mathrm{d}} \cup C_{31}^{+}\boldsymbol{D}_{2\mathrm{d}} \cup C_{31}^{-}\boldsymbol{D}_{2\mathrm{d}}$$

$$\boldsymbol{T}_{\mathrm{d}} = E\boldsymbol{C}_{3\mathrm{v}} \cup C_{2x}\boldsymbol{C}_{3\mathrm{v}} \cup S_{4x}^{+}\boldsymbol{C}_{3\mathrm{v}} \cup S_{4x}^{-}\boldsymbol{C}_{3\mathrm{v}}$$

$$\boldsymbol{C}_{3\mathrm{v}} = E\{E, \sigma_{de}\} \cup C_{31}^{+}\{E, \sigma_{de}\} \cup C_{31}^{-}\{E, \sigma_{de}\}.$$

Also

$$\overline{\boldsymbol{G}}^{\boldsymbol{k}} = S_{4x}^{-}\overline{\boldsymbol{G}}^{L}S_{4x}^{+} = S_{4x}^{-}\boldsymbol{C}_{3\mathrm{v}}S_{4x}^{+}$$

$$= \{E, C_{34}^{-}, C_{34}^{+}, \sigma_{de}, \sigma_{da}, \sigma_{dd}\}.$$

This group has a two-dimensional representation $D^{\boldsymbol{k}}$ corresponding to the representation L_3 of $\boldsymbol{C}_{3\mathrm{v}}$ given by

$$D^{\boldsymbol{k}}(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^{\boldsymbol{k}}(\sigma_{de}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad D^{\boldsymbol{k}}(C_{34}^{-}) = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}. \tag{3.4}$$

Returning to equation (3.2), let Δ be the representation $(X_1 \downarrow \{E, \sigma_{de}\}) \otimes (L_3 \downarrow \{E, \sigma_{de}\})$, then

$$\Delta(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Delta(\sigma_{de}) = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}. \tag{3.5}$$

It can be shown that

$$U_2 = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix} \tag{3.6}$$

reduces Δ to $A_g \oplus A_u$, the identity and alternating representations of $\{E, \sigma_{de}\}$.

Now induce up to $\bar{\boldsymbol{G}}^k$ taking as coset representatives $E, S_{4x}^- C_{31}^+ S_{4x}^+$, $S_{4x}^- C_{31}^- S_{4x}^+$. That is E, C_{34}^-, C_{34}^+. We obtain the following representations:

$$\begin{aligned} [A \uparrow \bar{\boldsymbol{G}}^k](\sigma_{de}) &= \begin{pmatrix} \pm 1 & 0 & 0 \\ 0 & 0 & \pm 1 \\ 0 & \pm 1 & 0 \end{pmatrix} \\ [A \uparrow \bar{\boldsymbol{G}}^k](C_{34}^-) &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \end{aligned} \tag{3.7}$$

where we take the $\pm$ signs corresponding to $A = A_g, A_u$ respectively. Since $(A_g \oplus A_u) \uparrow \bar{\boldsymbol{G}}^k$ gives the regular representation of $\bar{\boldsymbol{G}}^k$, it is easy to find matrices which decompose the above representations. It can be shown that

$$\begin{aligned} U_{3g} &= \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & 0 \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{2}} \end{pmatrix} \\ U_{3u} &= \begin{pmatrix} \sqrt{\frac{1}{3}} & 0 & -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} \end{pmatrix} \end{aligned} \tag{3.8}$$

We now have enough information to find the Clebsch–Gordan coefficients.

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