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Abstract

An energy band in a solid contains an infinite number of states which transform linearly as a space group representation induced from a finite dimensional representation of the isotropy group of a point in space. A band representation is elementary if it cannot be decomposed as a direct sum of band representations; it describes a single band. We give a complete classification of the inequivalent elementary band representations.

1 **Space groups.** A crystallographic space group is a discrete closed subgroup of the Euclidean group $E(n) = R^n \rtimes O(n)$ which contains a lattice of translations $T \sim Z^n$; when a choice of origin is made its elements can be written as $g = (t + v(R), R) \in E(n)$, with $R \in O(n)$, $t \in T$ and v(R) is either $= 0$ or a non-primitive translation $\notin T$. The quotient $G/T = P$ is the point group, a finite subgroup of $O(n)$. The action of P on $T \sim Z^n$ is given by an injective homomorphism $P \hookrightarrow GL(n, Z)$ up to a conjugation in $GL(n, Z)$, i.e., by a conjugation class of $GL(n, Z)$ subgroups isomorphic to P. Such a class is called an arithmetic class: there are 73 of them in $n = 3$ dimensions [1]. In each arithmetic class there is one symmorphic space group $G = T \rtimes P$. For such a group, with a suitable choice of origin, all $v(R)$'s can vanish. In the general case the action of G on a point x of space $\mathcal{E}$ is defined by

$$g.x = Rx + v(R) + t \tag{1}$$

2 **Band Representations.** Let $\psi(x - x_0)$ be the wave function of an electron localized around an atom sitting at x_0 in a crystal whose symmetry group is G. The wave functions $\psi(g^{-1}.(x - x_0))$, for all $g \in G$ are those of the corresponding electrons in all similar atoms of the crystal; they span a vector space $\mathcal{H}$ of functions which also contains the state vectors of delocalized electrons in a band. G acts linearly on $\mathcal{H}$; by definition of induced group representations, the linear representation of G on $\mathcal{H}$ is $\mathrm{Ind}_{G_{x_0}}^{G} \gamma_{G_{x_0}}^{(\rho)}$ where G_{x_0} is the isotropy group of x_0 and $\gamma_{G_{x_0}}^{(\rho)}$ is the linear representation of G_{x_0} on the space spanned by the functions $\psi(g^{-1}.(x - x_0))$, for all $g \in G_{x_0}$. This representation $\mathrm{Ind}_{G_{x_0}}^{G} \gamma_{G_{x_0}}^{(\rho)}$ is called a **band representation**. These representations are of great interest for solid state physics; they have been studied by des Cloizeaux [2], Zak [3], Evarestov and Smirnov [4]. The most interesting band representations are the **elementary** ones: those which cannot be decomposed into a direct sum of band representations, so they describe a **single** band [1]. Using Bloch functions as main tool, we are making a complete classification of

[1] Of course, as group representations, elementary band representations are highly reducible. So we prefer to avoid here the expression irreducible-band representations used as a synonym in [3] and [5].

elementary band representations [5]. We think worthwhile to present here a purely group theoretical method. Sections 3 and 4 recall the basic notions on space group geometry and on induced representations that we shall need. In section 5 we will begin the study of the band representations. Finally, in section 6 we establish the complete list of inequivalent elementary band representations.

3 Space group actions. Space $\mathcal{E}$ is partitionned into orbits by the action of the space group G. The isotropy groups of an orbit $G.x$ form a conjugation class $[G_x]$ of G-subgroups. Orbits are naturally classified by the conjugation class of their isotropy subgroups. The union of all orbits of the same type is called a stratum (see e.g., [6]). In physical problems the number of strata is usually finite: they can be listed. For space groups, this has been done in the International Tables for Crystallography [7]; there the strata are called "Wyckoff positions".

No translation leaves fixed $x \in \mathcal{E}$ so $G_x \cap T = \{1\}$ and $G_x \sim \sigma(G_x) \subset P$ where σ is the surjective homomorphism $\sigma : G \xrightarrow{\sigma} P$ of kernel T. Hence isotropy groups G_x are finite subgroups of G. If x is chosen as origin $G_x \subset O(n)$, the elements of G_x have vanishing non-primitive translations; hence $T.G_x$ is a symmorphic space group $\subset G$. One can also show that for the action on $\mathcal{E}$ of the space groups, the intersections of isotropy groups are isotropy groups.

There is a natural order (by inclusion up to a conjugation) on the set of conjugation classes of finite subgroups of an arbitrary group. Maximal finite subgroups of G are isotropy groups (consider the barycenter of any orbit of such a subgroup); the corresponding strata are closed: they are sets of symmetry centers, rotation (or skew- rotation) axes, symmetry (or glide-reflexion) planes, or, for 13 of the 230 space groups, there is only one stratum, the whole space $\mathcal{E}$ (see Table 1). The trivial subgroup is the minimal isotropy group and the corresponding stratum is called generic; it is open and dense.

230	104	63	5	13	38	2	4	1
dim 0	x				x	x		x
dim 1		x			x		x	x
dim 2			x			x	x	x
dim 3				x				

Table 1. Number of space groups with given dimension of closed strata

In 3 dimensions there are 32 geometric classes of point groups (i.e., conjugation classes in $O(3)$), forming only 18 isomorphic classes. Among the 32 point groups, 10 of them are polar groups, i.e., the stratum with an isotropy group $G_x \sim P_x$ has dimension ≥ 1 when P_x is a polar group; this dimension is:

$$3 \text{ for } C_1 \sim 1, \quad 2 \text{ for } C_s, \quad 1 \text{ for } C_2, C_3, C_4, C_6, C_{2v}, C_{3v}, C_{4v}, C_{6v}; \tag{2}$$

the dimension is 0 for the 22 non-polar groups. Assume that H_1 and H_2 are two non-polar isotropy groups; then $H_0 = H_1 \cap H_2$ is a polar isotropy group; the stratum $S([H_0])$ is the union of axes or planes or the whole space, minus the symmetry centers of $S([H_1])$ and $S([H_2])$.

The orbit space $W = \mathcal{E} \mid T$ is a n-dimensional torus represented by the "Wigner-Seitz cell" with opposite faces idendified. The action of G on $\mathcal{E}$ induces an action of $G/T = P$ on $\mathcal{E} \mid T = W$; the natural map $\phi : \mathcal{E} \xrightarrow{\phi} W$ is continuous, open, closed. If $q = \phi(x)$, then

$P.q = \phi(G.x)$ and $P_q = \sigma(G_x) \sim G_x$. One shows that the different connected components of a same P stratum in W are ϕ-images of different G-strata in $\mathcal{E}$. Except for the enantiomorphic pairs (there are 11 of them in dimension 3) different space groups define inequivalent actions of P on W.

Similarly, the quotient of the p-space $\mathcal{E}'$ modulo the reciprocal lattice T' is the Brillouin zone B with opposite faces identified. Moreover B carries a natural group structure $\hat{T}$, the dual group of T i.e., the set of all (one dimensional) irreducible representations of T with the group multiplication defined by the multiplication of the character values. With the notation of k for the wave vector of the T representation $t \mapsto e^{2\pi i k.t}$, the group law of $\hat{T}$ is the addition of k's with their coordinates defined modulo 1 (i.e., up to a vector of the reciprocal lattice). In the natural action of G on $\hat{T}$,T acts trivially, so the G and P orbits (and strata) on $B = \hat{T}$ are the same; moreover these actions are the same for all space groups of the same arithmetic class. Note also that $P_k = \sigma(G_k) = G_k/T$.

