STRUCTURE AND CLASSIFICATION OF BAND REPRESENTATIONS

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Abstract.

Band representations in solids are investigated in the general framework of induced representations by using the concepts of orbits (stars) and strata (Wyckoff positions) in their construction and classification. The connection between band representations and irreducible representations of space groups is established by reducing the former in the basis of quasi-Bloch functions which are eigenfunctions of translations but are not, in general, eigenfunctions of the Hamiltonian. While irreducible representations of space groups are finite-dimensional and are induced from infinite-order little groups G_k for vectors $\vec{k}$ in the Brillouin zone, band representations are infinite-dimensional and are induced from finite-order little groups G_r for vectors $\vec{r}$ in the Wigner-Seitz cell. This connection between irreducible representations and band representations of space groups sheds new light on the duality properties of the Brillouin zone and the Wigner-Seitz cell. As an introduction to band representations the induced representations of point groups are investigated in some detail. A connection is found between band representations of space groups and induced representations of point groups which is applied to the investigation of the equivalency of band representations. Based on this connection and on the properties of the crystallographic point groups a necessary condition is established for the inequivalency of band representations induced from maximal isotropy groups. For using this condition there is need for the induced representations of point groups and a full list of them is given in the paper. One is especially interested in irreducible-band representations which form the elementary building bricks for band representations. From the point of view of the physics, irreducible-band representations correspond to energy bands with minimal numbers of branches. A method is developed for finding all the inequivalent irreducible-band representations of space groups by using the induction from maximal isotropy groups. As a rule the latter leads to inequivalent

irreducible-band representations. There are, however, few exceptions to this rule. A full list of such exceptions is tabulated in the paper. With this list at hand one can construct all the different irreducible-band representations of any space group. A discussion is also given for irreducible-band representations of 2-dimensional space groups. For them we list the continuity chords of all their irreducible-band representations.

I. Introduction.

A symmetry group G occurs in physics through its action on manifolds M_i (which can be, in particular, space-time, phase-space, Hilbert space of states or discrete sets). This defines naturally linear representations of the group G on the spaces of scalar, vector or tensor valued functions on the manifolds M_i. Such representations are induced representations or direct sums or integrals of them. This emphasizes the wide occurrence of induced representations in physics. Moreover, for many physical groups, e.g. Poincaré group, Weyl-Heisenberg group, Euclidean group, space groups, point groups, most of their irreducible unitary representations can be obtained by means of the induction method from representations of their subgroups [1]. Consequently, induced representations have acquired an important rôle in representation theory in physics. Their wide use is partly explained by the fact that the induction method enables one to find representations of the full group from the knowledge of the representations of its subgroups. In this framework, the induced representations of a group G have the simple mathematical meaning of being generated from some elementary building bricks which are the irreducible representations of a family of subgroups of G. In physics one is usually concerned with irreducible representations of a symmetry group because they are directly connected with a set of states that belong to a single energy level [2]. Since induced representations are, as a rule, reducible they cannot, in general, be assigned to a single energy level of a system. There is, however, some analogy between the structure of physical systems and the structure of induced representations. This is connected with the fact that some physical systems consist of elementary building bricks with local symmetry H which is a subgroup of the symmetry G of the full system. Good examples of such systems are molecules or solids which consist of atoms or sets of atoms having as their local symmetry some subgroup of the full group G. The structure of such physical systems resembles the structure of induced representations in that both are built from some elementary building tricks. With this analogy in mind one should expect that induced representations could be assigned some direct physical meaning. This is actually the case, and as was first shown by des Cloizeaux [3], the induction process for space groups can be used in constructing a set of orbitals for spanning the space of all the eigenfunctions of an entire energy band of a solid. As was later shown by one of the authors [4,5] the representations built on these sets of orbitals have the physical meaning of corresponding to energy bands in a solid and as such they were called band representations. This shows that unlike irreducible representations that correspond to single energy levels, induced representations should, in general, correspond to sets of energy levels. In solids such a set of levels forms an energy band. Band representations present therefore a striking example of a correspondence between an induced representation and a set of energy levels that all belong to a well defined energy band.

Motivated by the correspondence between induced representations and energy bands in solids we investigate in this paper the structure and classification of induced representations of point groups and space groups. It is well known that irreducible representations of a space group can be obtained by induction from the little groups G_k which are isotropy groups of the vectors $\vec{k}$ in the Brillouin zone [6,7]. For an infinite crystal G_k is a subgroup of infinite order: it contains an infinite number of elements and is of finite index. In this paper our particular interest will be in a special class of induced representations which are induced from finite order little groups of the points in the space of the crystal. In the case of space groups these are the band representations. Being induced representations one can apply to them the concepts of orbits and strata [8,9] and treat them in the general framework of the induction theory [1,10].

In applications of group theory to physical problems one is usually interested in the reduction of representations into their irreducible components [6,11]. In the case of band representations a reduction of different nature arises which is related to their decomposition into band representations [4,5]. More generally, one can consider the reduction of a given induced representation into a direct sum of induced representations. For band representations the concept of an irreducible-band representation was introduced for the case where it does not reduce into a direct sum of other band representations [4]. Having in mind that band representations are reducible, some confusion might be avoided by using the hyphenated form irreducible-band representation. While irreducible representations of space groups are finite-dimensional and are induced from infinite-order subgroups (isotropy groups of $\vec{k}$-vectors in the Brillouin zone), irreducible-band representations are of infinite dimension and are induced from finite-order isotropy groups in the Wigner-Seitz cell. This connection between the two kinds of induced representations of space groups leads to a group-theoretical foundation for the structure and classification of energy bands in solids.

The outline of the paper is as follows : Section II deals with group actions and the connected subject of induced representations. A discussion is given of symmetry centers, orbits (stars), strata (Wyckoff positions) and their invariance groups (little groups, isotropy groups) are described. In particular, the concept of a closed stratum turns out to be of much importance in the derivation of irreducible-band representations. In this section a detailed discussion is also given of the related subject of induced representations. Formulas are derived for the characters of induced representations and much attention is payed to the very important Frobenius reciprocity theorem. In Section III we discuss induced representations of point groups. This section serves a twofold purpose : being of finite order, point groups can be easily utilized for defining different concepts of induced representations; also the results of this section are explicitly applied to the classification of band representations of space groups which is the main subject of this paper. In Section IV a description is given of the induction process of band representations and the concepts of equivalency of band representations and of irreducible-band representations are discussed. Section V deals with the connection between irreducible representations and band representations of space groups. This connection is obtained by reducing the band representations in the basis of quasi-Bloch functions which are eigenfunctions of the translations but unlike the Bloch functions are not, in general, eigenfunctions of the Hamiltonian [3,12]. In this basis the band representations reduce into finite-dimensional components ($\vec{k}$- components) whose characters are easily found in a closed form. The latter give the continuity chord of the band [5] which is the contents of a band representation in terms of irreducible representations of the space group. The k-component character of all the irreducible band representations are calculated for the diamond structure space group O_h^7. In Section VI we consider the problem of equivalent irreducible-band representations. Thus, we prove that band representations induced from irreducible representations of maximal isotropy groups are, in general, irreducible-band representations. The number of exceptions is relatively small and a listing of them is presented. A full list of irreducible-band representations which are equivalent is also given in this section. This together with the previous list gives us the information of all the inequivalent irreducible-band representations of space groups in 3 dimensions.

Section VII is a short description of space groups in 2 dimensions and of their inequivalent irreducible-band representations. Section VIII is a Summary. In tne Appendix the Mackey double coset method is compared with the reduction of band representations by means of quasi-Bloch functions.

II. Group Actions and Induced Representations.

A. Group Actions.

For the sake of completeness, let us recall the concepts which are basic in the study of group action. An action of G on M is defined by a function $G \times M \overset{\varphi}{\to} M$ satisfying

$$\varphi(1,m) = m \quad , \quad \varphi(g_1 g_2, m) = \varphi(g_1, \varphi(g_2, m)) \tag{1}$$

If G and M are manifolds, φ is a smooth map. We will often use the short notation $g.m$ for $\varphi(g,m)$ whenever there is no ambiguity about the way the group acts. When M is a vector space, a linear representation on M is a particular example of group action.

The orbit of m is the set of transforms of m by the group action. We denote that orbit $\varphi(G,m)$ or simply $G.m$. The isotropy group (also called stabilizer or little group) G_m of m is the set of elements of G which leave m invariant; one can show that it is a (closed) subgroup of G , i.e. $G_m \leq G$. One easily establishes that $G_{g.m} = gG_m g^{-1}$. So the set of isotropy groups of a G-orbit $G.m$ forms a conjugacy class of G-subgroups. That class is denoted by $[G_m]$. We say that the orbit $G.m$ is of type $[G_m]$.

An action of G on M partitions M into orbits. We denote by $M|G$ the set of orbits ($M|G$ is called the orbit space). The (disjoint) union of orbits of the same type is called a stratum. In other words, two points m and m' are in the same stratum iff their isotropy groups are conjugate. We denote by $M||G$ the set of strata. Clearly there is a natural injective map

$$M \| G \overset{\sigma}{\rightarrowtail} K_G \tag{2}$$

into the set of conjugacy classes of G subgroups. For many groups G : all finite groups, compact groups, space groups, Poincaré group , given two non conjugate subgroups A,B if $A \leq B' \in [B]$ where $[B]$ is the class of groups conjugate to B , then one cannot have $B' \leq A' \in [A]$. So there is a natural partial order, by inclusion up to a conjugation, on the set K_G of conjugation classes of subgroups of G . Equation (2) shows that we can order the strata under a G-action.

Most group actions met in physics have only a finite number of strata. Their classification is generally easy and always important. For instance, in the Lorentz group action in Minkowski space, there are three strata outside the origin (an orbit and a stratum by itself), those of space like, time like and light like vectors. The strata of the action of a crystallographic space group on the Euclidean space E are tabulated in the international Tables of X-Ray Crystallography [13] for dim $E = 2$ and 3 , under the name of Wyckoff positions and the corresponding conjugacy classes of isotropy groups are also given.

Since orbits are classified into types, we can define them per se without referring to the spaces M_i . Given a subgroup $H \leq G$ and an element $a \in G$, a left coset aH is the set of elements $\{ah, h \in H\}$. G is a disjoint union of left H-cosets and the set of cosets - the coset space - is denoted by $[G:H]$. It is an orbit of G for the action :

$$g\cdot(aH) = (ga)H \tag{3}$$

According to our definition that orbit is of type $[H]$. As is well known, if $H \triangleleft G$ (H is an invariant subgroup of G) , $[G:H]$ is a group (the quotient group $G|H$).

Given two actions φ and φ' of G on M and M' there is a natural action of G on the set of functions $F(M,M')$ defined on M and valued on M' . It is defined by

$$F(M,M') \ni f \longmapsto g \cdot f \quad , \quad \varphi'(g,f(m)) = (gf)(\varphi(g,m)) \tag{4}$$

or, in shorter notation,

$$(g \cdot f)(m) = g \cdot [f(g^{-1} \cdot m)] \tag{5}$$

(beware that the dot represents three different actions depending on the mathematical object placed at its right). Whenever $g \cdot f = f$, the functions f is said to be equivariant. When an equivariant isomorphism f exists between M and M', the two actions φ and φ' are said to be equivalent. One has

$$f(m) = g \cdot [f(g^{-1} \cdot m)] \tag{6}$$

This is the usual equivalence of linear representations when M and M' are vector spaces.

From that definition of equivalence, it is easy to prove that the actions of G on two orbits are equivalent if, and only if, the two orbits are of the same type.

In the present work, we are interested in the action of a crystallographic space group G on the Euclidean space E (also referred to as the $\vec{r}$-space or the position space). Except when we have to give explicit Tables, there is no reason to specify the dimension n of E.

