

CLIFFORD THEORY AND ITS APPLICATION  
TO THE REPRESENTATION THEORY OF  
CRYSTALLOGRAPHIC SPACE GROUPS.

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1. Introduction

This survey contains a comparative exposition of Clifford's theory of group representations and of the little group method, used by solid state physicists, for constructing space group representations. In particular we show that the little group method provides a nice application of the Clifford theory, albeit as a very special case.

Let  $H$  be a subgroup of finite index in a group  $G$ . Then Frobenius induction enables us to generate representations of  $G$  from those of  $H$ . In general such induced representations are not irreducible. By analyzing the case where  $H$  is an invariant subgroup, Clifford [6] was able to establish a procedure for obtaining all finite dimensional unitary irreducible representations (U.I.R.) of  $G$  from knowledge of all U.I.R. of  $H$  and certain projective representations of subgroups of the finite group  $G/H$ . Although Clifford disclaimed credit for the originality of many of his results, his work is regarded as an important landmark in group representation theory in that by organizing and generalizing the then current knowledge of special results he laid the foundations for much future work. It is worth noting at this point that some of Clifford's terminology differs in a possibly confusing way from that now in use. In particular he uses the term 'induce', where we would now use 'subduce' or 'restrict', and the term 'generate', where we would now use 'induce'. We shall stick to modern usage in this review. An up to date formulation of Clifford theory is to be found in the book by Curtis and Reiner [8].

Later Mackey found a general theory of unitary representations of locally compact topological groups incorporating a far reaching generalization of the Clifford method, which is particularly valid for so-called type I groups - a class of groups whose representation theory is in some sense nice, and which includes nearly all of the groups of mathematical physics. We refer the reader to Mackey [13] for an extensive account of his theory and to Coleman [7] for a summary of its main concepts, results and some applications in physics.

Turning now to space group representations, the first paper devoted to this subject was that of Seitz [14] in which he discussed the applicability of Schur's theory of representations of finite solvable groups. We recall that a finite solvable group  $G$  has a sub-invariant series

$$\{ e \} = G_0 \triangleleft G_1 \triangleleft \dots \triangleleft G_{r-1} \triangleleft G_r = G,$$

where  $G_i/G_{i-1}$  is a cyclic group for each  $i = 1, 2, \dots, r$ . It is true that the factor groups obtained by making three-dimensional space groups (or subgroups of these) finite using the Born-von Kármán periodic boundary conditions, fall into the above class of groups. These finite factor groups will be referred to in the sequel as "finite space groups", for contrast ordinary space groups will be called "infinite space groups". Schur's method works by stepping up the sub-invariant series for  $G$ , applying at each stage what we can now recognize as Clifford's theory. Seitz's paper just predates that of Clifford. Almost at once, Bouchaert, Smoluchowski and Wigner [3] applied the Seitz method to some specific space groups and incidentally also introduced such terms as 'reduced wave number vector', 'group of the wave vector' and 'small representation'.

This so-called little group method has now been refined and modernized by several authors. A good account of it has been given by Koster [11], and its relationship with Clifford theory recognized by Lomont [12], Jansen and Boon [9], Janssen [10]. The most detailed version is given by Bradley and Cracknell [5], who also take advantage of the Mackey Kronecker product theory for computing Clebsch-Gordan coefficients.

We conclude this introduction with a few remarks on the comparative merits of dealing with finite or infinite space groups. Our first point is that Clifford theory is valid not only for finite groups, but also for infinite groups as long as  $G/H$  is finite and where we only want to compute finite dimensional representations. Now if  $G$  is an infinite space group with translation subgroup  $T$  then  $G/T$  is certainly finite, and furthermore, all of the U.I.R. of  $T$  are known and are one-dimensional. That  $G$  only has finite dimensional U.I.R. is a special case of a theorem of Thoma [15]: A discrete group  $G$  is of type I - which implies that it has a nice representation theory - if and only if  $G$  contains an invariant Abelian subgroup  $M$  of finite index, and then the dimensions of the U.I.R. of  $G$  are bounded by  $|G/M|$ . Thus there is no mathematical objection to taking an infinite transla-

tion subgroup.