4 **Induced Representations.** We recall here the results (see e.g.,[8,9]) that we shall need concerning induced representations; we explain them first in the easier case of a finite group G with a subgroup H. The complex valued functions on G form an Hilbert space with the Hermitian scalar product ($|G|$ = cardinal of G):

$$\langle f|g\rangle_G = |G|^{-1} \sum_{x\in G} \bar{f}(x)g(x) \tag{3}$$

The central functions satisfy $f(x) = f(yxy^{-1})$; these functions form a sub-Hilbert space that we denote by $\mathcal{H}_G$. The characters $\chi_G^{(\alpha)}$ of the *unirreps* (=unitary irreducible representations) of G form an orthonormal basis of $\mathcal{H}_G$. So we can say that the characters separate the conjugation classes or ,equivalently, if we denote by $[x]_G$ the conjugation class of x in G and by $\hat{G}$ the set of equivalence classes of unirreps of G:

$$\forall\alpha \in \hat{G}, \quad \chi_G^{(\alpha)}(x) = \chi_G^{(\alpha)}(y) \Longleftrightarrow [x]_G = [y]_G \tag{4}$$

Let $CC[G]$ the set of conjugation classes of the group G; to each group homomorphism $H \xrightarrow{\xi} G$ corresponds a map: $CC[H] \xrightarrow{\bar{\xi}} CC[G]$. When H is subgroup of G, ξ is injective and we denote it by ι; the corresponding map $\bar{\iota}$ defines a linear map between the spaces of functions defined on $CC[G]$ and $CC[H]$: $\mathcal{H}_G \xrightarrow{\text{Res}} \mathcal{H}_H$. Res is a short for "Restriction"; indeed, if χ_G is the character of a linear representation of G, $\text{Res}_H^G \chi_G = \chi_G \circ \bar{\iota}$ is the character of the representation of H obtained from that of G by restriction to the elements of the subgroup H. The adjoint map is called $\mathcal{H}_H \xrightarrow{\text{Ind}} \mathcal{H}_G$; to any H-representation of character $\chi_H^{(\rho)}$ corresponds the induced representation of G. Its character is denoted by $\text{Ind}_H^G \chi_H^{(\rho)}$.

By definition of the adjoint of an operator we obtain Frobenius reciprocity relation:

$$\langle \text{Ind}_H^G \chi_H^{(\rho)} | \chi_G^{(\alpha)} \rangle_G = \langle \chi_H^{(\rho)} | \text{Res}_H^G \chi_G^{(\alpha)} \rangle_H \tag{5}$$

where $\langle\ |\ \rangle_K$ is the Hermitean scalar product in $\mathcal{H}_K$. It means that, in the reduction of $\text{Ind}_H^G \chi_H^{(\rho)}$ into a direct sum of unirreps of G, the multiplicity of $\chi_G^{(\alpha)}$ is equal to the multiplicity of $\chi_H^{(\rho)}$ in the restriction of $\chi_G^{(\alpha)}$ to H. From the associativity of linear maps one deduces the Induction Chain Rule:

$$H_k \subset H_{k-1} \subset ... \subset H_0 \subset G, \qquad \mathrm{Ind}_{H_k}^G \chi_{H_k}^{(\rho)} = \mathrm{Ind}_{H_0}^G(\mathrm{Ind}_{H_1}^{H_0}(...(\mathrm{Ind}_{H_k}^{H_{k-1}} \chi_{H_k}^{(\rho)})..)) \tag{6}$$

We can prove the

Lemma A. If, and only if, $CC[H] \xrightarrow{\iota} CC[G]$ is injective, Ind is injective i.e., inequivalent representation of H induce inequivalent representations of G.
Indeed $\bar{\iota}$ injective $\Leftrightarrow$ Res surjective; and from the general property Ker Ind = (Im Res)$^\perp$, Ind is injective.
Ind is always injective when G is Abelian. When H is a subgroup of a point group G, *Ind* is injective for the following 16 subgroups H of the point groups:

$$1, C_i, C_s, C_2, C_{2h}, C_{3v}, D_3, D_{3d}, T_d \tag{7}$$

$$C_{4v}, C_{6v}, D_6, D_{3h}, D_{6h}, O, O_h \tag{7'}$$

(For the subgroups of equation (7) $\bar{\iota}$ is injective when $G = O(3)$ so it is true a fortiori when G is a point group containing H).

Given a matrix representation $h \mapsto D(h)$ of $H \subset G$, one can write explicitly the matrices $\Delta(g)$ of the induced representation $\Delta = \mathrm{Ind}_H^G D$. First choose arbitrarily an element $s_i \in G$ in each left H-coset of G; $\Delta(g)$ is given by blocks Δ_{ij}:

$$G = \bigcup_i s_i H, \qquad \Delta = (\Delta_{ij}), \quad \Delta_{ij}(g) = D((s_i^{-1} g s_j)) \tag{8}$$

with the definition:

$$D((k)) = D(k) \text{ if } k \in H, \quad = 0 \text{ otherwise} \tag{8'}$$

so:

$$\dim\Delta = (\dim D) \times |G/H| \tag{8''}$$

where $|G/H|$ is the index of H in G. The character of the induced representation is:

$$tr\Delta(g) = \chi_G^{(\Delta)}(g) = \sum_{i=1}^{|G/H|} \chi_H^{(D)}((s_i^{-1} g s_i)), \text{ with } \chi_H^{(D)}((k)) = trD((k)) \tag{9}$$

If we denote by $[g]_G$ the conjugacy class of g in G, we see that:

$$[g]_G \cap H = \emptyset \Rightarrow \chi_G^{(\Delta)}(g) = 0 \tag{9'}$$

Let us first study the case $H \triangleleft G$ (where $\triangleleft$ reads "invariant subgroup"). Then there is a natural group homomorphism $G \xrightarrow{\varpi} \mathrm{Aut}H$. It defines an action of G on $\hat{H}$, the set of equivalence classes of unirreps of H. This action defines a linear representation of G on $\mathcal{H}_H$: for $n \in G, (n.\chi_H^{(D)})(h) = \chi_H^{(D)}(n^{-1}hn)$. Let G_D the isotropy group of the representation

D of H and $G.D$ the orbit. Since the set of elements of $H(\triangleleft G)$ is a disjoint union of G-conjugation classes, equation (8) becomes:

$$H \triangleleft G, \Delta = \mathrm{Ind}_H^G D;\ g \notin H, \chi_G^{(\Delta)}(g) = 0;\ h \in H, \chi_G^{(\Delta)}(h) = |\frac{G_D}{H}| \sum_{D' \in G.D} \chi_H^{(D')}(h) \quad (10)$$

Hence the **different** H-representations of the G-orbit $G.D$ induce the **same** representation of G. In the particular case $G_D = G$:

$$H \triangleleft G, G_D = G; \quad g \notin H, \chi_G^{(\Delta)}(g) = 0; \quad h \in H \chi_G^{(\Delta)}(h) = |G/H| \chi_H^{(D)}(h) \qquad (10')$$

This equation applies to the interesting particular case of G Abelian; adding the properties that the characters of one dimensional group representations never vanish, one obtains:
Theorem A. Induced representations of an Abelian group are equivalent if and only if they are induced from equivalent representations of the same subgroup.
This theorem generalizes Lemma A for Abelian groups.