The orbits of G in E are usually called the crystallographic orbits. In 3 dimensionsthe types of crystallographic orbits are tabulated in Ref. [14]. Usually we do not consider directly the orbit space. Rather we consider the orbit space of the translation subgroup T of G. It is $E|T$, an n-dimensional torus which can be referred to as the Wigner-Seitz torus since it is nothing else than a Wigner-Seitz cell in which parallel boundaries are identified. (The fundamental domains of the translation groups were studied by Dirichlet, Fedorov, Voronoy and Delone).

It is quite clear that G also acts on the WS torus, but the invariant subgroup T acts trivially on it. It is the quotient group $P = G/T$ (the point group) which acts effectively on the WS torus. This means that only the unit element 1 of P acts trivially.

Let us denote by π the group homomorphism $G \xrightarrow{\pi} P = G/T$ and by φ the mapping $E \xrightarrow{\varphi} WS = E/T$. Let $G_{\vec{r}}$ be the isotropy group of $\vec{r} \in E$. It is clear that, if $\vec{q} = \varphi(\vec{r})$,

$$\pi(G_{\vec{r}}) = P_{\vec{q}}$$

and, since $G_{\vec{r}} \cap T = 1$, $P_{\vec{q}}$ is isomorphic to $G_{\vec{r}}$.

We must emphasize that $P_{\vec{q}}$ cannot be confused with $G_{\vec{r}}$ not only because $\vec{q} \in WS$ and $\vec{r} \in E$ are different or because $P_{\vec{q}}$ is a subgroup of P (a quotient group) and $G_{\vec{r}}$ a subgroup of G , but also mainly because a given $P_{\vec{q}}$ can be the image of two (or more) non conjugate isomorphic subgroups $G_{\vec{r}}$ and $G_{\vec{r}'}$. If one considers the action of G (instead of P) on WS , the orbits and strata are the same but the isotropy subgroup $P_{\vec{q}}$ is replaced by the group $G_{\vec{q}} = \pi^{-1}(P_{\vec{q}}) = T \cdot P_{\vec{q}}$ which is a symmorphic space group.

To summarize, we have therefore the following vocabulary : G_r (for simplicity we shall omit the vector signs on $\vec{r}$ and $\vec{q}$) is the isotropy group of the vector $\vec{r}$ in the Euclidean space E ; P_q is the isotropy group of the vector $\vec{q}$ in the Wigner-Seitz cell; finally, $G_q = T \cdot P_q$ is a symmorphic space group. It is clear that G_r is a subgroup of G , while P_q is a subgroup of P . The above vocabulary will be used throughout the paper.

We have shown that in the action of a space group G on the physical space, the isotropy groups $G_{\vec{r}}$ are finite, so they belong to the subset $K_G^F \subset K_G$ of conjugation classes of finite G subgroups.

Let us remark that any finite subgroup F of G cannot contain a pure translation; we can then prove that the maximal conjugation classes of K_G^F are conjugation classes of isotropy subgroups. Indeed let F_m be such a maximal finite subgroup of G and $\vec{x}$ an arbitrary point of E . The barycenter $\vec{b}$ of the orbit $F_m\vec{x}$ is invariant by F_m so $F_m \leq G_{\vec{b}}$ which is finite. The maximality of F_m implies $F_m = G_{\vec{b}}$.

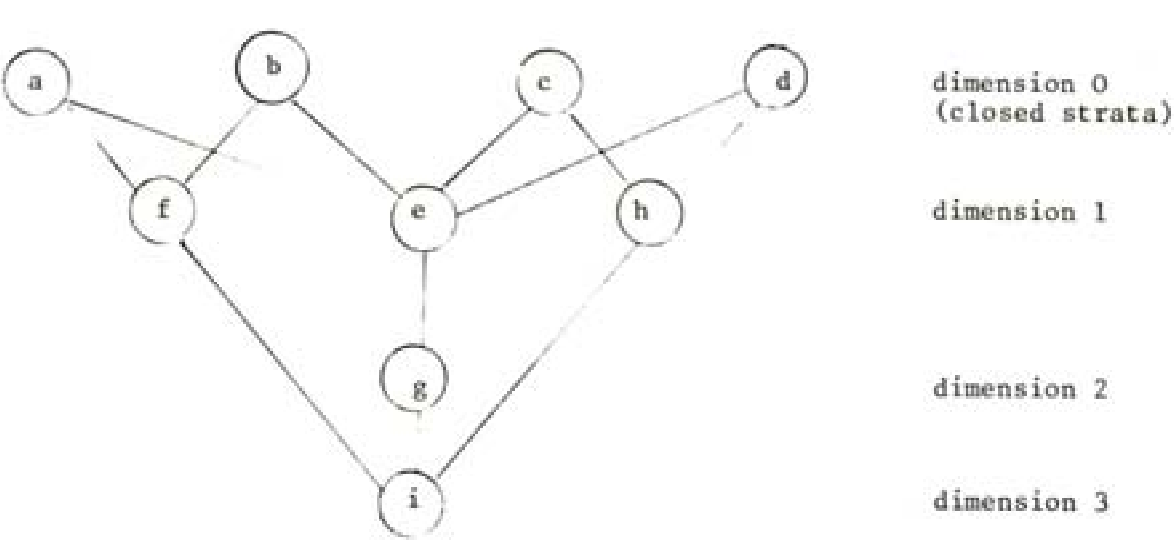
In general, an intersection of little groups is not a little group, but this is the case for finite groups [9] and the proof can be easily extended to space groups.

The dimension of the stratum of $G_{\vec{r}}$, isomorphic to P_q is the multiplicity of the trivial representation in the vector representation of the point group P_q . The Table 1 gives this dimension for the 32 point groups.

As we already said the strata are called the Wyckoff positions in the International Tables for X-Ray Crystallography [13] and the number of free parameters of a position is the dimension of the stratum. As before let us denote by $[G_r]$ the class of groups conjugate to G_r in G . Every space group has only one 3-dimensional stratum, that of $[\{1\}]$ (the trivial group) : it is open dense [8]. The strata corresponding to maximal conjugation classes of finite G-subgroups are topologically closed [8]. They correspond to symmetry points, rotation axes or reflection planes [3,4]. We give in Table 2 a statistics of the dimension of the closed strata of space groups in 3 dimensions.

There are 183 space groups whose closed strata have the same dimension (or is unique). Among them, 13 have only one stratum, the whole space; hence their only symmorphic subgroups are in T . These 13 space groups are tabulated in Table 3. This Table contains also the 5 space groups with closed strata of dimension 2. There are 2 space groups with closed strata of dimension 0 and 2 , 6 of dimension 1 and 2 and 38 of dimension 0 and 1 (See Table 2). There is only one group (# 57 with the international symbol Pbcm) which contains closed strata of all possible dimensions 0,1 and 2 (See Table 3).

Let us illustrate all these properties by presenting the partial ordered set of Wyckoff positions of the diamond group (#227) $Fd\bar{3}m = O_h^7$. Reference [13] gives a list of nine strata denoted by the letters a,b,...,i . The only closed Wyckoff positions are a,b,c and d with the corresponding maximal isotropy groups $[G_a]$, $[G_b]$, $[G_c]$ and $[G_d]$ (See Table 4). On the other hand, i is the (3-dimensional) generic open stratum corresponding to the trivial little group 1. None of the groups in Table 4 is contained in a larger stability subgroup. Thus, f contains all the points of the type (x,0,0) except (0,0,0) which belongs to a and $(\frac{a}{2},\frac{a}{2},\frac{a}{2})$ which belongs to b (the letter a is used here with two meanings : in the symmetry site it denotes the lattice constant and as a separate letter it denotes the type of the symmetry site). Therefore f has less symmetry than a or b . The following diagram illustrates the above results (See [13]).



A number of examples of zero-dimensional strata are given in Table 3 for the hexagonal closed packed structures ($P6_3/mmc$) and 4 cubic groups : the simple cubic (Pm3m) , the face-centered (Fm3m) , the diamond-structure (Fd3m) and the body centered-cubic (Im3m) . Three of these space groups are symmorphic, while two (the hexagonal closed packed and the diamond structure) are non-symmorphic. We would like to point out that the simple cubic and the face-centered cubic groups have two different closed strata with the full cubic symmetry m3m . This is not the case with the body-centered cubic group which has only one closed stratum with the symmetry m3m .

In conclusion of this subsection we make a number of remarks about notations. Space group elements are denoted by $(\alpha|\vec{t})$ where α is a point group element and $\vec{t}$ a translation. $(\alpha|\vec{t})$ of the space group G acts on the vectors $\vec{r}$ in the Euclidean space E in the following way :

$$(\alpha|\vec{t})\vec{r} = \alpha\vec{r} + \vec{t} \tag{7}$$

A little group G_r (or isotropy group) of $\vec{r}$ contains all those elements $(\gamma|\vec{v}(\gamma))$ of G (where $\vec{v}(\gamma)$ is the particular translation of γ) for which

$$(\gamma|\vec{v}(\gamma))\vec{r} = \gamma\vec{r} + \vec{v}(\gamma) = \vec{r} \tag{8}$$

$\vec{r}$ is called a symmetry center. For a general point $\vec{r}$, G_r contains the unit element only. Any space group G can be decomposed into cosets with respect to a chosen origin O (T is the group of pure translations)

$$G = T + (\gamma_2|\vec{v}(\gamma_2))T + \ldots + (\gamma_s|\vec{v}(\gamma_s))T \tag{9}$$

where $(\gamma_j|v(\gamma_j))$, $i = 1,2,\ldots,s$ are called the representative elements, and we shall keep them fixed with well defined partial translations $\vec{v}(\gamma_i)$. In general, $(\gamma|\vec{v}(\gamma))$ in (8) is not one of the representative elements in (9) and it can differ from the latter by a Bravais lattice vector. The fact that the vector $\vec{r}$ has a non-trivial little group means that the space group G has point group elements with $\vec{r}$ as the origin. In other words, the elements $\gamma_1^{(r)}, \gamma_2^{(r)}, \ldots, \gamma_f^{(r)}$ of G_r are pure point group elements when written with respect to $\vec{r}$ as an origin

$$\gamma_m^{(r)}\vec{r} = \vec{r} \ , \quad m = 1,2,\ldots,f \tag{10}$$

The representative element $(\gamma_m|\vec{v}(\gamma_m))$ which we have fixed in advance (See (9)) with respect to the origin O will, in general, leave $\vec{r}$ unchanged only up to a vector of the Bravais lattice

$$(\gamma_m|\vec{v}(\gamma_m)\vec{r} = \vec{r} + \vec{R}_r^{(\gamma_m|\vec{v}(\gamma_m))} \tag{11}$$

where $\vec{R}_r^{(\gamma_m|\vec{v}(\gamma_m))}$ is by definition a Bravais lattice vector which depends both on the radius vector $\vec{r}$ and the representative element $(\gamma_m|\vec{v}(\gamma_m))$.

As mentioned before the symmetry centers in the Wigner-Seitz cell are denoted by $\vec{q}$. Correspondingly, the vectors of the orbit of $\vec{q}$ in the unit cell are

$$\vec{q}_1 = \vec{q} \ , \ \vec{q}_2 = (\alpha_2|\vec{v}(\alpha_2))\vec{q}, \ldots, \vec{q}_m = (\alpha_m|\vec{v}(\alpha_m))\vec{q} \tag{12}$$

where the elements $(\alpha_m|\vec{v}(\alpha_m))$ appear in the decomposition of the space group G with respect to the group G_q

$$G = G_q + (\alpha_2|\vec{v}(\alpha_2))G_q + \cdots + (\alpha_m|\vec{v}(\alpha_m))G_q \tag{13}$$

The vectors $\vec{q}$ in (12) form what is called a star in the unit cell of the Bravais lattice. Correspondingly, also the stratum of a $\vec{q}$-vector with the little group G_q is limited to a unit cell of the Bravais lattice. With this limitation a stratum coincides with the Wyckoff positions of the International Tables [13]. Wyckoff positions in a unit cell of the Bravais lattice, play an important rôle in band representations of space groups. This is very much the same as the rôle of strata in the Brillouin zone of the reciprocal lattice for irreducible representations of space groups [7,11]. It was already pointed out (See (10)) that the little group G_r when written with respect to the symmetry center $\vec{r}$ has only pure point group elements. The following relation exists between elements $\gamma^{(r)}$ with respect to r and $(\gamma|v(\gamma))$ with respect to the fixed origin O (See (9))

$$(\gamma|\vec{v}(\gamma)) = (\gamma^{(r)}|\vec{R}^{(\gamma|\vec{v}(\gamma))} \quad , \tag{14}$$

Ref. (14) gives the transition for elements of G_r from the r-origin to the common O-origin. The reason the Bravais lattice vector $\vec{R}_r^{(\gamma|\vec{v}(\gamma))}$ appears in Rel. (14) is because the representative elements $(\gamma(\vec{v}(\gamma))$ are fixed once and forever by (9). Different centers $\vec{r}$ will correspondingly lead to different $\vec{R}_r^{(\gamma|\vec{v}(\gamma))}$ for a given element $(\gamma|\vec{v}(\gamma))$. The vectors $\vec{R}_r^{(\gamma|\vec{v}(\gamma))}$ as will be seen later, play an important rôle in band representations of space groups.