On the other hand a real crystal is finite in extent and, if perfect and opposite faces identified, is invariant under a finite space group. However, the spacings in the resulting discrete energy spectrum are too fine to be resolved experimentally and are blurred by imperfections anyway. It is usual to interpolate and assume the spectrum is a piece-wise continuous function of the wave-vector. The set of U.I.R. of an infinite space group, because it contains subsets of U.I.R. which correspond to every finite crystal, can accommodate both the discrete and the continuous points of view for the energy spectrum. There are more serious problems with a finite space group for the spectrum of an electron moving in a crystal potential under the additional influence of a uniform magnetic field.

The best reason for considering finite space groups is pedagogical in nature. The fact is that the theory of finite space group representations, including proofs of results, can be rigorously discussed within the scope of finite group theory at a little above the elementary level. The added sophistication and confidence required to make the transition to a rigorous infinite group treatment is not usually considered justified in view of the practical success of the finite approach. For example, although the present author, in [ 2 ], demonstrated rigorously the validity of the Herring reality criterion for infinite space group representations, without the risky summation over the translations, he would not wish to impose his proof on a beginner!

In the main part of this review we state most results without proof. For this, the distinction between finite and infinite space groups is immaterial.

In the next two sections we give an account of the structure and results of Clifford theory and little group theory. To assist the easy comparison of results, each section is divided into manageable subsections in such a way that subsection 3( $\alpha$ ) is a special case of subsection 2( $\alpha$ ), for  $\alpha = a, b \dots e$ . Note that 3(e) is very much simpler than 2(e).

## 2. Clifford Theory

If  $G$  is a group, denote by  $G^*$  its unitary dual, namely the set of equivalence classes of U.I.R. of  $G$ .

(a) Let  $G/H = P$  be a finite group. Write  $G = \bigcup H p_i$ , with coset representatives  $p_i$  and cosets  $\bar{p}_i = H p_i$  forming the quotient group  $P$ . A product  $\bar{p}_i \bar{p}_j = \bar{p}_k$  in  $P$  is equivalent to a relation  $p_i p_j = h(p_i, p_j) p_k$ ,

where  $h(p_i, p_j) \in H$ .

(b) Let  $\overline{D} \in H^*$  denote the equivalence class of  $D$ , a U.I.R. of  $H$ . The action of  $g \in G$  on  $D$ , and hence on  $\overline{D}$ , is defined by  $D_g : h \rightarrow D(g^{-1}hg)$  for all  $h \in H$ . The totality  $\{\overline{D}_g : g \in G\}$  forms the orbit of  $\overline{D}$  in  $H^*$ .

(c) To each  $D$  (resp.  $\overline{D} \in H^*$ ) associate its Inertia Group or Stabilizer  $G_D = \{g \in G : D_g \text{ is unitarily equivalent to } D\}$  (resp.  $G_{\overline{D}} = \{g \in G : \overline{D}_g = \overline{D}\}$ ). Then : i)  $G_D = G_{\overline{D}}$  ; (ii)  $G_D$  contains  $H$  ; (iii)  $G_D/H = P_D$  is a subgroup of  $P$ .

(d) Let  $D'$  be any U.I.R. of  $G_D$  such that the subduced representation  $D' \downarrow H$  is a multiple of  $D$  - the subduction property. Then the induced representation  $D' \uparrow G$  is a U.I.R. of  $G$ . All of  $G^*$ , with no repetitions, is obtained by picking one  $\overline{D}$  from each orbit in  $H^*$  under the action of  $G$ , and for each such  $\overline{D}$  using one  $D'$  from each equivalence class of U.I.R. of  $G_D$  with the subduction property.

To implement the above we need to know how to find representations of the inertia group which possess the subduction property. This we now describe.

(e) If  $g \in G_D$  there exists a unitary transformation  $T(g)$ , such that  $D(h) = T(g) D(g^{-1}hg) T(g)^{-1}$  for all  $h \in H$ . By Schur's lemma  $g \rightarrow T(g)$  is a unitary irreducible projective representation (U.I.P.R.) of  $G_D$ , whose restriction to  $H$  is  $D$  if we make the choice  $T(h) = D(h)$  for  $h \in H$ . Denote the factor system by  $\omega$ .

Let  $G \rightarrow S(g)$  by a U.I.P.R. of  $G_D$  with factor system  $\omega^{-1}$  and such that  $S \downarrow H$  is a multiple of the trivial representation. Then the U.I.R. of  $G_D$  defined by  $D'(g) = T(g) \otimes S(g)$ , for all  $g \in G_D$ , has the subduction property. The converse is also true.