We can now deal with the general case for computing the character of an induced representationfrom the character of the unirreps of H. To complete (9') we need only to know the characters of the conjugation classes $[h]_G$ for all $h \in H$. Let $N_G(H)$ be the normalizer of H in G. From the coset decompositions one defines the positive integer $c(h)$ for any $h \in H$:

$$G = \bigcup_\alpha s_\alpha N_G(H), \quad N_G(H) = \bigcup_i r_i H, \quad c(h) = \#\{s_\alpha, s_\alpha^{-1} h s_\alpha \in H\} \qquad (11)$$

Another way to compute $c(h)$ is:

$$c(h) = \frac{|G|}{\#[h]_G} / \frac{|N_G(H)|}{\#[h]_{N_G(H)}} = \frac{|C_G(h)|}{|C_{N_G(H)}(h)|} \qquad (11')$$

where the centralizer of h in G, $C_G(h)$ is the subgroup formed by the elements which commute with h. From (9) and (11) we obtain:

$$\chi_G^{(\Delta)}(h) = \sum_\alpha \sum_i \chi_H^{(D)}((r_i^{-1} s_\alpha^{-1} h s_\alpha r_i)) = c(h)\, \mathrm{Ind}_H^{N_G(H)} \chi_H^{(D)}(h) \qquad (12)$$

with, from equation (10):

$$\mathrm{Ind}_H^{N_G(H)} \chi_H^{(D)}(h) = \frac{|N_G(H)_D|}{|H|} \sum_{D' \in N_G(H).D} \chi_H^{(D')}(h) \qquad (13)$$

In plain words we have found that in the induced representation, the character of a group element conjugate to $h \in H$ is a multiple of the character of h in the direct sum of the H-representations in the $N_G(H)$ orbit of the character $\chi_H^{(D)}$ of the inducing representation. The positive integer $c(h)$ defined in equation (11) is independent from the choice of the representation of H. So the remark following equation (10) generalizes to:

Theorem B. The unirreps in $\hat{H}$ belonging to the same orbit of the normalizer $N_G(H)$, induce equivalent representations of G.

The converse of this theorem is not true: as we have seen Ind is not injective when $\bar{\iota}$ is not. However all elements of G which conjugate two elements not conjugated in H may be outside the normalizer $N_G(H)$. Moreover the induced representation from a unirrep might be equivalent to the induced representation from a reducible representation of the same subgroup. In point groups, the only exceptions to the converse of theorem B are (we follow reference [11] for the labelling of the unirreps of the point groups):

$$\mathrm{Ind}_{D_4}^{O}\,\chi_{D_4}^{(5)} \sim \mathrm{Ind}_{D_4}^{O}(\chi_{D_4}^{(2)} \oplus \chi_{D_4}^{(4)}), \quad \mathrm{Ind}_{D_{2d}}^{T_d}\,\chi_{D_{2d}}^{(5)} \sim \mathrm{Ind}_{D_{2d}}^{T_d}(\chi_{D_{2d}}^{(2)} \oplus \chi_{D_{2d}}^{(4)}),$$

$$\mathrm{Ind}_{D_{4h}}^{O_h}\,\chi_{D_{4h}}^{(5)} \sim \mathrm{Ind}_{D_{4h}}^{O_h}(\chi_{D_{4h}}^{(2)} \oplus \chi_{D_{4h}}^{(4)}), \quad \mathrm{Ind}_{D_{4h}}^{O_h}\,\chi_{D_{4h}}^{(10)} \sim \mathrm{Ind}_{D_{4h}}^{O_h}(\chi_{D_{4h}}^{(7)} \oplus \chi_{D_{4h}}^{(9)}) \qquad (14)$$

We will find more exceptions in space groups and list in table 3 those related to elementary band representations.

From the properties of induced representations it is evident that equivalent representations of conjugate subgroups induce equivalent G-representations. But the converse is not true as the chain induction property already shows. Another obvious counterexample is given by the induction from the regular representation from any G-subgroup H: one obtains the regular representation of G. In this paper we will only be interested by the following problem: given a unirrep $\chi_H^{(\rho)}$ of a subgroup H, find all conjugate classes $[H']_G$ of G-subgroups (which do not contain H) and representations $\chi_{H'}^{(D)}$ (which might be reducible), such that $\mathrm{Ind}_H^G\,\chi_H^{(\rho)} \sim \mathrm{Ind}_{H'}^G\,\chi_{H'}^{(D)}$. Equations (9') and (12) are very relevant; in section 5 we will solve this problem for band representations. Here we make only some remarks. For simplicity, let us assume that H is its own normalizer in G : $N_G(H) = H$. If $\forall h \in H, \chi_H^{(\rho)}(h) \neq 0$ (for example $\rho \in \hat{H}$ is a one dimensional unirrep), (9') shows that every element of H should be conjugate to an element of H'; an example of such a case is studied in the:

Lemma B. Equivalent representations of non conjugate, isomorphic: $H \xrightarrow{i} H'$, subgroups of G induce equivalent representations if $i(h)$ and h are conjugate for every $h \in H$.

In any unirrep $\chi_G^{(\alpha)}$ of G, conjugate elements have the same characters, so $\mathrm{Res}_H^G\,\chi_G^{(\alpha)} \sim \mathrm{Res}_{H'}^G\,\chi_G^{(\alpha)}$; we complete the proof of the theorem by using Frobenius reciprocity (5).

This lemma does not apply to point groups; however, as we shall see later, it can apply to some finite groups and to a dozen of space groups in the search of equivalent elementary band representations: table 4 gives the list of occurences.

For the point groups it is easy to find all solutions to the problem we have defined. Indeed we need only to consider the 9 isomorphic classes of non Abelian point groups. Moreover any multidimensional unirrep $\chi_H^{(\rho)}$ of a point group H is monomial, i.e. induced from a one dimensional representation of a subgroup, e.g., $\chi_H^{(\rho)} \sim \mathrm{Ind}_K^H\,\chi_K^{(\alpha)}$; then a solution for any subgroup $H' \supset K$ is $\chi_{H'}^{(D)} = \mathrm{Ind}_K^{H'}\,\chi_K^{(\alpha)}$. The only solutions not obtained by this method are:

$$\mathrm{Ind}_{S_4}^{D_{2d}}\,\chi_{S_4}^{(3)} \sim \mathrm{Ind}_{S_4}^{D_{2d}}\,\chi_{S_4}^{(4)} \sim \mathrm{Ind}_{D_2}^{D_{2d}}\,\chi_{D_2}^{(2)} \sim \mathrm{Ind}_{D_2}^{D_{2d}}\,\chi_{D_2}^{(3)} \sim$$

$$\sim \mathrm{Ind}_{C_{2v}}^{D_{2d}} \chi_{C_{2v}}^{(2)} \sim \mathrm{Ind}_{C_{2v}}^{D_{2d}} \chi_{C_{2v}}^{(4)} \sim \chi_{D_{2d}}^{(5)} \tag{15}$$

and the similar cases obtained from the isomorphisms $D_{2d} \approx D_4 \approx C_{4v}$ or by chain induction to larger point groups: D_{4h}, T_d, O, O_h.

5 **Induced space group representations.** There is no difficulty for constructing representations of space groups induced from a subgroup of finite index, e.g., one obtains the unirreps of a space group G by induction from (one dimensional) representations k of T: this yields $|P|$ dimensional representations $\Gamma^{(k,1)}$ of G; their restriction to T contains all representations belonging to the orbit $G.k = P.k$. The representation $\Gamma^{(k,1)}$ is irreducible if k belongs to the generic stratum in B. If not, the $P.k$ orbit has $|P/P_k|$ elements and each k appears with a multiplicity $|P_k|$. For a fixed k one has a representation of G_k which contains all "allowed" [2] unirreps of G_k, each one with a multiplicity equal to its dimension. To summarize: the unirreps of G are labelled :

$$\Gamma^{(k,\alpha)} = \mathrm{Ind}_{G_k}^{G} \chi_{G_k}^{(\alpha)}, \quad k \in B, \alpha \in \text{ allowed } \hat{G}_k \tag{16}$$

$$k' \in G.k,\ \alpha \sim \alpha' \Longleftrightarrow \Gamma^{(k',\alpha')} \sim \Gamma^{(k,\alpha)} \tag{16'}$$

A space group has a continuous infinity of unirreps and the decomposition of a unitary representation into unirreps requires a direct integral on the Brillouin zone $B = \hat{T}$.