B. Induced representations.

We recall the definitions and the main properties of induced representations in the simple case of finite groups [10]. For this let us consider first an orbit [G:H] with $Hm_o = m_o$ and the set of real or complex valued functions defined on it. They form a vector space $E_H^{(o)}$ of dimension $|G|/|H|$ where $|G|$ and $|H|$ are the orders of the groups G and H respectively. The corresponding action of G on $c \in E_H^{(o)}$ is defined by

$$(g\cdot c)(m) = c(g^{-1}\cdot m) \tag{15}$$

So, if $n = |G|/|H|$ different functions are taken as a basis of $E_H^{(o)}$, (for instance, the functions c_m defined by $c_m(m') = \delta_{mm'}$), the matrices of the G-representation are $n \times n$ permutation matrices. This representation is denoted by $\mathrm{Ind}_H^G(1_H)$ or by $\mathrm{Ind}_H^G(\gamma_H^{(o)})$ where 1_H or $\gamma_H^{(o)}$ denote the trivial representation of H. Obviously, the representations $\mathrm{Ind}_{H'}^G(1_{H'})$ where $H' = gHg^{-1}$ are equivalent since they are obtained from one-another by a change of basis in $E_H^{(o)}$. When the orbit is $[G:1]$ the corresponding induced representation $\mathrm{Ind}_G^G(1_G)$ is the regular representation of G, and its vector space can be identified with the space of functions on the group.

As an example of constructing induced representations, consider the action of G on a manifold M. On the Hilbert space H_M of square integrable functions on M, the corresponding action of G is

$$\forall g \in G, \quad \forall x \in M, \quad \forall f \in H_M \quad (g\cdot f)(x) = f(g^{-1}x) \tag{16}$$

Let $\psi \in H_M$ with isotropy group $G_\psi = H$, i.e.

$$h \in H \Leftrightarrow \psi(h^{-1}x) = \psi(x) \quad \forall x \in M \tag{17}$$

If we denote by p the surjective map $G \xrightarrow{p} [G:H]$ which maps every group element on its coset $p(g) = g\cdot H$, a section s is a map $[G:H] \xrightarrow{s} G$ such that $p.s = I_{[G:H]}$ the identity on the orbit $[G:H]$. In other words, a section is obtained by choosing one representative s_m for each coset. We use the short notation s_m for $s(m)$, $m \in [G:H]$ and $\psi_m(x)$ for the function $(s_m\psi)(x)$. The functions of the orbit $G\cdot\psi$ generate a vector space $E_H^{(o)}$ and the ψ_m form a basis of this vector space. Let $f \in E_H^{(o)}$

$$f = \sum_m c(m)\psi_m \qquad m \in [G:H] \tag{18}$$

and

$$\begin{aligned}(g.f)(x) &= \sum_m c(m)\psi_m(g^{-1}x) = \\ &= \sum_m c(m)\psi(s_m^{-1}g^{-1}x)\end{aligned} \tag{19}$$

And let $h(g,m) \in H$ be defined by

$$g \cdot s_m = s_{g \cdot m} h(g,m) \tag{20}$$

Then (19) can be written with the use of (17) as follows

$$(g \cdot f)(x) = \sum_m c(m)\psi(s_{g \cdot m}^{-1} x) = \sum_m c(m)\psi_{g \cdot m}(x) = \sum_m c(g^{-1} \cdot m)\psi_m(x)$$

This shows that the coordinates of the function $f \in E_H^{(o)}$ are transformed under g exactly as in Equation (15) and that the G-linear representation on $E_H^{(o)}$ is the induced representation $\mathrm{Ind}_H^G(\gamma^{(o)})$.

A more general kind of induced representation is obtained from the representation of H on the vector space $V_H^{(\alpha)}$: $h \to D^{(\alpha)}(h)$; the character of this representation is $\chi_H^{(\alpha)}(h) = \mathrm{Tr}\, D^{(\alpha)}(h)$. We consider now the Hilbert space $H_M^{(\alpha)}$ of functions defined on M and valued in $V_H^{(\alpha)}$, with the G-action again defined by (16) but with vector functions $\underline{f}$:

$$g \cdot \underline{f}(x) = \underline{f}(g^{-1}x) \tag{21}$$

Instead of the scalar function ψ with little group H defined in (17) we have to choose an H-equivariant $\underline{\psi} \in H_M^{(\alpha)}$, which means a $\underline{\psi}$ satisfying

$$\forall h \in H \quad \underline{\psi}(h^{-1}x) = D^{(\alpha)}(h)\underline{\psi}(x) \tag{22}$$

We call $E_H^{(\alpha)}$ the vector space of functions spanned by the orbit $G.\underline{\psi}$ (with the action in (21)). If the representation $D_H^{(\alpha)}$ is irreducible, the $D^{(\alpha)}(h)\underline{\psi}(x) = \underline{\psi}(h^{-1}x)$ span the vector space $V_H^{(\alpha)}$ and

$$\dim E_H^{(\alpha)} = \frac{|G|}{|H|} \dim V_H^{(\alpha)} \tag{23}$$

The linear representation of G on $E_H^{(\alpha)}$ is denoted by $\mathrm{Ind}_H^G(\gamma_H^{(\alpha)})$. One can choose a basis $\{\psi_i(x)\}$ of functions in $V_H^{(\alpha)}$ ($\psi_i(x)$ are the components of the vector $\underline{\psi}(x)$) and define as before

$$\psi_{i,m}(x) = \psi_i(s_m^{-1}x) \tag{24}$$

From (22) we obtain, for these basis vector functions

$$\psi_{j,m}(h^{-1}x) = \sum_i \psi_{i,m}(x) D_{ij}(h) \tag{25}$$

If

$$f(x) = \sum_{i,m} c_i(m)\psi_{i,m}(x) \quad , \tag{26}$$

then

$$(g\cdot f)(x) = \sum_{i,m} c_i(m)\psi_{i,m}(g^{-1}x) = \sum_{i,m} c_i(m)\psi_i(s_m^{-1}g^{-1}x) \tag{27}$$

and from (20), (24) and (25) (definition (20) is used)

$$\begin{aligned}(g\cdot f)(x) &= \sum_{i,j,m} \psi_j(s_{g\cdot m}^{-1}x)\ D_{ji}(h(g,m))c_i(m) = \\ &= \sum_{i,j,m} \psi_{j,g\cdot m}(x)\ D_{ji}(h(g,m))c_i(m) = \\ &= \sum_{i,j,m} \psi_{j,m}(x)\ D_{ji}(h(g,g^{-1}\cdot m))c_i(g^{-1}\cdot m)\end{aligned} \tag{28}$$

Comparing to Rel. (26) this shows that the vector valued function $[G:H] \otimes V_H^{(\alpha)}$ of components $c_i(m)$ in the basis $\psi_{i,m}$ is transformed by g into

$$(g.c)_i(m) = \sum_j D_{ij}(h(g,g^{-1}m))c_j(g^{-1}m) \tag{29}$$

where (20) becomes : $h(g,g^{-1}m) = s_{g\cdot m}^{-1}\, g s_m$. This gives explicitly the matrix

$\Delta(g)$ on $E_H^{(\alpha)} = \bigoplus_m V_m^{(\alpha)}$ with $V_m^{(\alpha)} = s_m V_H^{(\alpha)}$. It is made of blocks Δ_{mn} , $i \leq m$, $n \leq N = \frac{|G|}{|H|}$, each block is a $d \times d$ matrix with $d = \dim V_H^{(\alpha)}$ and

$$\Delta_{mn}(g) = \begin{cases} D(s_m^{-1} g s_n) & \text{if} \quad s_m^{-1} g s_n \in H \\ 0 & \text{if} \quad s_m^{-1} g s_n \notin H \end{cases} \tag{30}$$

Note that

$$\dim \mathrm{Ind}_H^G(\gamma_H^{(\alpha)}) = \dim(\gamma_H^{(\alpha)}) \times (\text{Index } H \text{ in } G) \tag{31}$$

This explicit expression yields the character $\chi_G^{(\Delta)}$ of the induced representation $\Delta = \mathrm{Ind}_H^G \, \gamma_H^{(\alpha)}$. Indeed

$$\mathrm{Tr}\, \Delta(g) = \chi_G^{(\Delta)}(g) = \frac{1}{|H|} \sum_{\substack{s \in G \\ s^{-1} g s \in H}} \chi_H^{(\alpha)}(s^{-1} g s) \tag{32}$$

Let $N_G(H)$ be the normalizer of H in G . $N_G(H)$ acts on $\hat{H}$, the dual of H ($\hat{H}$ is the set of equivalence classes of unitary irreducible representations of H). Thus, for $n \in N_G(H)$ we have $(n\chi^{(\ell)})(h) = \chi^{(\ell)}(nhn^{-1})$. It follows that

$$\chi^{(\Delta)}(h) = \sum_{\ell' \in \text{ orbit } N_G(H)\ell} \chi^{(\ell')}(h) \quad , \quad h \in H \tag{33}$$

Hence, irreducible representations of H which do not belong to the same orbit of $N_G(H)$ induce inequivalent representations of G .

It should be pointed out that we have defined an induced representation as a construction procedure from a given representation of a subgroup, and a representation is said to be induced if such a construction exists. In that case, as we will see, this procedure is, in general, not unique : a given representation can be induced from representations of different subgroups or even from different representations of a given subgroup.