The problem is therefore reduced to finding (i) the intertwining transformations  $T(g)$  ; and (ii) suitable projective representations  $S$  of  $G_D$ .

Having chosen  $T(h) = D(h)$ ,  $h \in H$ , and putting  $T(hp_i) = D(h) T(p_i)$  for  $h \in H$ ,  $\overline{p}_i \in P_D$ , (i) is reduced to a finite problem. Its solution is discussed by Backhouse [ 1 ] .

To clarify (ii) we note that the factor system  $\omega$  satisfies  $\omega(h', hp_i) = \omega(hp_i, h') = 1$  for  $h, h' \in H$  and  $\overline{p}_i \in P_D$ . This leads to the conclusion that  $\omega$  is essentially a factor system on  $P_D$ . The same is true of  $\omega^{-1}$ . Noting this, which implies  $S(hp_i) = S(h) S(\overline{p}_i)$ , for all  $h \in H$ ,  $\overline{p}_i \in P_D$ , we therefore only require  $S$  on the coset representatives of  $H$  in  $P_D$ . However,  $S(p_i p_j)$  equals  $\omega^{-1}(p_i, p_j) S(\overline{p}_i) S(\overline{p}_j)$ , but on the other hand equals  $S(h(p_i, p_j) p_k) = S(\overline{p}_k)$ . It follows that we

can recover  $S$  from an  $\omega^{-1}$ -representation of  $P_D$ . Again this is a finite problem.

We must emphasize that the analysis depended on choosing  $T(h) = D(h)$ , for all  $h \in H$ . In certain special cases an alternative choice is possible, leading to a simpler analysis.

Case 1:  $H$  Abelian. The analysis takes a completely different course right from the start.  $D$  is one-dimensional, so we can choose  $T(g) = 1$  for all  $g \in G_D$ . This eliminates  $T$  from the argument.

If  $D'$  has the subduction property, we can write  $D'(hp_i) = D(h) D'(p_i)$ , noting that  $D(h)$  is purely a scalar. It is clear that  $D'(p_i) D'(p_j) = D(h(p_i, p_j)) D'(p_k)$ , and if we put  $D''(\overline{p}_i) = D'(p_i)$  then  $D''$  is a U.I.P.R. of  $P_D$  with specified factor system.

Case 2:  $G$  is the semi-direct product of  $H$  with  $P$ , written  $G = H \otimes P$ . The main analysis of (e) applies, but now  $p_i \rightarrow T(p_i)$  is actually a U.I.P.R. of  $P_D$  with some factor system  $\omega$ . If  $p_i \rightarrow S(p_i)$  is a U.I.P.R. of  $P_D$  with factor system  $\omega^{-1}$ , then U.I.R. of  $G_D$  with the subduction property are of the form

$$D'(hp_i) = D(h) T(p_i) \otimes S(p_i),$$

for all  $h \in H$ ,  $p_i \in P_D$ .

Case 3:  $G = H \otimes P$  with  $H$  Abelian. We can use either the analysis of case 1 or case 2 to obtain

$$D'(hp_i) = D(h) S(p_i),$$

for all  $h \in H$ ,  $p_i \in P_D$ , where  $h \rightarrow D(h)$  is one-dimensional and  $p_i \rightarrow S(p_i)$  is a U.I.R. of  $P_D$ .

The Clifford theory described above, regarded as a recipe for constructing all finite dimensional U.I.R. of  $G$  from those of  $H$  can break down if we withdraw some of the hypotheses and requirements. However, it remains a sound method for constructing some, if not all, the irreducible representations of  $G$ , possible infinite-dimensional and non-unitary, as long as  $G/H$  is countable. Otherwise Mackey theory is required.

### 3. Little Group Theory for Crystallographic Space Groups

Let  $T$  denote a discrete translation group whose elements  $\underline{t}$  are regarded as Euclidean 3-vectors, and let  $P$  denote a point group whose elements  $R_i$ ,  $i = 1, 2, \dots$  |  $P$  | act naturally on Euclidean 3-space.