It is also possible to extend all results of the theory of induced representations of finite groups to the space group representations induced from finite dimensional representations of finite subgroups; for instance one can work explicitly on the space $\mathcal{H}'_G$ of functions on the space group G which are different from zero only on a finite subset of G; the space $\mathcal{H}'_G$ is a Hilbert space with the scalar product $\sum_{x \in G} \bar{f}(x) g(x)$. This Hilbert space carries the regular representation of G. Let H a finite subgroup of G; one knows how to define a sub-representation $h \mapsto D(h)$ of the regular representation of H on the space $\mathcal{H}'_H$. The functions on H define functions on G with zero value on the elements of G which are not in H; this identifies $\mathcal{H}'_H$ as a sub-Hilbert space of $\mathcal{H}'_G$. We define a set of functions on G that we denote by $f_x, x \in G$:

$$\forall f \in \mathcal{H}'_H \subset \mathcal{H}'_G, \forall x, y \in G, \quad f_x(y) = f(x^{-1}y) \tag{17}$$

These functions form a sub-Hilbert space of $\mathcal{H}'_G$ which carries the unitary representation $x \mapsto \Delta(x)$ of G which is the induced representation from the H-representation D:

$$\Delta = \mathrm{Ind}_H^G D_H, \quad \Delta(x) f_y = f_{xy}, \tag{18}$$

These induced representations satisfy Frobenius reciprocity. It is true that band representations are realized on another space of functions: the functions on $\mathcal{E}$ which decrease fastly enough at infinity; they form a Hilbert space, but when one makes an infinite sum of them (for instance to compute Bloch functions) one must take care of the problem of

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[2] "allowed" means here that the restriction to T of the G_k-representation is a multiple of the T-representation $k \in B = \hat{T}$.

convergence. We assume here that the two realizations of the induced representation Δ are equivalent.

Two points r and r' of $\mathcal{E}$ on the same translation orbit yield equivalent band representations; so these can be labelled by points of the Wigner Seitz cell W:

$$B^{(q,\rho)} = \mathrm{Ind}_{G_q}^{G}\chi_{G_q}^{(\rho)}, \quad q \in W, \rho \in \hat{G}_q \sim \hat{P}_q \tag{19}$$

$$q' \in \mathrm{Stratum}(q), \rho' \sim \rho \Longrightarrow B^{(q',\rho')} \sim B^{(q,\rho)} \tag{19'}$$

All q's of the same G-stratum yield equivalent band representations. The problem is to find which representations are elementary and, among those, which are the (q,ρ) labels of equivalent pairs.

Let us now study some consequences of the application of Frobenius reciprocity to band representations. We can compute $m_{q,\rho}^{k,\alpha}$ the multiplicity of the G unirrep $\Gamma^{(k,\alpha)}$ in the band representation $B^{(q,\rho)}$. For this we need a formula due to Mackey (see e.g.,[8]) which tells how to commute *Res* and *Ind*. We also need to use double cosets of G for G_q and G_k; they are the subsets $G_q s G_k \subset G$ for arbitrary $s \in G$. If $P_q \triangleleft P$ (respectively $P_k \triangleleft P$), then $T.G_q \triangleleft G$ ($G_k \triangleleft G$) and the double cosets are simple left (right) cosets of the G-subgroup $G_q.G_k = G_k.G_q$. With the definition $K_s = sG_ks^{-1} \cap G_q$ and the use of the adjoint identity and of Mackey's formula (we denote by $[G_q : G : G_k]$ the set of double cosets):

$$m_{q,\rho}^{k,\alpha} = \langle \mathrm{Res}_{G_q}^{G} \mathrm{Ind}_{G_k}^{G} \chi_{G_k}^{(\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q} = \sum_{s\in[G_q:G:G_k]} \langle \mathrm{Ind}_{K_s}^{G_q} \mathrm{Res}_{s^{-1}K_s s}^{G_k} \chi_{G_k}^{(\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q} =$$

$$= \sum_s \langle \mathrm{Res}_{s^{-1}K_s s}^{G} \chi_{G_k}^{(\alpha)} | \mathrm{Res}_{K_s}^{G_q} \chi_{G_q}^{(\rho)} \rangle_{K_s} = \sum_s |K_s|^{-1} \sum_{g\in K_s} \bar{\chi}_{G_k}^{(\alpha)}(s^{-1}gs)\chi_{G_q}^{(\rho)}(g) \tag{20}$$

When k is in the generic stratum of B the corresponding $m_{q,\rho}^{k,\alpha}$ is the number of branches of the band; equation (20) yields:

$$\text{number of branches in the band} = |P/P_q|.\mathrm{dim}(\chi_{G_q}^{(\rho)}) \tag{21}$$

When $k = 0$, the translations are represented trivially, $G_0 = G$, so the corresponding G-unirreps are simply the P-unirreps. Then:

$$m_{q,\rho}^{0,\alpha} = \langle \mathrm{Res}_{P_q}^{P} \chi_P^{(\alpha)} | \chi_{P_q}^{(\rho)} \rangle_{P_q} = \langle \chi_P^{(\alpha)} | \mathrm{Ind}_{P_q}^{P} \chi_{P_q}^{(\rho)} \rangle_P \tag{22}$$

Hence the necessary condition for equivalence of band representations:

$$B^{(q',\rho')} \sim B^{(q,\rho)} \Longrightarrow \mathrm{Ind}_{P_q}^{P} \chi_{P_q}^{(\rho)} \sim \mathrm{Ind}_{P_{q'}}^{P} \chi_{P_q'}^{(\rho')} \tag{23}$$

(In section 2, we have defined: $P_q = \sigma(G_q)$).

On any stratum of the Brillouin zone B, the $m_{q,\rho}^{k,\alpha}$'s are constant: at least it is evident on each connected component of a stratum since $m_{q,\rho}^{k,\alpha}$ is on it an integer valued continuous function. Since the number of strata on B is finite and for each stratum the number of values of α is also finite we need only to apply equation (20) a finite number of time for comparing the m components of two band representations; if their respective components are all equal, the two band representations are equivalent.

The characters of the infinite band representations are not defined and, for instance, the equations (9') and (12) have no meaning. To avoid this difficulty we will prove a lemma which allows us to use these equations for finite groups G_ν's. These groups are considered by solid state physicists when they use the periodic boundary conditions introduced first by Born and von Karman. For any integer ν consider νT, the subgroup of T formed by the translations $\nu t, t \in T$. It is an invariant subgroup of G and we define $G_\nu = G/\nu T$. By the surjective homomorphism $G \xrightarrow{\beta_\nu} G_\nu$ the translations $T \triangleleft G$ are sent unto $T_\nu = T/(\nu T) \approx (Z_\nu)^3$ and the Brillouin zone is replaced by $B_\nu = \hat{T}_\nu \sim (Z_\nu)^3$. Paradoxically the choice of ν is critical, even if it is very large: for instance if ν is relatively prime to $|P|, G_\nu = T_\nu \rtimes P$ even if G is not symmorphic. However one can prove that if (in three dimensions) ν is taken as a multiple of 12, non isomorphic space groups have non isomorphic G_ν and there is a natural bijective map between the strata of the action of G on B and that of G_ν on B_ν. May be, as it is done heuristically for many problems of solid state physics, one could replace the study of the band representations of the countable space group G by those of the countable set of finite groups $G_{12\nu}$ and one could formally define the limit $\nu \to \infty$. Here we will be rigourous; we only need to prove lemma C below. Since the isotropy groups G_q contain no translations, $\beta_\nu(G_q) \approx G_q$; to simplify our expressions we will identify these two groups and write $G_q \subset G_\nu$.