We recall that the Kernel of a G-representation is the invariant subgroup K of G (for an invariant subgroup the notation is used $K \triangleleft G$) whose elements are represented by the identity matrix. Thus, for $k \in K$, $\chi^{(\Delta)}(k) = \dim \Delta$. From (32) one obtains

$$\mathrm{Ker}(\mathrm{Ind}_H^G \gamma_H^{(\alpha)}) = \bigcap_{g\in G} g(\mathrm{Ker}\, \gamma_H^{(\alpha)})g^{-1} \tag{34}$$

where the right-hand side is the largest G-invariant subgroup contained in the H-invariant subgroup $\mathrm{Ker}\,\gamma_H^{(\alpha)}$. If $H \triangleleft G$ (i.e. H invariant subgroup of G), the conjugation in G induces a group-homomorphism $G \to \mathrm{Aut}\, H$. This action of G on H yields also an action of G on $\hat{H}$, the dual of H i.e. the set of equivalence classes of unitary irreducible representations. (In what follows they will be called unireps of H). Indeed, g transforms $h \to D(h)$ into $h \to D(ghg^{-1})$. Then from Rel. (32) one easily finds

$$H \triangleleft G : \chi_G^{(\Delta)}(g) = \begin{cases} 0 & \text{when } g \notin H \\ \sum\limits_{\alpha' \in G.\gamma_H^{(\alpha)}} \chi_H^{(\alpha')}(g) & \end{cases} \tag{35}$$

where $G\cdot\gamma_H^{(\alpha)}$ is the G-orbit of $\gamma_H^{(\alpha)}$ in $\hat{H}$. In particular, when $H = 1 \triangleleft G$, we have the well known case of the regular representation

$$\chi^{(R)}(g) = |G|\ \delta_{1,g} \tag{36}$$

When G is Abelian, every subgroup is an invariant subgroup and G acts trivially on it

$$G \text{ abelian},\ \Delta = \mathrm{Ind}^G \gamma_H^{\prime\alpha\prime} \quad \chi^{(\Delta)}(g) = \begin{cases} 0 & \text{if } g \notin H \\ \dfrac{|G|}{|H|}\, \chi_H^{(\alpha)}(g) & \text{if } g \in H \end{cases} \tag{37}$$

Given a linear representation $g \to \Gamma(g)$ of G, its restriction to H (i.e. $g \in H$) yields a linear representation of H whose character is denoted by

$$\chi_H^{(\Gamma)} = \mathrm{Res}_H^G \, \chi_G^{(\Gamma)} \tag{38}$$

Let $\chi_G^{(\Gamma)}$ and $\chi_H^{(\alpha)}$ be the characters of linear representations of G and H respectively. From equation (32) one can compute the scalar product of the G-characters :

$$\langle \chi_G^{(\Gamma)}, \mathrm{Ind}_H^G \chi_H^{(\alpha)} \rangle_G = \frac{1}{|G||H|} \sum_{\substack{g \in G \\ s^{-1}gs \in H}} \chi_G^{(\Gamma)}(g^{-1}) \chi_H^{(\alpha)}(s^{-1}gs) =$$

$$= \frac{1}{|H|} \frac{1}{|G|} \sum_s \chi_G^{(\Gamma)}(sh^{-1}s^{-1}) \chi_H^{(\alpha)}(h)$$

(due to the change of variable $s^{-1}gs = h$) . Since $\chi_G^{(\Gamma)}(sh^{-1}s^{-1}) = \chi_G^{(\Gamma)}(h^{-1})$ we obtain the Frobenius reciprocity relation :

$$\langle \chi_G^{(\Gamma)}, \mathrm{Ind}_H^G \chi_H^{(\alpha)} \rangle_G = \langle \mathrm{Res}_H^G \, \chi_G^{(\Gamma)}, \chi_H^{(\alpha)} \rangle_H \tag{39}$$

We denote K_G the Hilbert space of unitary central functions ξ on G i.e. $\xi(g_1 g_2) = \xi(g_2 g_1)$ so $\xi(g_1 g_2 g_1^{-1}) = \xi(g_2)$ and $\overline{\xi}(g) = \xi(g^{-1})$ with the scalar product $\langle \xi, \eta \rangle_G = \frac{1}{|G|} \sum_g \xi(g^{-1}) \eta(g)$, it is well known that the characters of the irreducible representations form an orthonormal basis of K_G ; so when $\chi_H^{(\alpha)}$ and $\chi_G^{(\Gamma)}$ are characters of irreducible representations equation (39) reads : The multiplicity of the unirep $\gamma_G^{(\Gamma)}$ in $\mathrm{Ind}_H^G \, \gamma_H^{(\alpha)}$ is equal to the multiplicity of $\gamma_H^{(\alpha)}$ in $\mathrm{Res}_H^G \, \gamma_G^{(\Gamma)}$.

As an application we prove Lemma 1 which will be useful for us later.

Lemma 1. If $\gamma_H^{(\alpha)}$ is a unirep of H of dimension d, $\mathrm{Ind}_H^G \, \gamma_H^{(\alpha)}$ is a direct sum of G unireps of dimension $\geq d$.

Indeed, if $d' = \dim \gamma_G^{(\rho)}$ (a G-unirep) is smaller than d, the decomposition of $\mathrm{Res}_H^G \gamma_G^{(\rho)}$ into a direct sum of H unireps does not contain those of dimension $> d'$ so $\langle \mathrm{Res}_H^G \chi_G^{(\rho)}, \chi_H^{(\alpha)} \rangle_H = 0$ and the Frobenius reciprocity proves the lemma (χ is the character of the representation γ).

Another way to interpret (39) is to state the

Frobenius reciprocity theorem : The linear operators $K_H \xrightarrow{\mathrm{Ind}_H^G} K_G$ and $K_G \xrightarrow{\mathrm{Res}_H^G} K_H$ are adjoint of each other :

$$(\mathrm{Ind}_H^G)^\dagger = \mathrm{Res}_H^G \quad , \quad \mathrm{Ind}_H^G = (\mathrm{Res}_H^G)^\dagger \tag{40}$$

This relation will be very useful for computing the tables of induced representations (See Table 5). All equations established for finite groups can be extended to compact groups if $\frac{1}{|G|} \sum_g$ is replaced by the Haar integral and, when they have a meaning, to discrete groups, e.g. the space groups. Obviously $\mathrm{Res}_H^{G_k} \ldots \mathrm{Res}_{G_2}^{G_1} \mathrm{Res}_{G_1}^{G} = \mathrm{Res}_H^G$. Taking the adjoint we have the chain induction theorem

$$H < G_k < \cdots < G_2 < G_1 < G : \mathrm{Ind}_H^G \gamma_H^{(\alpha)} = \mathrm{Ind}_{G_1}^G \; \mathrm{Ind}_{G_2}^{G_1} \ldots \mathrm{Ind}_H^{G_k} (\gamma_H^{(\alpha)}) \tag{41}$$

When a group G has an Abelian invariant subgroup $A \triangleleft G$ (e.g. space group, A is the translation subgroup), there is a systematic method for constructing the unireps of G. We have already defined $\hat{G}$, the dual of G, i.e. the set of equivalent classes of unireps of G. For an Abelian group $\hat{A}$ is itself a group and $\hat{\hat{A}} = A$. For example $\hat{Z} = U(1)$ the group of complex phases, since for any k, $n \to e^{ikn}$ ($k \bmod 2\pi$) is a unirep of Z (the additive group of integers). Similarly, for the translation group $T \sim Z^3$ of a space group $\hat{T} \sim U(1)^3$ has the structure of a 3 dimensional torus of coordinates k_i, $i = 1,2,3$, $0 \leq k_i < 1$ (i.e. k defined mod 1) in a basis where the translations $t \in T$ have integer coordinates; the vector $k(k_1,k_2,k_3)$ defines the representation

$$t \to \exp(ik.t) = \exp(i \sum_j k_j n_j) \qquad (42)$$

The torus of $\vec{k}$ is the Brillouin zone, but too often its group structure is neglected.

For a general Abelian group A we denote by k an element of $\hat{A}$. If $A \triangleleft G$, as we have seen G acts on $\hat{A}$. Let $k \in \hat{A}$ and G_k its isotropy group. One can choose a unirep $\gamma^{(\alpha)}_{G_k}$ of G_k and form the induced representation $\mathrm{Ind}^G_{G_k} \gamma^{(\alpha)}_{G_k}$. One proves that this G-representation is irreducible and moreover that for space groups and all physical symmetry groups mentioned in the Introduction (e.g. point groups) one so obtains irreducible representations of G. For any $\vec{k}$ of the Brillouin zone of the space group G, G_k is itself a space group, usually called the "little space group"; it contains the translation subgroup T of G, since T acts trivially on its dual and $P_k = G_k/T$ is called the "little point group" of k. The unireps of G_k can all be computed by induction, if necessary, and so on. Since $\hat{T}$ contains only one-dimensional unireps of T and since T has a finite index in G_k which by itself has a finite index $\left|\frac{G}{G_k}\right|$ in G, so $\dim(\mathrm{Ind}^G_{G_k}(\gamma^{(\alpha)}_{G_k}))$ is finite and one shows that it is a divisor of $|P|$ (so, in three dimensions, it is a divisor of 48). Hence, equation (39), Frobenius reciprocity, applies to space groups.

We recall here a theorem of Mackey [10] on induced representations which also can be extended to space groups. Let H and K be two subgroups of G; the set of elements HxK is called the double coset of x. Note that $x \in HxK$; if $y \in HxK$ i.e. $y = hxk$, $h \in H$, $k \in K$, $x = h^{-1}yk^{-1}$ so $x \in HyK$; finally $y = hxk$, $z = h'yk' \to z = k'hxkk'$, so to be in the same double coset is an equivalence relation and G is a disjoint union

$$G = \bigcup_{s\in[H:G:K]} HsK \tag{43}$$

where $[H:G:K]$ is the set of double cosets. We denote $K_s = sKs^{-1} \cap H$.
Then Mackey has proven

$$\mathrm{Res}_H^G \, \mathrm{Ind}_K^G \, \gamma_K^{(\alpha)} = \bigoplus_{s\in[H:G:K]} \mathrm{Ind}_{K_s}^H \, \mathrm{Res}_{s^{-1}K_s s}^K \, \gamma_K^{(\alpha)} \tag{44}$$

Remark that $K_s < H$ and $s^{-1}K_s s = K \cap s^{-1}Hs \leq K$. As an application let us compute the multiplicity of the irreducible representation of $\gamma_H^{(\rho)}$ in the above representation defined in (44) :

$$\langle \mathrm{Res}_H^G \, \mathrm{Ind}_K^G \, \gamma_K^{(\alpha)} | \gamma_H^{(\rho)} \rangle_H = \sum_s \langle \mathrm{Ind}_{K_s}^H \, \mathrm{Res}_{s^{-1}K_s s}^K \, \gamma_K^{(\alpha)} | \gamma_H^{(\rho)} \rangle_{K_s} =$$

$$= \sum_s \langle \mathrm{Res}_{s^{-1}K_s s}^K \, \gamma_K^{(\alpha)} | \mathrm{Res}_{K_s}^H \, \gamma_H^{(\rho)} \rangle_{K_s} = \sum_s \frac{1}{|K_s|} \sum_{g\in K_s} \bar{\chi}_K^{(\alpha)}(s^{-1}gs)\chi_H^{(\rho)}(g) \tag{45}$$

We can apply these relations to the crystallographic group G , with $H = G_k$ and $K = G_x = P_q$. For instance when $\vec{k} = 0$, $H = G_k = G$ so $s = 1$, $K_s = P_q$; moreover the translations are represented trivially so $\gamma_G^\alpha \equiv \gamma_P^\alpha$. Equation (45) reads for this case

$$\langle \mathrm{Res}_{P_q}^G \, \gamma_G^{(\alpha)} \mid \gamma_{P_q}^{(\rho)} \rangle_{P_q} = \langle \mathrm{Res}_{P_q}^P \, \gamma_P^{(\alpha)} | \gamma_{P_q}^{(\alpha)} \rangle_{P_q} = \frac{1}{|P_q|} \sum_{g\in P_q} \bar{\chi}_P^{(\alpha)}(g)\chi_{P_q}^{(\rho)}(g) \tag{46}$$

A necessary condition of the equivalence of the band representations $\mathrm{Ind}_{G_x}^G \gamma_{P_q}^{(\rho)}$ and $\mathrm{Ind}_{G'_x}^G \gamma_{P'_q}^{(\rho')}$ is $\mathrm{Ind}_{P_q}^P \gamma_{P_q}^{(\rho)} \sim \mathrm{Ind}_{P'_q}^P \gamma_{P_q}^{(\rho')}$.

Obviously the operator Ind_H^G commutes with $\oplus$, i.e. direct sums and tensor products of representations

$$\mathrm{Ind}_H^G(\gamma_H^{(\alpha)} \oplus \gamma_H^{(\beta)}) = \mathrm{Ind}_H^G \gamma_H^{(\alpha)} \oplus \mathrm{Ind}_H^G \gamma_H^{(\beta)} \tag{47}$$

$$\mathrm{Ind}_H^G \gamma_H^{(\alpha)} \otimes \gamma_H^{(\beta)} = \mathrm{Ind}_H^G \gamma_H^{(\alpha)} \otimes \mathrm{Ind}_H^G \gamma_H^{(\beta)} \tag{48}$$

As we pointed out in the Introduction, for many groups in physics, every irreducible representation is an induced representation so every representation is a direct sum of induced representations. A physically more relevant decomposition of an induced representation is into a direct sum of induced representations from the same subgroup. As the relation of chain induction (41) shows a given induced representation can be considered as induced from different representations of different (i.e. non-conjugate) subgroups. It may also happen that some of these subgroups do not form an increasing chain of subgroups (or more precisely, in the partially ordered set K of conjugacy classes of subgroups). We are led to the concept of irreducible-induced G-representations. (The hyphen is essential and avoids confusion with a representation which is both irreducible and induced). By definition, such a representation is not equivalent to an induced representation of G from a reducible representation of a subgroup.