(a) A space group  $G$  has set of elements  $\{\{\underline{t} + \underline{v}(R_i), R_i\} : \underline{t} \in T, R_i \in P\}$ , with coset decomposition  $\cup \{\underline{v}(R_i), R_i\}$  relative to the translation subgroup. The vectors  $\underline{v}(R_i)$  are non-primitive translations.

The action  $\underline{x} \rightarrow \underline{t} + \underline{v}(R_1) + R_1 \underline{x}$  on Euclidean 3-space determines the product rule in G. Thus, in particular,

$$\begin{aligned} \{ \underline{v}(R_1), R_1 \} \{ \underline{v}(R_j), R_j \} &= \{ \underline{v}(R_1) + R_1 \underline{v}(R_j), R_1 R_j \} \\ &= \{ \underline{m}(R_1, R_j) + \underline{v}(R_1 R_j), R_1 R_j \}, \end{aligned}$$

where  $\underline{m}(R_1, R_j) \in T$ . We also have the conjugation

$$\{ \underline{t} + \underline{v}(R), R \} \{ \underline{t}', 1 \} \{ \underline{t} + \underline{v}(R), R \}^{-1} = \{ R \underline{t}', 1 \},$$

where 1 denotes the identity in P.

(b) A U.I.R. of T is of the form  $\chi^{\underline{k}} : \underline{t} \rightarrow \exp(-i\underline{k} \cdot \underline{t})$ , where  $\underline{k}$  belongs to the first Brillouin zone of T. The latter can be regarded as the dual of T and is topologically equivalent to a 3-torus.

The action of G on  $\chi^{\underline{k}}$  is given by

$$\begin{aligned} \chi^{\underline{k}}_{\{ \underline{t}, \underline{v}(R), R \}} &: \underline{t} \mapsto \chi^{\underline{k}}(R^{-1} \underline{t}') = \exp(-i\underline{k} \cdot R^{-1} \underline{t}') \\ &= \exp(-iR\underline{k} \cdot \underline{t}'), \end{aligned}$$

which can be written as  $\chi^{R\underline{k}}(\underline{t}')$ .

The orbit of  $\chi^{\underline{k}}$  corresponds to the Star of  $\underline{k}$ , namely the vectors  $\{ R\underline{k} : R \in P \}$ .

(c) To each  $\underline{k}$  we associate its Little Group  $G^{\underline{k}} = \{ \{ \underline{t} + \underline{v}(R), R \} : R\underline{k} \equiv \underline{k} \text{ modulo reciprocal lattice} \}$ . Evidently  $T \triangleleft G^{\underline{k}}$ , so we may form  $G^{\underline{k}}/T = \bar{G}^{\underline{k}}$ , the Little Co-group of k.  $G^{\underline{k}}$  is also called the group of the wave vector  $\underline{k}$ .

(d) An Allowable or Small Representation  $D^{\underline{k}}$  is a U.I.R. of  $G^{\underline{k}}$  such that  $D^{\underline{k}} \downarrow T$  is a multiple of  $\chi^{\underline{k}}$ . For each such  $D^{\underline{k}}$ ,  $D^{\underline{k}} \uparrow G$  is a U.I.R. Other members of the star of  $\underline{k}$  give rise to equivalent U.I.R. of G.

(e) The calculations  $D^{\underline{k}}(\underline{t} + \underline{v}(R), R) = \exp(-i\underline{k} \cdot \underline{t}) D^{\underline{k}}(\underline{v}(R), R)$  and  $D^{\underline{k}}(\underline{v}(R_1), R_1) D^{\underline{k}}(\underline{v}(R_j), R_j) = \exp[-i\underline{k} \cdot \underline{m}(R_1, R_j)] D^{\underline{k}}(\underline{v}(R_1, R_j), R_1 R_j)$ , where  $R, R_1, R_j$  belong to the little co-group, imply that allowable representations simply arise from projective representations of the little co-group with pre-determined factor systems. In particular the factor systems are trivial in the symmorphic case.

A bonus from the little group method is that it provides an easy labelling scheme for the U.I.R. of space groups. In fact to each U.I.R. we associate a  $\underline{k}$ -vector and an integer, or equivalent, label from some suitable list of projective representations of the finite point groups. We can use those defined in Bradley and Cracknell [ 5 ]

or the more compact tabulations of Michel and Mozryzmas (these proceedings). This easy labelling is particularly useful for the working out of Kronecker products and selection rules - see for example Bradley [4] .

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