Lemma C. If $\mathrm{Ind}_{G_q}^{G} \chi_{G_q}^{(\rho)} \sim \mathrm{Ind}_{G_{q'}}^{G} \chi_{G_{q'}}^{(D)}$, then for any ν, $\mathrm{Ind}_{G_q}^{G_\nu} \chi_{G_q}^{(\rho)} \sim \mathrm{Ind}_{G_{q'}}^{G_\nu} \chi_{G_{q'}}^{(D)}$ .Equivalently $\mathrm{Ind}_{G_q}^{G_\nu} \chi_{G_q}^{(\rho)} \not\sim \mathrm{Ind}_{G_{q'}}^{G_\nu} \chi_{G_{q'}}^{(D)} \Rightarrow \mathrm{Ind}_{G_q}^{G} \chi_{G_q}^{(\rho)} \not\sim \mathrm{Ind}_{G_{q'}}^{G} \chi_{G_{q'}}^{(D)}$

We remark that [3] for $k \in B_\nu = \mathrm{Ker}\,\hat{\nu}$ i.e., for the wave vectors of the Brillouin zone $k \in B$ such that $\nu k = O$ (many physicist prefer to say " modulo the reciprocal lattice") the kernel of the G-unirrep $\Gamma^{(k,\alpha)}$ contains νT so $\Gamma^{(k,\alpha)}$ is also a unirrep of G_ν and all unirreps of G_ν can be so obtained. By Frobenius reciprocity, the assumption of the lemma is equivalent to $\forall(k,\alpha) \in \hat{G}, m_{q,\rho}^{k,\alpha} = m_{q',D}^{k,\alpha}$. Since this is true for all $k \in B_\nu$, by Frobenius reciprocity applied to the group G_ν we conclude the proof of the lemma.

6 The elementary bands representations.

Elementary band representations must be induced from unireps of G_q since $\mathrm{Ind}_H^G \chi_H^{(0)} = \mathrm{Ind}_H^G \chi_H^{(1)} \oplus \mathrm{Ind}_H^G \chi_H^{(2)}$ when $\chi_H^{(0)} = \chi_H^{(1)} \oplus \chi_H^{(2)}$. If G_q is not a maximal finite G-subgroup, i.e. $G_q < G_r$ maximal, then from the chain induction:

$$B^{(q,\rho)} \sim B^{(r,\sigma)} \quad \text{with } \chi_{G_r}^{(\sigma)} = \mathrm{Ind}_{G_q}^{G_r} \chi_{G_q}^{(\rho)} \tag{24}$$

This band representation might be elementary; in any case we have the necessary condition:

Lemma 1. Elementary bands representations are induced from unirreps of maximal isotropy subgroups of space groups.

To determine the exact sufficient conditions we will need the following results.

Lemma 2. For non-polar isotropy subgroups: $N_G(G_q) = G_q$.

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[3] The dual of the exact sequence $O \to T \xrightarrow{\nu} T \to T_\nu \to O$ is $O \leftarrow \hat{T} \xleftarrow{\hat{\nu}} \hat{T} \leftarrow \hat{T}_\nu \leftarrow O$,i.e., $B_\nu = \hat{T}_\nu = \mathrm{Ker}\,\hat{\nu} \subset B$.

Indeed all points of the normalizer orbit $N_G(G_q).q$ have same isotropy group G_q. Assume that G_q is a strict sugroup of its normalizer; so there exists $q' \neq q$ with $G_{q'} = G_q$; then all points of the line $\lambda q' + (1-\lambda)q$ are left fixed by G_q which is therefore a polar group.

The finite order elements of space groups belong to ten conjugation classes in $O(3)$. They are called the geometric classes of the elements. The notation used in the international crystallographic tables [7] for labelling them is given in equation (25). It is usual to denote by $\mathcal{E}^g$ the set of points in our space which are fixed by g. This set is a linear sub-manifold of $\mathcal{E}$ whose dimension $d(g)$ depends only on the geometric class of g. This dimension is given in (25').

$$\text{geometric classes}: \; 1,\; 2,\; 3,\; 4,\; 6,\; \bar{1},\; m,\; \bar{3},\; \bar{4},\; \bar{6} \tag{25}$$

$$\text{d(g)} \qquad : \; 3,\; 1,\; 1,\; 1,\; 1,\; 0,\; 2,\; 0,\; 0,\; 0 \tag{25'}$$

(1 is the identity, $2,3,4,6$ are rotations of this order, $\bar{1}$ is the space inversion, $\bar{3},\bar{4},\bar{6}$ are the product of the space inversion by the corresponding rotation; m is used instead of $\bar{2}$ and means "mirror" reflection). The elements whose $d(g) = 0$ are called *non polar elements*; they leave invariant a unique point of $\mathcal{E}$.

Similarly, if H is a subgroup of a space group, we denote by $\mathcal{E}^H$ the linear manifold set of the points fixed by H. Obviously: $\mathcal{E}^H = \cap_{h\in H}\mathcal{E}^h$; so when $h \in H$, $\mathcal{E}^H \subset \mathcal{E}^h$. We say that an element g of the isotropy group G_x is *dominant* when $\mathcal{E}^g = \mathcal{E}^{G_x}$; e.g. non polar elements are dominant in their groups G_x (those are non polar); similarly (non trivial) rotations are dominant in their groups if those are polar. We denote by $S[G_x] = S[G_q]$ the stratum corresponding to these isotropy groups. There are only six point groups P_q without dominant elements:

$$D_2, D_3, D_4, D_6, T, O \tag{26}$$

Lemma 3. $\mathcal{E}^g \cap S[G_x] = \emptyset \Leftrightarrow [g]_G \cap G_x = \emptyset$, i.e. g is not conjugate to an element of G_x. We prove the equivalent statement $\mathcal{E}^g \cap S[G_x] \neq \emptyset \Leftrightarrow [g]_G \cap G_x \neq \emptyset$. Proof $\Rightarrow$: $r \in \mathcal{E}^g \cap S[G_x]$, so $g \in G_r$. Conversely $\Leftarrow$: $\exists k \in G, kgk^{-1}.x = x$ so $g.k^{-1}x = k^{-1}x \in \mathcal{E}^g \cap S[G_x]$. Finally we consider explicitly the conjugation class of an element of finite order g by taking as origin a point that it leaves fixed, for instance the barycenter of an orbit; so $g = (0, G)$. It is easy to compute (see [9]):

$$(s + v(A), A)(0,G)(s + v(A), A)^{-1} = ((I - AGA^{-1})(s + v(A)), AGA^{-1}) \tag{27}$$

This equation shows that g_1 and g_2 are conjugated in G if and only if $G_1 = \sigma(g_1), G_2 = \sigma(g_2)$ are conjugated in P.

We study now when a band repsentation induced from a unirrep of a maximal isotropy group can be equivalent to another band representation. We first deal with the case:
i) *equivalence of band representations at the same site* $q \in W$.

From lemma 2 and theorem B we must study the action of the normalizers of the polar maximal isotropy groups on the set $\hat{G}_q$ of their unirreps. From (27), for the normalizer of a G-subgroup $H : \sigma(N_G(H)) \subset N_P(\sigma(H))$. Given a subgroup H of an arbitrary group

G, one defines the centralizer $C_G(H)$ as the set $\{g \in G, \forall h \in H, gh = hg\}$. There is a natural injective map:$N_G(H)/(H.C_G(H)) = Q_G(H) \hookrightarrow \mathrm{Out}H$, the group of classes of outer automorphisms of H. In the case of a space group G and an isotropy subgroup G_q, if a translation is in $N_H(G_q)$, it is in $C_H(G_q)$, so ($\approx$ means isomorphic groups):

$$Q_G(G_q) \approx \sigma(N_G(G_q))/(\sigma(G_q).\sigma(C_G(G_q))) \tag{28}$$

This group acts effectively on $\hat{P}_q$. When G_q is a polar maximal isotropy group with a strictly larger normalizer, on the axis or more generally the linear manifold whose every point is fixed by G_q, the action of $N_G(G_q)$ is not trivial and must be without fixed points; so $\sigma(N_G(G_q))$ must be polar and moreover G must contain a screw rotation or a glide reflexion

In dimension 3, from the list of the ten polar groups (given in equation (2)) and the determination of their normalizer in the point groups which can contain them, one finds easily that there are only four non polar point groups with a non trivial Q_G, and that in the four cases: $Q_G \approx Z_2$. In the next equation we give the list of these four polar isotropy groups and, for each of them, the pairs of their unirreps which are exchanged by the action of $Q_G(G_q)$ or $N_G(G_q)$ on $\bar{G}_q$:

$$C_{2v}(2,4),\ C_4(3,4),\ C_3(2,3),\ C_6(2,3)(5,6). \tag{29}$$

Note that all these unirreps have dimension one. There are only 52 space groups with non Abelian point groups and polar maximal isotropy groups; in 15 of them there are pairs of equivalent band representations: they are listed in table 2.