Lemma 2. Irreducible-induced representations are induced representations from irreducible representations of maximal subgroups.

This is obvious; if $H < M < G$, M maximal (strict) subgroup of G and $\gamma_H^{(\alpha)}$ is an irreducible representation of H . By (41) $\mathrm{Ind}_H^G \gamma_H^{(\alpha)} = \mathrm{Ind}_M^G (\mathrm{Ind}_H^M \gamma_H^{(\alpha)})$ and for $\mathrm{Ind}_H^G \gamma_H^{(\alpha)}$ to be irreducible-induced it is required that $\mathrm{Ind}_H^M \gamma_H^{(\alpha)}$ be irreducible.

This lemma 2 gives a necessary condition for irreducible-induced representations which is far from sufficient. As we shall see, an induced representation from an irreducible representation of a maximal subgroup may be equivalent to an induced representation from a reducible representation of another maximal subgroup.

It is easy to give a strong sufficient condition. We recall that when $H < G$, the number of H cosets is called the index of H in G . For finite groups the index of H in G is $|G|/|H|$.

Lemma 3. If $H < G$ with prime index p then for any one-dimensional representation $\gamma_H^{(\alpha)}$ of H, $\mathrm{Ind}_H^G \gamma_H^{(\alpha)}$ is an irreducible-induced representation.

Note that H is a maximal subgroup : indeed if there were M, $H < M < G$ the index of H in M and the index of M in G would both divide p. Similarly, as given in Eq. (31) the dimension of an induced representation is the product (Index of H) $\times$ (dim of H-representation), so $\mathrm{Ind}_H^G \gamma_H^{(\alpha)}$ can be equivalent only to an induced representation from a one-dimensional one of a subgroup of index p. For a finite Abelian group, we have a complete classification.

Theorem 1. The inequivalent irreducible-induced representations of a finite Abelian group A are all the induced representations from one-dimensional representations of maximal subgroups. By lemma 2, this is a necessary conditon. From equation (37) we see that such an induced representation defines uniquely the inducing subgroup and representation.

III. Induced representations of point groups.

Let us start this section by describing some general properties of irreducible representations of point groups. Mathematicians have proven that the unireps of supersolvable groups are monomial, i.e. they are either one-dimensional or induced from one-dimensional representations of subgroups [10]. For such monomial representations there exists a basis in the carrier space such that all matrices of the unireps have all elements vanishing except one in each line and column which is equal to a phase. A group is supersolvable if it contains a chain of k subgroups satisfying (again, $\lhd$ reads invariant subgroups) :

$$\text{a)}\ \ 1 = G_k \quad \text{b)}\ G_o = G \ \text{ for all } \ i,\ k \leq i \leq 1 \quad \text{c)}\ G_i \lhd G \quad \text{d)}\ G_{i-1}/G_i \ \text{ is cyclic} \tag{49}$$

Note that when c) is replaced by the weaker condition c') $G_i \lhd G_{i-1}$, G is solvable. The point groups in 2 dimensions are supersolvable : there are 10 of them. Among the 32 point groups in 3 dimensions, only the five cubic groups are not supersolvable; but they are solvable. Indeed the 32 geometric classes are defined as conjugation classes of subgroups in O(3) , but they define only 18 group-isomorphic classes; 9 of them are Abelian; five others are supersolvable.

$$\left.\begin{array}{lll} C_{3v} \sim D_3\ ,\ C_{4v} \sim D_4 \sim D_{2d}\ ,\ C_{6v} \sim D_6 \sim D_{3d} \sim D_{3h} & 1 \lhd C_n \lhd D_n & D_n/C_n \sim Z_2 \\ D_{4h}\ ,\ D_{6h} \qquad 1 \lhd C_n \lhd D_n \lhd D_{nh} & D_{nh}/D_n \sim Z_2\ . & \end{array}\right\} \tag{50}$$

The 5 cubic groups form 4 isomorphic classes T , T_h , $T_d \sim O$, O_h of solvable groups :

$$1 \lhd C_2 \lhd D_2 \lhd T \lhd O \lhd O_h \qquad \frac{D_2}{C_2} \sim \frac{O}{T} \sim \frac{O_h}{O} \sim Z_2\ \frac{T}{D_2} \sim Z_3 \tag{51}$$

but C_2 is not an invariant subgroup of T ! However, all unireps of the cubic point groups are monomial : indeed the 2 and 3 dimensional ones are both orthogonal and with integer elements.

We remark that the ten point groups in 2 dimensions are isomorphic to point groups in 3 dimensions. In dimension > 3 many point groups are still supersolvable or solvable, but not all. For example, the symmetry groups of the icosahedron is a 4-dimensional point group and is not solvable.

As an introduction to band representations of space groups (Sections IV-VI) we discuss in this section induced representations of crystallographic point groups (in what follows they will be called point groups). The latter are finite order groups and it is easy to demonstrate on them different concepts connected with induced representations. In addition, as will be shown later, there is a close relation between band representations of space groups and induced representations of point groups. The subject will be considered both for abstract point groups and for their action on the physical $\vec{r}$-space. When considered abstractly, any representation of the subgroup H of G can be used in constructing induced representations according to the formulas of the previous section. However, a more restrictive type of induced representations is obtained by considering the action of the point group G on the space $\vec{r}$, and by dealing with functions $\psi(\vec{r})$.

For abstract point groups one starts with a representation $\gamma_H^{(\alpha)}$ of H and by using Formula (32) one finds the character of the induced representation $\mathrm{Ind}_H^G(\gamma_H^{(\alpha)})$. It is convenient to give the contents of the latter by listing the irreducible representations of G it contains. For this purpose the Frobenius reciprocity theorem (40) is of much use. By using this theorem we have constructed Tables 5 of all induced representations of point groups (See Ref. (15) for notations). Reference to these tables is given in Section VI where they are extensively used in establishing the equivalency (or inequivalency) of band representations.

In the case of the action of the point group G on the space $\vec{r}$ it is instructive to distinguish between two kinds of induced representations. One of them refers to any subgroup H of G while the other one is when H is a little group in $\vec{r}$-space. In analogy with space groups we shall call the latter band representations of point groups. These induced representations should play the same role for molecules [3] as band representations of space groups play for solids. As a rule, not all subgroups of a given point group are little groups in $\vec{r}$-space and, correspondingly, one can talk about induced representations, in general, and about band representations, in particular.

In the framework of assigning induced representations to sets of energy levels of a physical system it is of interest to deal with irreducible-induced representations. The latter were already defined in Section II as induced representations which cannot be written as a direct sum of induced representations from the same subgroup. The restriction to the same subgroup is essential and it is added keeping in mind the possible application to band representations. Thus, an irreducible-band representation (of a point group or space group) cannot be written as a sum of band representations for a single isotropy group. As already mentioned before, to avoid confusion the words irreducible and induced (or irreducible and band) are connected by a hyphen because an irreducible-induced representation might be reducible despite of the fact that it cannot be reduced into induced representations. On the other hand, a reducible-induced representation is always reducible. In a similar way one talks about irreducible-band representations. They are the ones that cannot be written as direct sums of band representations. Being induced from an isotropy group of a symmetry center the basis functions of a band representation should be expected to correspond to some set of energy levels that belong to a well defined part of the energy spectrum. Correspondingly, an irreducible-band representation should correspond to a minimal set of such energy levels. Thus, in a solid there is a correspondence between an irreducible-band representation and a band of energy labels. In general, irreducible-induced representations should play the same rôle in the framework of induced representations as the irreducible representations of a group play in the framework of representations.

In order to demonstrate the difference between induced representations and band representations of point groups let us consider the construction of all irreducible-induced representations of the point group T_d. The maximal subgroups of this group are T, D_{2d} and C_{3v}. In Table 6 we list all the induced representations of Td from its maximal subgroups. The notations of the irreducible representations of point groups are taken from Ref. 15. In the column on the very right of Table 6 the irreducible-induced representations of T_d are listed. It is seen that the latter (8 in number) are all induced from one-dimensional representations of the maximal subgroups of T_d (this is in accordance with Theorem 2 which is given below). It is also instructive to consider the irreducible-band representations of T_d. They are induced from maximal isotropy groups of T_d, which are C_{3v} and C_{2v}. In Table 7 we list the band representation of T_d. All of them are irreducible-band representations, e.g. they cannot be reduced into band representations. There is therefore a difference between induced representations from maximal subgroups and band representations which are induced from maximal isotropy subgroups. While for the latter only irreducible band representations are obtained, in the former case we have also reducible-induced representations when inducing from maximal subgroups. It turns out that the feature of having only irreducible-band representations when inducing from maximal isotropy groups holds with very few exceptions for all crystallographic point groups in 3 dimensions. This feature is of much importance for space groups because for the latter all maximal finite order subgroups are isotropy groups (See Section II A).

In what follows we give a classification of all irreducible-induced representations of point groups. Among them we shall also obtain the irreducible representations. From Theorem 1, we know the results for Abelian point groups. We shall prove that we can extend it to all 2 or 3 dimensional point groups, but some of the obtained representations might be equivalent.

Theorem 2. The irreducible-induced representations of 2 or 3 dimensional point groups are induced representations from one dimensional representations of maximal subgroups. We know it for Abelian groups. Outside the five cubic groups, the non-Abelian point groups have irreducible representations of dimension 1 or 2. (We shall refer to it as property I_a). Moreover, each such point group P has an Abelian maximal subgroup A of index 2. Indeed $P \leq D_{nh}$ with $n = 3,4$ or 6 . Define $A_P = P \cap C_{nh}$ (since $D_{nh}/C_{nh} = Z_2$, $P/A_P = Z_2$) . Let $\gamma_P^{(\alpha)}$ be a two-dimensional irreducible representation of P . $\mathrm{Res}_A^P \gamma_P^{(\alpha)} = \gamma_A^{(\alpha_1)} + \gamma_A^{(\alpha_2)}$ and by Frobenius reciprocity $\mathrm{Ind}_A^P \gamma_A^{(\alpha_1)} = \mathrm{Ind}_A^P \gamma_A^{(\alpha_2)} = \gamma_P^{(\alpha)}$. So every 2-dimensional representation of P is induced from a one-dimensional representation of A . Let M be a maximal subgroup of P and $\gamma_M^{(\rho)}$ a 2-dimensional irreducible M-representation. From property I_a and Lemma 1, $\mathrm{Ind}_M^P \gamma_M^{(\rho)}$ is a direct sum of $\frac{|P|}{|M|}$ 2-dimensional irreducible representations of P and therefore it is the induction from A to P of the direct sum of $|P|/|M|$ one-dimensional representations of A .

II. We now use the following properties of the Cubic groups.

II_a the dimension of their irreducible representations is ≤ 3 .

II_b their order is 3×2^k $(k = 2,3,4)$.

Let C be a cubic group; all subgroups S of index 3 are Sylow groups [10] of C and therefore all conjugate. Hence all 3-dimensional irreducible representations of C are induced from 1-dimensional representations. If $\gamma_H^{(a)}$ is a 3-dimensional irreducible representation of $H < C$, by II_a and Lemma 1, $\mathrm{Ind}_H^C \gamma_H^{(a)}$ is a direct sum of 3-dimensional irreducible representations of C and it is therefore an induced representation from a direct sum of representations of H .