$101 = P4_2cm$	a	C_{2v}	2,4	$108 = I4cm$	a	C_4	3,4	$159 = P31c$	a	C_3	2,3
	b	C_{2v}	2,4		b	C_{2v}	2,4	$161 = R3c$	a	C_3	2,3
$103 = P4cc$	a	C_4	3,4	$130 = P/4ncc$	c	C_4	3,4	$165 = P\bar{3}c1$	d	C_3	2,3
	b	C_4	3,4	$137 = P4_2/nmc$	d	C_{2v}	2,4	$184 = P6cc$	a	C_6	3,4
$105 = P4_2mc$	a	C_{2v}	2,4	$138 = P4_2/ncm$	e	C_{2v}	2,4				5,6
	b	C_{2v}	2,4	$158 = P3c1$	a	C_3	2,3		b	C_3	2,3
107$= I4mm$	b	C_{2v}	2,4		b	C_3	2,3	$185 = P6_3cm$	b	C_3	2,3
					c	C_3	2,3	$220 = I\bar{4}3d$	c	C_3	2,3

Table 2. Equivalent band representations induced from the *same* polar maximal isotropy group G_q by unirreps froming an orbit of the normalizer $N_G(G_q)$. There are 23 pairs of them belonging to 15 space groups. After the n^o and the symbol of the space group, the columns of this table give the Wyckoff position, the corresponding isotropy group and its unirreps (notation of [11]) yielding equivalent elementary band representations.

Lemma A suggests another possibility for obtaining equivalent band representations at the same site: the map between the set of conjugation classes $CC(G_q) \xrightarrow{\bar{\iota}} CC(G)$ is not injective; we do know that this cannot happen when $\bar{\sigma} \circ \bar{\iota}$ (with $CC(G) \xrightarrow{\bar{\sigma}} CC(P)$)

is injective, which is the case for the 16 geometric classes of G_q listed in equations (7,7'). The following geometric classes of isotropy group can be also excluded for our search of equivalent band representations at the same site, not given in table 2:

$$C_3, C_4, S_4, C_6, C_{3i}, C_{3h}, C_{6h}, C_{4h}, T_h. \tag{30}$$

For the three first groups, the only elements which can be conjugated are group generators, so the conjugating elements are in the normalizer and we have already studied these cases; this argument can be extended to C_6 because any $g \in G$ which conjugates the elements of order 3 has to preserve the rotation axis and therefore it conjugates also the two generators (of order 6). The five other groups have non polar elements: these cannot be exchanged by a conjugating $g \in G$ not in the isotropy group because q is a point isolated in its stratum and $g.q \neq q$. So only the rotations of order respectively 3,3,3 and 6, 4,3 can be conjugated by an element outside the isotropy group. This yields the following kernel for *Ind* acting on $\mathcal{H}_{G_q}$:

$$\chi^{(2)}_{C_{3i}} + \chi^{(5)}_{C_{3i}} - \chi^{(3)}_{C_{3i}} - \chi^{(2)}_{C_{3i}}, \quad \chi^{(2)}_{C_{3h}} + \chi^{(5)}_{C_{3h}} - \chi^{(3)}_{C_{3h}} - \chi^{(2)}_{C_{3h}}, \quad \chi^{(2)}_{C_{6h}} + \chi^{(9)}_{C_{6h}} - \chi^{(4)}_{C_{6h}} - \chi^{(10)}_{C_{6h}},$$

$$\chi^{(5)}_{C_{6h}} + \chi^{(11)}_{C_{6h}} - \chi^{(6)}_{C_{6h}} - \chi^{(12)}_{C_{6h}}, \quad \chi^{(3)}_{C_{4h}} + \chi^{(7)}_{C_{4h}} - \chi^{(4)}_{C_{4h}} - \chi^{(8)}_{C_{4h}}, \quad \chi^{(2)}_{T_h} + \chi^{(6)}_{T_h} - \chi^{(3)}_{T_h} - \chi^{(7)}_{T_h}, \tag{31}$$

Hence different sum of two unirreps can induce equivalent non elementary band representations, but this cannot happen with one unirrep only. Therefore we have only 7 geometric classes of isotropy groups to sudy; we give their list, the corresponding unirreps wich induce equivalent representations and the point groups of the possible space groups where this equivalence could occur:

$$T(2,3) \subset O, T_d, O_h; \quad D_{4h}(5, 2\oplus 4)(10, 7\oplus 9) \subset O_h; \quad D_{2d}(5, 2\oplus 4) \subset T_d; \quad D_4(5, 2\oplus 4) \subset O;$$

$$D_{2h}(2,3)(6,7) \subset D_{4h}, T_h, O_h; \quad C_{2v}(2,4) \subset C_{4v}, D_{2d}, D_{4h}, T_h, T_d, O_h;$$

$$D_2(2,3) \subset D_4, D_{2d}, D_{4h}, T, T_h, O, T_d, O_h. \tag{32}$$

A systematic study of the partial ordering of the Wyckoff positions in the potential case yields 34 pairs of equivalent band representations . They appear in 25 space groups. (We remark that the isotropy groups D_4, D_{2d}, D_{4h} do not occur; they were the only ones with two dimensional representations). We tabulate these cases in table 3.

ii) *equivalence of band representations at different sites of W.*

We want first to prove some inequivalence; lemma C allows us to work with the finite Born von Karman groups $G_{12\nu}$. By definition of different sites $q \neq q'$, the strata $S[G_q]$ and $S[G_{q'}]$ have no common points, so from lemma 3 a dominant element $g \in G_q$ is not conjugate to any element of $G_{q'}$; then equation (9') shows that it has character zero for any band representation induced from $G_{q'}$ (the inducing representation might be reducible). Therefore if the dominant element $g \in G_q$ has a non zero character in the band representation $B^{(q,\rho)}$ induced from a unirrep of a maximal isotropy group, this representation is inequivalent to any band representation at an other site, therefore it is elementary (from tables 2 and 3 this property is not spolied by equivalences at the same site). This is the case of

$90 = P42_12$	a	D_2	2,3	$127 = P/4mbm$	c	D_{2h}	2,3	**197** $= I23$	b	D_2	2,3
	b	D_2	2,3		c	D_{2h}	6,7	$201 = Pn\bar{3}$	d	D_2	2,3
97 $= I422$	d	D_2	2,3		d	D_{2h}	2,3	**204** $= Im\bar{3}$	b	D_{2h}	2,3
$100 = P4bm$	b	C_{2v}	2,4		d	D_{2h}	6,7		d	D_{2h}	6,7
$102 = P4_2nm$	a	C_{2v}	2,4	$128 = P4/mnc$	d	D_2	2,3	$208 = P4_232$	a	T	2,3
$109 = I4_1md$	a	C_{2v}	2,4	$130 = P4/ncc$	a	D_2	2,3	**209** $= F432$	c	T	2,3
$113 = P\bar{4}2_1m$	c	C_{2v}	2,4	$133 = P4_2/nbc$	c	D_2	2,3	**211** $= I432$	d	D_2	2,3
$117 = P\bar{4}b2$	c	D_2	2,3	$135 = P4_2/mbc$	d	D_2	2,3	$218 = P\bar{4}3n$	a	T	2,3
	d	D_2	2,3	$140 = I4/mcm$	d	D_{2h}	2,3	$219 = F\bar{4}3c$	a	T	2,3
$120 = I\bar{4}c2$	a	D_2	2,3		d	D_{2h}	6,7		b	T	2,3
	d	D_2	2,3	$142 = I4_1/acd$	b	D_2	2,3	$228 = Fd\bar{3}c$	c	T	2,3
								$230 = Ia\bar{3}d$	c	D_2	2,3

Table 3. Pairs of equivalent band representations induced from the same maximal isotropy group G_q, by unirreps which do not form an orbit of the normalizer $N_G(G_q)$. There are 34 pairs of them belonging to 25 space groups. After the n^o and the symbol of the space group, the columns of this table give the Wyckoff position, the corresponding isotropy group and its unirreps (notation of [11]) yielding the pair of band representations.

induced representations from one dimensional unirreps $\chi_{G_q}^{(\rho)}$: indeed the characters of one dimensional representations do not vanish, and equation (12) shows that the character of the induced representation is a multiple of that of the inducing representation except when the normalizer $N_G(G_q)$ has non trivial orbits in $\hat{G}_q$, i.e. for the cases listed in equation (29). The latter do not yield exceptions: indeed the dominant elements $2, 2, 3, 3, 3$ have respectively $-2, -2, -1, -1, -1$ as characters in the direct sums of the unirreps given in (29), and the corresponding characters of the band representation are a multiple of these values. Thus we have proven:

Lemma 4. At a site q whose isotropy group is not listed in (26), all band representations induced from one dimensional unirreps are elementary and inequivalent except for the 57 pairs listed in tables 2 and 3.

Remark that the character of (the dominant) space inversion never vanishes in a unirrep of G_q since $\bar{1}$ is in the center of the group and is therefore represented by a multiple of the identity. Other dominant elements may have vanishing character in a unirrep of G_q. In the next equation we list the multidimensional unirreps of point groups in which all dominant elements have vanishing characters:

$$D_{2d}(5), \quad T_d(3) \tag{33}$$

These two representations are two dimensional; we can enlarge lemma 4 to:

Theorem 1. At a site q whose isotropy group is not listed in (26), all band representations induced from unirreps of G_q are elementary except possibly those induced from the two

2-dimensional unirreps listed in (33).

We now study the maximal isotropy groups whose geometrical classes are listed in equation (26). If two groups satisfy lemma B, i.e. they are isomorphic, not conjugate but their corresponding elements are pairwise conjugate; hence these two groups belong to the same geometric class. The search for such pairs of maximal isotropy groups can be made from the study of the partial ordered set of strata (the Wyckoff positions listed in [7]). We find 17 such pairs belonging to 14 space groups; they are listed in table 4. This corresponds to 63 pairs of equivalent band representations.

22	$= F222$	D_2	a ≡ b	118	$= P\bar{4}n2$	D_2	c ≡ d	210	$= F4_132$	T	a ≡ b
		D_2	c ≡ d	163	$= P\bar{3}1c$	D_3	c ≡ d			D_3	c ≡ d
68	$= Ccca$	D_2	a ≡ b	182	$= P6_322$	D_3	c ≡ d	212	$= P4_332$	D_3	a ≡ b
70	$= Fddd$	D_2	a ≡ b	196	$= F23$	T	a ≡ b	213	$= P4_132$	D_3	a ≡ b
94	$= P4_22_12$	D_2	a ≡ b			T	c ≡ d	214	$= I4_132$	D_2	c ≡ d
98	$= I4_122$	D_2	a ≡ b	203	$= Fd\bar{3}$	T	a ≡ b				

Table 4. Pairs of maximal isotropy groups which satisfy lemma B: they are isomorphic, not conjugate, but their corresponding elements are pairwise conjugated. There are 17 pairs of such isotropy groups belonging to 14 space groups. They yield 63 pairs of equivalent band representations. After the n^o and the symbol of the space group, the columns of this table give the isotropy group and the pair of Wyckoff positions. All band representations induced from the equivalent unirreps of these pairs of subgroups are equivalent.

When we search for equivalence of band representations, lemma C shows that working with the Born von Karman groups G_ν yields a necessary condition; then we have to check in each case if it is sufficient (as a matter of fact it will always be so), for instance we verify the equality of the $m_{q,\rho}^{k,\alpha}$ components. The isotropy groups G_q of the eight geometric classes listed in (26) and (33) are non polar, so they are equal to their normalizer in G. To continue our study of equivalence of a band representation $B^{(q,\rho)}$ induced from a maximal isotropy group G_q, with another one induced from a non conjugate maximal isotropy group $G_{q'}$, we have to consider the multidimensional unirreps of G_q because they have elements with zero character. When their elements with non vanishing character form a subgroup (we call it K_q) we list these representations in the equations (34) giving also the representation $\mathrm{Res}_{K_q}^{G_q}\chi_{G_q}^{(\rho)}$):

$$C_3(2\oplus 3) \subset D_3(3),\; C_6(3\oplus 4) \subset D_6(3),\; C_6(5\oplus 6) \subset D_6(6), \tag{34}$$

$$D_2(2\oplus 3\oplus 4) \subset T(4),\; T(2\oplus 3) \subset O(3),\;\; T(2\oplus 3) \subset T_d(3), \tag{34'}$$

$$C_2^z(2\oplus 2) \subset D_4(5),\; C_2^z(2\oplus 2) \subset D_{2d}(5) \tag{34"}$$

It is only in the 3-dimensional unirreps of O that the elements with non vanishing characters do not form a group; we give in the next equation the geometric class of elements with zero character:

$$[3] \quad \text{in } O(4), O(5). \tag{35}$$

There are only five space groups which contain O as maximal isotropy groups; by studying the partial ordering of their Wyckoff positions we find in two of them that the elements with non vanishing characters in the 3-dimensional representations of O (i.e. the elements of order $\neq 3$) are *all* conjugate to the elements of another isotropy group, namely D_4, but a class of rotations of order 2 in D_4 is not conjugate to that of O. So exceptions can only arise for the unirreps of D_4 in which the order 2 rotations have vanishing characters. This is the case with the 2-dimensional unirrep $D_4(5)$; it is induced from $C_4(3)$ or $C_4(4)$ and this C_4 subgroup is the intersection $C_4 = O \cap D_4$ so the two corresponding exceptions will appear in the family of non elementary band representations given in table 7 (groups 207, 211).

The equations (34) have been divided in three cases on the following grounds:
i) in (34) and (34') the unirreps of G_q is induced by the corresponding one dimensional representation of K_q
ii) in (34') the K_q's are non polar and have no dominant elements. In the other cases, they are polar, cyclic and therefore have a dominant elements
We first study the partial ordering of Wyckoff positions for the space groups which contain T, O or T_d as maximal isotropy groups, looking for pairwise conjugation of the elements of the corresponding K_q: this yields 4 pairs of equivalent elementary band representations, also listed in table 5. Note that none of them concern $D_2(2 \oplus 3 \oplus 4) \subset T(4)$.

209 $=F432$ a $O(3) \sim$ b $O(3)$	216 $=F\bar{4}3m$ a $T_d(3) \sim$ b $T_d(3)$ c $T_d(3) \sim$ d $T_d(3)$	227 $=Fd3m$ a $T_d(3) \sim$ b $T_d(3)$

Table 5. Pairs of elementary equivalent band representations induced from unirreps of maximal isotrophy groups whose elements with non vanishing characters are pairwise conjugate. There are 4 pairs belonging to 3 space groups. After the n^o and the symbol of the space group, the columns of this table give for each pair the Wyckoff positions, the isotropy group and its unirrep.