II_c Only the groups O_h and $O \sim T_d$ have maximal subgroups with two-dimensional irreducible representations. For the other, induction from a 2-dimensional representation of a subgroups leads (from Lemma 1) to a direct sum of 3-dimensional representations. As we have just seen, this is a reducible-induced representation equivalent to an induction from the Sylow group S of a direct sum of one-dimensional representations.

II_d The 2-dimensional representations of the cubic groups have a kernel D_2 or D_{2h}. Induction from an index 2 cubic subgroup can lead only (Lemma 1) to a direct sum of representations of dim 2 or 3. The latter are excluded because their kernel is too small (trivial or generated by the space inversion). A direct sum of 2-dimensional representations are reducible into monomial representations in T_h or T (the only index 2 subgroup) for O_h or T_d. On the other hand, the 2-dimensional representations of the index 3 subgroups of these groups have as kernel $\{I\}$ or $\{I,-I\}$. So the 6-dimensional induced representation in a cubic group cannot be the direct sum of three 2-dimensional irreducible representations of the cubic group. They have to be the direct sum of 2 or 3-dimensional representations. Then the argument after II_b applies.

We are left to study the induction from the 2-dimensional representations of index 4 maximal subgroups of cubic groups: D_{3d} for O_h, $D_3 \sim C_{3v}$ for $O \sim T_d$. We simply verify the reducibility.

Of course, "Theorem 2" applies only to a finite number of groups and representations. It can, however, be simply verified for all the others.

The problem left is that of equivalence of irreducible-induced representations. The proof of Theorem 2 gives a class of equivalence : The 2-dimensional irreducible representations are induced from 2 non-equivalent one-dimensional representations of an Abelian subgroup. So these representations induce the same irreducible-induced (it is irreducible in the usual meaning) representation. This is also true for 3-dimensional irreducible representations induced from an Abelian group. (Those of T_h from D_{2h}). It was essential in the proof of Theorem 2 to use the fact that multidimensional irreducible representations of a given dimension are induced from a unique subgroup (the index 2 maximal Abelian subgroups A_p ; The Sylow group S or T_h or T for Cubic groups). This explains why there are very few equivalent irreducible-induced representations induced from different maximal subgroups and where to look for exceptions : In (non Abelian) non-cubic groups which have non conjugate Abelian subgroups of index 2; those groups are D_{4h} , $D_4 \sim C_{4v} \sim D_{2d}$. For Abelian groups we have proven the inequivalence of all induced representations from unireps of maximal subgroups.

In conclusion of this Section we summarize the inequivalent irreducible-induced representations of crystallographic point groups in 3 dimensions by giving their statistics side by side with the numbers of the corresponding irreducible representations. This information is presented in Table 8.

IV. Band Representations of Space Groups.

The space group G acts on a $\psi(\vec{r})$ in the following way

$$(\alpha|\vec{t})\psi(\vec{r}) = \psi((\alpha|t)^{-1}\vec{r}) \tag{52}$$

When the $\psi(\vec{r})$ are square integrable functions, Rel. (52) defines a linear action of G on the Hilbert space $L^2(R^3)$. A band representation is obtained by acting with G on a square integrable function $\psi(\vec{r})$ [4]. Like an orbit for the action of G on the space R^3 (Rel. (1)) one can also define an orbit $G(\psi)$ for the action of G on $\psi(\vec{r})$ (Rel.(52)). This orbit, $G(\psi)$, spans a G-invariant subspace of $L^2(R^3)$. It carries the band representation $G(\psi)$. Such a representation is called an induced representation of G . More explicitly, a band representation is defined as an induced representation of G in the following way : it is an induced representation of G from a representation of a finite isotropy subgroup H of G . Thus in Table 4, T_d is a finite subgroup of O_h^7 and it is a little group of the symmetry center $\vec{r}_a = (000)$. In the language of bases, the induction process for a band representation of a space group is described as follows. Let $\psi_j^{(w,\rho)}(\vec{r})$, $j = 1,2,\ldots,p$ be the basis functions for a representation $\gamma^{(\rho)}$ of G_w (Since $\vec{r}$ appears now in the wave function, we denote by $\vec{w}$ the symmetry center)

$$\gamma^{(w)}\psi_j^{(w,\rho)}(\vec{r}) = \sum_{j'=1}^{p} D_{j'j}^{(\rho)}(\gamma)\psi_{j}^{(w,\rho)}(\vec{r}) \tag{53}$$

where $\gamma^{(w)}$ are the elements of G_w with respect to the symmetry center $\vec{w}$. By using Rel. (14) one can rewrite Rel. (53) with respect to the common origin O.

$$(\gamma_m|\vec{v}(\gamma_m))\psi_j^{(w,\rho)}(\vec{r}) = \sum_{j'=1}^{p} D_{j'j}^{(\rho)}(\gamma)\psi_{j'}^{(w,\rho)}(\vec{r}-\vec{R}^{(\gamma_m|\vec{v}(\gamma_m))}) \tag{54}$$

A band representation is the induced representation $\mathrm{Ind}_{G_w}^{G}(\gamma^{(\rho)})$. The basis of this induced representation is

$$\psi_j^{(w_1,\rho)}(\vec{r}) \equiv \psi_j^{(w,\rho)}(\vec{r}) \ , \quad \psi_j^{(w_2,\rho)}(\vec{r}) = (\alpha_2|\vec{v}(\alpha_2))\psi_j^{(w,\rho)}(\vec{r}),\ldots,$$

$$\psi_j^{(w_m,\rho)}(\vec{r}) = (\alpha_m|\vec{v}(\alpha_m))\psi_j^{(w,\rho)}(\vec{r}) \tag{55}$$

plus all those functions that are obtained by applying to (55) all the translations of T . In Rel. (55) $(\alpha_s|\vec{v}(\alpha_s))$ are the representative elements in the decomposition of G with respect to $G_q = G_w \cdot T$ in Rel. (13).

The concept of a closed stratum aquires much importance in the framework of irreducible-band representations [16]. Thus, it will be shown in Section VI that band representations induced from irreducible representations of maximal isotropy groups (which are little groups of closed strata) are as a rule irreducible-band representations. There are relatively few exceptions of this rule. It might, however, happen that some irreducible-band representations induced in such a way will turn out to be equivalent. This question is discussed in detail in Section VI. If one looks for irreducible-band representations only then it is sufficient to consider induction from isotropy groups for closed strata. This follows from Lemma 2 of Section IIB. Qualitatively, the reason for this is that any little group $G_{w'}$ of an open stratum is, by definition, a subgroup of a little group G_w of a closed stratum. This means that an open stratum does not add any irreducible-band representations that cannot be obtained from a closed stratum. In looking for irreducible-band representations it is therefore sufficient to consider only closed strata. Thus, for the diamond structure space group O_h^7 one has to consider only the four closed strata in Table 4 when constructing its irreducible-band representations.

From the point of view of the band structure of a solid irreducible-band representations correspond to energy bands of minimal possible degeneracy. In this sense the irreducible-band representations form the building bricks for any band representations and correspondingly for any composite energy bands. The reduction of a band representation into irreducible-band representations is therefore of much importance in the physical structure of composite energy bands. From here we have also the importance of closed strata since the symmetry centers of the latter are the only relevant centers [4] in the construction of the irreducible-band representations.

V. Reduction of Band Representations.

Any band representation is infinite-dimensional and therefore reducible. It can be reduced into finite-dimensional representations of G (in general, still reducible ones) by forming the following Bloch sums, or the quasi-Bloch functions [3,12] , from the basis function in (55). (We replace $\vec{w}$ by $\vec{q}$ since we use star-vectors in a single Wigner-Seitz cell. See Rel. (12)).

$$\psi_{jk}^{(q_s,\rho)}(\vec{r}) = \sum_{\vec{R}_n} \exp(i\vec{k}.\vec{R}_n)\psi_j^{(q_s,\rho)}(\vec{r}-\vec{R}_n) \quad , \tag{56}$$

where $s = 1,2,\ldots,m$ labels the vectors in the star, and $j = 1,2,\ldots,p$ labels the functions in the representation $\gamma^{(\rho)}$. It is easy to check that the quasi-Bloch functions(56) form bases for finite-dimensional representations of G . What is, however, more interesting is that the $p \times m$ quasi-Bloch functions in (56) for a fixed k form a basis for a representation of G_k , in general, a reducible one. Indeed, let $(\beta|\vec{v}(\beta))$ be an element of G_k . For any element of G one can write [11]

$$(\beta|\vec{v}(\beta))(\alpha_m|\vec{v}(\alpha_m)) = (\alpha_n|\vec{v}(\alpha_n))(\gamma|\vec{v}(\gamma)) \tag{57}$$

where the elements $(\alpha_s|\vec{v}(\alpha_s))$ appear in the decomposition (13) and $(\gamma|\vec{v}(\gamma))$ is an element of G_w up to a Bravais lattice vector. By using Rels. (54), (56) and (57) and the fact that $\beta\vec{k} = \vec{k}$ up to a vector of the reciprocal lattice, we find

$$(\beta|\vec{v}(\beta))\psi_{jk}^{(q_m,\rho)}(\vec{r}) = \exp(-i\vec{k}\cdot\alpha_n\vec{R}_q^{(\gamma|\vec{v}(\gamma))})\sum_{j'=1}^{p} D_{j'j}^{(\rho)}(\gamma)\psi_{j'k}^{(q_n,\rho)}(\vec{r}) \tag{58}$$

Rel. (58) defines a $pm \times pm$ matrix connecting Bloch-like functions for the vector $\vec{k}$. This means that the pm functions $\psi_{jk}^{(q_s,\rho)}$. (Rel. (56)) form a basis for a pm-dimensional representation of G_k . It is convenient to look at the matrix in Rel. (58) as consisting of block matrices of dimension p. Thus the only non-vanishing block-matrix in the m-th column is in the n-th row and it equals $\exp(-i\vec{k}\cdot\alpha_n\vec{R}_q^{(\gamma|\vec{v}(\gamma))})\, D^{(\rho)}(\gamma)$, where γ is determined by Rel. (57). The representation of G_k as defined by Rel. (58) will be denoted by $D^{(q^*,\rho)}(k)$ and called the k-component of the band representation (q^*,ρ). The result we have is that by forming linear combinations (Rel. (56)) of the basis functions $\psi_j^{(q_s,\rho)}(\vec{r})$ for the band representation (q^*,ρ), the latter reduces into finite-dimensional representations of G_k. The difference between the quasi-Bloch functions $\psi_{jk}^{(q_s,\rho)}(\vec{r})$ in Rel. (56) and the Bloch functions $\psi_{nk}(\vec{r})$ is that the latter are also eigenfunctions of the Hamiltonian. Correspondingly, $\psi_{nk}(\vec{r})$ form bases for irreducible representations of G_k, while for the quasi-Bloch functions the representations of G_k are, in general, reducible ones.