When the K_q's are polar and their elements are pairwise conjugated with a subgroup $L_{q'}$ of another maximal isotropy group $G_{q'}$, these two groups are conjugate because all their non trivial elements are dominant. Then by a conjugation on $G_{q'}$ they can be brought to coincide: $K_q = L_{q'} \subseteq G_q \cap G_{q'}$. When the last relation is an equality, we denote this group by $G_{qq'}$; as an intersection of isotropy groups it is a polar isotropy group. This is the case of the groups of (34) because the K_q subgroups are maximal. We have to study those of (34"): indeed C_2^z is not a maximal subgroup of D_4 or D_{2d}, so the intersection can be strictly larger. If $G_r \approx D_4$ the points of the z-axis containing r have isotropy group C_4: indeed since the rotations of order 4 around the z-axis leaves the point r fixed, they leave all points of the z-axis fixed; moreover this isotropy group cannot contain other elements (such as a reflection plane) because these elements should be also in the isotropy group of r. Since the non conjugate group $G_{q'}$ contains C_2^z, it must contain C_4, the isotropy group of the z-axis so $G_{qq'} = G_q \cap G_{q'} = C_4$. By a similar sequence of arguments when $C_2^z \subseteq G_q \cap G_{q'}$ for two pairs of non conjugate maximal isotropy groups and $G_q \approx D_{2d}$ one proves that $G_{qq'} = C_{2v}$. So we can replace equation (34") by:

$$C_4(3 \oplus 4) \subset D_4(5),\ C_{2v}(2 \oplus 4) \subset D_{2d}(5) \tag{36}$$

in which the subgroup is $G_{qq'}$.

By searching among the list of non polar point groups, one finds that the only unirreps of point groups induced by any one of the unidimesional representations of the subgroups $G_{qq'}$ listed in (34) and (36), are exactly the 2-dimensional unirreps listed in the same equations for the groups G_q. This yields equivalent elementary band representations induced from non conjugate maximal isotropy groups with a common z-axis, and belonging to the same geometric classes: D_3, D_6, D_4 or D_{2d}.

There are 33 pairs of such equivalent band representations. They belong to 23 space groups. They are listed in table 6. Note however that five of those pairs are implicitly contained in table 4.

89 $= P422$	ab	D_4	5	126 $= P4/nnc$	ab	D_4	5	163 $= P\bar{3}1c$	cd	D_3	3*
	cd	D_4	5	129 $= P4/nmm$	ab	D_{2d}	5	**177** $= P622$	ab	D_6	5
97 $= I422$	ab	D_4	5	134 $= P4_2/nnm$	ab	D_{2d}	5			D_6	6
111 $= P\bar{4}2m$	ac	D_{2d}	5	137 $= P4_2/nmc$	ab	D_{2d}	5		cd	D_3	3
	bd	D_{2d}	5	141 $= I4_1/amd$	ab	D_{2d}	5	182 $= P6_322$	ab	D_3	3
115 $= P\bar{4}m2$	ad	D_{2d}	5	**149** $= P312$	ab	D_3	3		cd	D_3	3*
	bc	D_{2d}	5		cd	D_3	3	210 $= F4_132$	cd	D_3	3*
119 $= I\bar{4}m2$	ab	D_{2d}	5		ef	D_3	3	212 $= P4_332$	ab	D_3	3*
	cd	D_{2d}	5	**150** $= P321$	ab	D_3	3	213 $= P4_132$	ab	D_3	3*
121 $= I\bar{4}m2$	ab	D_{2d}	5	**155** $= R32$	ab	D_3	3	214 $= I4_132$	ab	D_3	3
125 $= P4/mcc$	ab	D_4	5	**162** $= P\bar{3}1m$	cd	D_3	3				
	cd	D_{2d}	5								

Table 6. List of the 33 pairs of equivalent elementary band representations induced from two dimensional unirreps of non conjugate maximal isotropy groups belonging to the same geometric class. These pairs belong to 23 space groups. The pairs marked with a * are already implicitly contained in table 4. After the n^o and the symbol of the space group, the columns of this table give the Wyckoff positions, the maximal isotropy group and its two dimensional unirrep.

Finally the one dimensional unirreps of the groups $G_{qq'}$ listed in equations (34) and (36) may induce a reducible representation of $G_{q'}$. In that case the band representation $B^{(q,\rho)}$ is not elementary. There are 40 such band represenntations induced from the 2-dimensional unirreps of maximal isotropy groups listed in equations (34) and (36). They

124 $= P4/mcc$	a	D_4	5	188 $= P\bar{6}c2$	a	D_3	3	**211** $= I432$	b	D_4	5
	a	D_4	5		c	D_3	3		c	D_3	3
131 $= P4_2/mmc$	e	D_{2d}	5		e	D_3	3	**215** $= P\bar{4}3m$	c	D_{2d}	5
	f	D_{2d}	5	190 $= P\bar{6}2c$	a	D_3	3		d	D_{2d}	5
132 $= P4_2/mcm$	b	D_{2d}	5	192 $= P6/mcc$	a	D_6	5	**217** $= I\bar{4}3m$	b	D_{2d}	5
	d	D_{2d}	5				6	222 $= Pn3n$	b	D_4	5
139 $= I4/mmm$	d	D_{2d}	5		c	D_3	3	223 $= Pm3n$	c	D_{2d}	5
140 $= I4/mcm$	a	D_4	5	193 $= P6_3/mcm$	d	D_3	3		d	D_{2d}	5
	b	D_{2d}	5	**207** $= P432$	c	D_4	5		e	D_3	3
163 $= P\bar{3}1c$	a	D_3	3		d	D_4	5	224 $= Pn3m$	d	D_{2d}	5
165 $= P\bar{3}c1$	a	D_3	3	208 $= P4_232$	b	D_3	3	226 $= Fm3c$	c	D_{2d}	5
167 $= R\bar{3}c$	a	D_3	3		c	D_3	3	228 $= Fd3c$	b	D_3	3
				210 $= F4_132$	c	D_3	3	**229** $= Im3m$	d	D_{2d}	5
					d	D_3	3	230 $= Ia3d$	b	D_3	3

Table 7. List of the 40 bands representations induced from unirreps of maximal isotropy groups and *not elementary*; they belong to 25 space groups. After the n^o and the symbol of the space group, the columns of this table give the Wyckoff position, the maximal isotropy group and its two dimensional unirrep.

belong to 25 space groups. They are listed in table 7. They are the only counter examples to the converse of lemma 1.

This ends our systematic search for equivalences of band representations induced from unirreps of maximal isotrpy groups, and proves the:

Main Result. All band representations induced from unirreps of maximal isotropy groups are *elementary*, except for the 40 of them (listed in table 7), and *inequivalent* except for 152 pairs: 57 at the same site (listed in tables 2 and 3) and 95 at inequivalent sites (listed in tables 4,5 and 6).

The same study can be performed for dimension 2; it can be useful in surface physics. All the 132 band representations induced from the inequivalent unirreps of the maximal isotropy groups are elementary and inequivalent but one pair of them.

7 **Final remark.** It is not obvious that the mathematical equivalence (i.e. the existence of an intertwining operator) found for the elementary band representations always corresponds to the needs of physics. Indeed it is physically natural to choose a basis which diagonalizes the translations; then the basis functions are the Bloch functions: they are obtained by taking the Fourier transform of the electron wave functions over the translation group, so they are defined over the Brillouin zone B. Of course this procedure is rigourous only with the use of Born von Karman groups; for the infinite space groups the Bloch functions are not basis of the Hilbert space $\mathcal{H}$ carrying the band representation but they are basis of the finite dimensional integrand whose $\mathcal{H}$ is the direct integral on B. Then, **in this** basis, there does not exist an intertwining operator between some pairs of equivalent band representations (except if we consider "generalized" Bloch functions defined on a double covering of the Brillouin zone). The equivalence for which we can find an intertwining

operator (whose elements are in general continuous functions on B) are those of tables 2,6 and also 7; this corresponds to 23+33=56 pairs of equivalent representations. For the other pairs of mathematically equivalent elementary band representations, we can say that they have the same continuity chord but they seems to us *physically inequivalent* (for more details see [5]).

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