It is easy to find the character $\chi_k^{(q^*,\rho)}$ of the k-component $D^{(q^*,\rho)}(\vec{k})$ in (58). The reason for this is that to the character $\chi_k^{(q^*,\rho)}$ only those block matrices contribute which are on the diagonal of $D^{(q^*,\rho)}(\vec{k})$. Thus, for finding the character $\chi^{(q^*,\rho)}(\beta|\vec{v}(\beta))$ of the element $(\beta|\vec{v}(\beta))$ in Rel. (58) we have to check for which $(\alpha_r|\vec{v}(\alpha_r))$ Rel. (57) becomes

$$(\beta|\vec{v}(\beta))(\alpha_r|\vec{v}(\alpha_r)) = (\alpha_r|\vec{v}(\alpha_r))(\gamma|\vec{v}(\gamma)) \tag{59}$$

When Rel. (59) holds the representation (58) can be rewritten

$$(\beta|\vec{v}(\beta))\psi_{jk}^{(q_r,\rho)}(\vec{r}) = \exp(-i\vec{k}\cdot\vec{R}_{q_r}^{(\beta|\vec{v}(\beta))})\sum_{j'=1}^{p} D_{j'j}^{(\rho)}(\gamma)\psi_{jk}^{(q_r,\rho)}(\vec{r}) \tag{60}$$

From here the following formula can be obtained for the character $\chi_k^{(q^*,\rho)}$ of the k-component for a band representation $D^{(q^*,\rho)}$ (See Formula (32))

$$\chi_k^{(q^*,\rho)}[(\beta(\vec{v}(\beta))] = \sum_n \exp(-i\vec{k}\cdot\vec{R}_{q_n}^{(\beta(\vec{v}(\beta))})\, \chi^{(\rho)}(\alpha_n^{-1}\beta\,\alpha_n) \tag{61}$$

where the summation is over all those n for which $\alpha_n^{-1}\beta\alpha_n$ is a point group element of G_w. This is a very simple formula for calculating the character $\chi_k^{(q^*,\rho)}$. The only thing we have to know in addition to the character $\chi^{(\rho)}(\gamma)$ of the irreducible representation $\gamma^{(\rho)}$ of G_w are the phases $\exp(-i\vec{k}\cdot\vec{R}^{(\beta|\vec{v}(\beta))})$. The latter are easily found and, for example, in Ref. (5) they are listed for all the closed strata of O_h^7. We use this example and formula (61) for calculating the characters $\chi_k^{(q^*,\rho)}$ of the k-components $D_k^{(q^*,\rho)}$ of all the irreducible-band representations $D^{(q^*,\rho)}$ of the space group O_h^7. The results of this calculation are listed in Table 9.

The k-components $D_k^{(q^*,\rho)}$ of the band representations $D^{(q^*,\rho)}$ give a partial reduction of the latter. Having the character $\chi_k^{(q^*,\rho)}$ of the k-components of $D^{(q^*,\rho)}$ it is easy to carry out their complete reduction and to find the irreducible representations of G that are contained in $D^{(q^*,\rho)}$. In fact, the irreducible representations of G are themselves induced representations $\mathrm{Ind}_{G_k}^{G}(\gamma_\mu)$, where γ_μ is an irreducible representation of the little space group G_k for the point $\vec{k}$ in the Brillouin zone. Thus, the irreducible representations of G are labelled by the G-orbit in the Brillouin zone (or the $\vec{k}$-star) and an irreducible representation of G_k. The contents of the irreducible representations of G_k in the k-component of $D^{(q^*,\rho)}$ can be found according to the elementary formula in the algebra of characters. Given a band representation $D^{(q^*,\rho)}$, we first use formula (61) for finding the character $\chi_k^{(q^*,\rho)}$ of its k-component. Having $\chi_k^{(q^*,\rho)}$, we can then find how many times, $n_\mu^{(q^*,\rho)}(k)$, the irreducible representation γ_μ of G_k with the character $\chi^{(k,\mu)}$ is contained in the band representation $D^{(q^*,\rho)}$. This is given by the elementary formula from the algebra of characters [2] :

$$n_\mu^{(q^*,\rho)}(k) = \frac{1}{|g_k|} \sum_{(\beta|\vec{v}(\beta))} \chi_k^{(q^*,\rho)}(\beta|\vec{v}(\beta))\, \chi^{(k,\mu)*}(\beta|\vec{v}(\beta)) \qquad (62)$$

where $|g_k|$ is the order of $\frac{G_k}{T}$ and the summation is over the representative elements in the decomposition of G_k with respect to the translation group T

$$G_k = T + (\beta_2|\vec{v}(\beta_2))T + \ldots + (\beta_{g_k}|\vec{v}(\beta_{g_k}))T \tag{63}$$

Formula (62) gives the full reduction of the band representation $D^{(q^*,\rho)}$ into the irreducible representations of G_k . This is the relevant information in $D^{(q^*,\rho)}$ from the point of view of the symmetry of the energy band as a whole entity. By knowing how the band representation $D^{(q^*,\rho)}$ reduces into irreducible representations of G_k we know the symmetries of the Bloch functions for the particular band at different points in the Brillouin. These symmetries of all Bloch functions of an energy band form what is called the continuity chord of the band representation [5] . Thus, by means of formula (62) one can calculate the continuity chord of any band representation.

Since band representations are infinite-dimensional, no simple conventional criterion can be used for telling whether or not two band representations are equivalent. A possible way of doing this is by using the characters of their k-components. Thus, the characters of the k-components of two equivalent band representations are equal, and vice-versa, if they are equal, the band representations are equivalent. The character of the k-component, $\chi_k^{(q^*,\rho)}$, specifies therefore fully the band representation.

Having in mind that the character $\chi_k^{(q^*,\rho)}$ identifies the band representation, one should also be able to use it in the reduction process of a reducible band representation into irreducible-band representations. Thus, given a band representation, D , and its k-component character χ_k , one can immediately check whether D is a reducible band representation by comparing χ_k with the list of the characters $\chi_k^{(q^*,\rho)}$ of all the irreducible-band representations of the given space group. If χ_k equals to one of the $\chi_k^{(q^*,\rho)}$, then it belongs to an irreducible-band representation. Otherwise D is a reducible-band representation. For finding which of the $\chi_k^{(q^*,\rho)}$ are contained in χ_k (when the latter belongs to a reducible-band representation) one can simply use the elementary formula for characters in the reduction of representations (like Formula (62)). Next section deals in detail with the use of formula (61) for finding all inequivalent irreducible-band representations.

We have shown that a band representation is an induced representation from a finite order subgroup of the space group. As such it is an infinite-dimensional representation with a basis consisting of an infinite set of localized orbitals. We have also shown that by going to a basis of extended quasi-Bloch functions (Rel. (56)) the infinite-dimensional band representation reduces into a direct integral over $\vec{k}$ of finite-dimensional representations of the space group. This feature of going from infinite-dimensional matrices to finite-dimensional ones (of small dimension, in general) by utilizing eigenfunctions of the translation group (Bloch-like functions) is encountered in many problems in solid state physics. It is well known, that in solids one can alternately use either localized orbitals (Wannier function), or extended functions (Bloch functions). Let us show that a similar situation exists also for band representations and that the latter can be defined by employing directly quasi-Bloch functions. Like in the original definition, we start with an irreducible representation $\gamma^{(\rho)}$ of the isotropy group G_r of the Wyckoff position $\vec{r}$. (Since $\vec{r}$ appears in the wave function we shall use instead the notations G_w and $\vec{w}$). This representation and its basis function $\psi_j^{(w,\rho)}(\vec{r})$, $j = 1,2,\dots,p$ are given by Rels. (53) and (54). By using the decomposition $(G_q = T \cdot P)$

$$G = G_q + (\alpha_2|\vec{v}(\alpha_2))G_q + \dots + (\alpha_m|\vec{v}(\alpha_m))G_q \tag{64}$$

one can define the functions $\psi_j^{(w_s,\rho)}(\vec{r})$ for $j = 1,\dots,p$

and $s = 1,\ldots,m$ (See Rel. (55)). For those localized orbitals we define the quasi-Bloch functions $\psi_{jk}^{(q_s,\rho)}(\vec{r})$ (See Rel. (56)). We have here mp such functions. As was shown in Section V, these quasi-Bloch functions form a basis for a representation of G_k (See Rel. (58)). Clearly, this representation (of dimension mp) is, in general, a reducible representation of G_k. Having a representation of G_k one can employ the usual induction method for inducing a representation of the full space group. By going through this process for each $\vec{k}$ in the Brillouin zone we obtain a direct integral (over $\vec{k}$) of finite-dimensional representation of G. They together form the band representation of G for the fixed couple of indices (q,ρ). In other words, by fixing (q,ℓ) we define the set of mp Bloch functions (Rel. (56)). They form a basis of a representation of G_k. From this representation of G_k we induce a representation of G. This process has to be repeated for the continuum of k-vectors in the Brillouin zone. It reminds one very much of the application of translational symmetry in the solution of problems in solid state physics [18]. Instead of having to deal with an infinite-dimensional matrix for the Hamiltonian one obtains an infinite number of finite-dimensional matrices corresponding to different $\vec{k}$-vectors in the Brillouin zone.

The two following remarks are of interest. First, the two approaches to band representations (localized functions and extended functions) can be unified when using the kq-representation [4,5]. Given a wave function $\psi(\vec{r})$ in the $\vec{r}$-representation, its kq-representation $C(\vec{k},\vec{q})$ is

$$C(\vec{k},\vec{q}) = \Omega^{-1/2} \sum_n \exp(i\vec{k}\cdot\vec{R}_n)\psi(\vec{r}-\vec{R}_n) \tag{65}$$

where $\vec{k}$ and $\vec{q}$ are the quasi-momentum and the quasi-coordinate correspondingly, and Ω is the volume of a unit cell of the reciprocal lattice. The action of a space group element $(\alpha|\vec{v}(\alpha))$ on $C(\vec{k},\vec{q})$ is as follows [4]

$$(\alpha|\vec{v}(\alpha))\ C(\vec{k},\vec{q}) = C(\alpha^{-1}\vec{k},(\alpha|\vec{v}(\alpha))^{-1}\vec{q}) \qquad (66)$$

If we define the $C_j^{(w_s,\rho)}(\vec{k},\vec{q})$ functions for the localized orbitals $\psi_j^{(w_s,\rho)}(\vec{r})$ (Rel. (55)) then the following is clear : on one hand, the basis $C_j^{(w_s,\rho)}(\vec{k},\vec{q})$ leads to the original definition of a band representation via the induction from the finite order group G_w ; on the other hand, for elements $(\beta|\vec{v}(\beta))$ of G_k the functions $C_j^{(w_s,\rho)}(\vec{k},\vec{q})$ transform exactly like Bloch functions for a given $\vec{k}$ (this follows from Rel. (66); one should also pay attention to the fact that under a pure translation $(E|\vec{R}_m)$ any $C(\vec{k},\vec{q})$ goes into $\exp(-i\vec{k}\cdot\vec{R}_m)\ C(\vec{k},\vec{q}))$. We see therefore, that the kq-functions unify the two alternative approaches to band representations.

The other remark relates to the construction of irreducible representations of G_k . In the quasi-Bloch functions approach to the band representations we have shown that the set of mp functions (Rel. (56)) form a basis of a representation of G_k . In general, this representation is reducible. However, there are many cases where we obtain irreducible representations of G_k . This is of particular interest when one deals with non-symmorphic space groups. Because then this construction can serve as a method for finding irreducible representations of non-symmorphic G_k .

VI. Irreducible-Band Representations of Space Groups in 3 Dimensions

In this section we consider the problem of finding all inequivalent irreducible-band representations of space groups in 3 dimensions. As was shown in the previous section the contents of a band representation, or its continuity chord [5] , is fully defined by the character χ_k of its k-component (Formula 61). In particular, this means that two band representations (q,ρ) and (q',ρ') (In what follows we shall use q in the Wigner-Seitz cell instead of $\vec{r}$ for denoting representations and bases) are equivalent if their k-component characters are equal :

$$\chi_k^{(q,\rho)}(\beta|\vec{v}(\beta)) = \chi_k^{(q',\rho')}(\beta|\vec{v}(\beta)) \tag{67}$$

for all elements $(\beta|\vec{v}(\beta))$ $(\beta\vec{k} = \vec{k}$ up to a vector of the reciprocal lattice) of the space group and all vectors $\vec{k}$ in the Brillouin zone. On the other hand, if Rel. (67) does not hold (for this it is sufficient for it not to hold even at one point $\vec{k}$ in the Brillouin zone) then the two band representations (q,ρ) and (q',ρ') are inequivalent. This fact will extensively be used in verifying the inequivalency of band representations. It was already pointed out that for finding the irreducible-band representations of a space group it is sufficient to consider the induction from irreducible representations of maximal isotropy groups only. However, two things might happen. First, some of the band representations induced in such a way might turn out to be reducible-band representations [17]. Second, among the irreducible-band representations induced from irreducible representations of maximal isotropy groups some might be equivalent. In order to find all the inequivalent irreducible-band representations of a space group the following procedure will be used : We construct all the band representations for all the closed strata and we exclude the above-mentioned two kinds : 1) the reducible-band representations and 2) the equivalent ones. It turns out that there are relatively few band representations that are induced from maximal isotropy groups and that belong to these two kinds of band representations. In what follows we shall call them the exceptional ones. Since relatively few are exceptional it is not hard to tabulate them. Knowing this list and knowing that all irreducible-band representations are induced from irreducible representations of maximal isotropy groups one can deduce the full list of all the inequivalent irreducible-band representations.

To find the list of all exceptional band representations doesn't seem to be a simple matter. In what follows we shall give some arguments and some observations which when put together lead to the following criterion :

Let (q,ρ) be a band representation induced from an irreducible representation $\gamma^{(\rho)}$ of a maximal isotropy subgroup G_r . A sufficient and necessary condition for another band representation $D^{(q')}$ (the latter can also be a reducible-band representation) induced from a representation γ' of a non-conjugate maximal isotropy group $G_{r'}$ to be equivalent to (q,ρ) is for a subgroup $G_{r''} = G_r \cap G_{r'}$ ($G_r \cap G_{r'}$ is the intersection of G_r and $G_{r'}$) to exist such that both $\gamma^{(\rho)}$ and γ' are induced representations from a representation γ'' of $G_{r''}$.

Before presenting arguments for proving the criterion let us make the following two remarks. First, one can prove that an intersection of two isotropy groups G_r and $G_{r'}$ is by itself an isotropy group. The second remark is about crystallographic point groups in 3 dimensions. For them, as was already mentioned in Section 3, all irreducible multidimensional representations are by themselves induced representations from one-dimensional representations [19]. This means that $\gamma^{(\rho)}$ in the formulation of the criterion is either one-dimensional or, when multidimensional, it is inducible from a one-dimensional representation. Correspondingly, all irreducible-band representations can be induced from one-dimensional representations of finite order subgroups. However, it should be kept in mind that the latter are not necessarily isotropy groups when $\gamma^{(\rho)}$ is multidimensional. Thus, as will be verified below, for all the space groups of the cubic system the multidimensional irreducible representations of the cubic point groups are induced from one-dimensional representations of non-isotropy groups.

The proof of the sufficiency condition of the criterion is immediate because if two band representations are induced from a single representation γ'' of an isotropy subgroup $G_{r''}$ then they are certainly equivalent.

For proving the necessary part of the criterion there does not seem to exist a simple formal and compact way of doing it. The proof of this part of the condition will consist of a number of pieces of which some are of quite general nature, while others are less general and in a few cases the proof is by exhaustion. The general strategy will be first to prove that when $\gamma^{(\rho)}$ and γ' are not induced from a single representation γ'' then (q,ρ) and $D^{(q')}$ are inequivalent. From here it will follow that when (q,ρ) and $D^{(q')}$ are equivalent they are necessarily induced from γ''. This will complete the proof of the necessary part of the criterion.

The proof contains the following parts :

<u>Part 1</u>. The space group is assumed to have an Abelian point group P which is the quotient group G/T (See Section II). In this case also all the isotropy groups are Abelian. Since all α_n commute with β , Formula (61) will assume the following form

$$\chi_{k}^{(q,\rho)}(\beta|\vec{v}(\beta)) = \chi^{(\rho)}(\beta) \sum_{n} \exp(-i\vec{k}\cdot\vec{R}_{q_n}^{(\vec{\beta}|v(\beta))}) \qquad (68)$$

Here $\chi^{(\rho)}(\beta)$ is a character for a one-dimensional representation of the point group of G_r (since G_r is assumed to be Abelian, all its irreducible representations are one-dimensional). Formula (68) shows that the character χ_k of the induced representation is zero for elements not belonging to G_r and it is given by $\chi^{(\rho)}(\beta)$ multiplied by a sum of the phase factors when β is an element of G_r. It is therefore clear that when $P_{r'} \neq P_r$ (P_r point group of G_r), the equality

$$\chi_k^{(q,\rho)}(\beta|\vec{v}(\beta)) = \chi_k^{(q')}(\beta|\vec{v}(\beta)) \tag{69}$$

does not hold. But also when $P_{r'} = P_r$ (isotropy groups which are non-conjugate but have the same point groups), Equality (69) cannot hold because of the different phase factors in the sum of Rel. (68) for $\vec{q}' \neq \vec{q}$. For seeing this we assume that G_r and $G_{r'}$ are isomorphic non-conjugate isotropy groups, and that $P_r = P_{r'}$. For simplicity we can assume that $\vec{r}' = 0$. Then the stars of $\vec{r}'$ and $\vec{r}$ in the Wigner-Seitz cell will be (See decomposition (13))

$$\vec{q}' = 0 \quad , \quad \vec{v}(\alpha_2) \ , \ldots , \ \vec{v}(\alpha_m) \tag{70}$$

$$\vec{q} \ , \ (\alpha_2|\vec{v}(\alpha_2))\vec{q} \ , \ldots , \ (\alpha_m|\vec{v}(\alpha_m))\vec{q} \tag{71}$$

The sum in Rel. (68) will correspondingly become : for $\vec{q}' = 0$ (we denote it by Σ_o)

$$\Sigma_o = \sum_n \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{v(\alpha_n)}) \tag{72}$$

and for $\vec{q}$

$$\Sigma \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q_n}) \tag{73}$$

where $\vec{q}_n = (\alpha_n|\vec{v}(\alpha_n))\vec{q}$. It is convenient to rewrite the sum in (73) in the following way

$$\sum_n \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q_n}) = \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q}) \sum_n \exp(-i\vec{k}\cdot[\vec{R}^{\beta}_{q_n} - \vec{R}^{\beta}_{q}]) \tag{74}$$

One can see that

$$\vec{R}^{\beta}_{q_n} - \vec{R}^{\beta}_{q} = \vec{R}^{\beta}_{v(\alpha_n)} + \alpha_n \vec{R}^{\beta}_{q} - \vec{R}^{\beta}_{q} \tag{75}$$

where we have explicitly used the fact that β and α_n commute (P is abelian). With the aid of Expression (75), Rel. (74) becomes

$$\sum_n \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q_n}) = \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q}) \exp(-i[\alpha_n^{-1}\vec{k}-\vec{k}]\cdot\vec{R}^{\beta}_{q})\Sigma_o \tag{76}$$

From here the following useful result is obtained : For all those $\vec{k}$-vectors for which

$$\alpha_n^{-1}\vec{k}-\vec{k} = \vec{K} \tag{77}$$

where $\vec{K}$ is a vector of the reciprocal lattice and for all α_n in the star of $\vec{q}$ (See Rel. (71)), Rel. (74) becomes

$$\sum_n \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q_n}) = \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q}) \Sigma_o \tag{78}$$

Since there is always a β for which $\vec{R}^{\beta}_{q} \neq 0$ (otherwise $G_{r'}$ would be equal to G_r) , one can see that if the $\vec{k}$-vectors satisfying Rel. (77) form a basis in $\vec{k}$-space we have

$$\sum_n \exp(-i\vec{k}\cdot\vec{R}^{\beta}_{q_n}) \neq \Sigma_o \tag{79}$$

which means that in such cases the band representations induced from G_r and $G_{r'}$ are inequivalent. It turns out that for most G_r in Abelian groups the $\vec{k}$-vectors for which Formula (78) holds form a basis in $\vec{k}$-space. In the few cases when Formula (78) doesn't lead to the inequality (79) we have checked directly that this inequality still holds. It follows that for space groups with Abelian P band representations induced from maximal G_r and $G_{r'}$ (even when $P_r = P_{r'}$) are inequivalent. This completes the proof of Part 1. Among the 230 space groups 103 of them have Abelian P .

Part 2. $\gamma^{(\rho)}$ is a one-dimensional representation of a maximal isotropy group G_r. This part is a generalization of Part 1 and actually contains the latter. Part 2 we are going to prove by using explicitly the induction tables (Table 5) of point groups. The latter contain all the induced representations of point groups induced from maximal subgroups. Table 5 is constructed in such a way that one can find from it the information for induction from maximal isotropy groups of space groups with non-Abelian point groups P . It is for this reason that we have also added the induction tables for the Abelian groups D_{2h}, D_2 and C_{2v}. The idea of using these tables is as follows : for $\vec{k} = o$ in the Brillouin zone the quasi-Bloch functions $\psi_{jo}^{(q_r,\rho)}$ in Rel. (56) form a basis for an induced representation of the point group $G_{k=o}$ induced from the representation $\gamma^{(\rho)}$ of the point group G_r. This statement is easy to check because, in general, it is true for any point $\vec{k}$ for which G_r is a subgroup of G_k. Clearly, when $\vec{k} = o$, G_r is always a subgroup of $G_{k=o}$ and it follows that the character formula (61) for $\vec{k} = o$ will give the character of the induced representation of $G_{k=o}$ from the representation $\gamma^{(\rho)}$ of G_r (See also Formula (32)) :

$$\chi_o^{(q,\rho)}(\beta|\vec{v}(\beta)) = \sum_n \chi^{(\rho)}(\alpha_n^{-1}\beta\alpha_n) \tag{80}$$

where again the summation is on all those n for which $\alpha_n^{-1}\beta\alpha_n$ is an element of G_r. From Rel. (67) the following theorem follows :

Theorem 3. A necessary condition for two band representations induced from $\gamma^{(\rho)}$ and $\gamma^{(\rho')}$ to be equivalent is for $\gamma^{(\rho)}$ and $\gamma^{(\rho')}$ to induce the same representation of P . From this theorem we conclude that if for the band representations (q,ρ) and $D^{(q')}$ (as defined in the criterion) the characters (80) are not equal this means that they are inequivalent band representations. To prove Part 2 one can therefore proceed as follows. One first checks in the induction tables (Table 5) whether $\gamma^{(\rho)}$ and γ' of the point groups P_r and $P_{r'}$ of the isotropy groups G_r and $G_{r'}$ correspondingly induce equivalent representations of the point group P for the space group under discussion. If they are non-equivalent then the band representations (q,ρ) and $D^{(q')}$ are also non-equivalent and the proof of part 2 for these cases is finished. When $\gamma^{(\rho)}$ and γ' induce equivalent representations, it turns out that for an overwhelming majority of space groups this happens when P_r is a subgroup of $P_{r'}$. However, in this case it is easy to check that the equality of the characters doesn't hold for $\vec{k} \neq o$ (Rel. (67)). Indeed, since G_r is not a subgroup of $G_{r'}$, some of the point group elements of the former will have to appear with different translations from those of the latter (for some point group elements of $G_{r'}$ which coincide with those of G_r). This being the case we will have different phase factors $\exp(-i\vec{k}\cdot\vec{R}_{q_n}^{(\beta|v(\beta))})$ in Rel.(61) for the induction from the groups G_r and $G_{r'}$ (for some β belonging to the intersections $G_r \cap G_{r'}$) and correspondingly Rel. (67) will not hold for $k \neq o$. This means that when P_r is a subgroup of $P_{r'}$, the band representations $D^{(q,\rho)}$ and $D^{(q')}$ should be expected to be inequivalent. We have checked that this is actually the case As was already pointed out there are a few cases where P_r is not a subgroup of $P_{r'}$ and still $\gamma^{(\rho)}$, and γ' induce equivalent representations of P . All these latter cases were checked one-by-one by using Rel. (67) and we have proven that under conditions of Part 2 the band representations $D^{(q,\rho)}$ and $D^{(q')}$ are inequivalent.

Part 3. $\gamma^{(\rho)}$ is a multidimensional irreducible representation of a maximal subgroup G_r . This part is very interesting and two cases can appear. As was already pointed out being a multidimensional irreducible representation $\gamma^{(\rho)}$ is by itself an induced representation for point groups in 3 dimensions [19]. Let $\gamma^{(\rho)}$ be inducible from γ'' of a subgroup $G_{r''}$ of G_r . The two above-mentioned cases are when $G_{r''}$ is either not an isotropy group or when it is one. In case one it is possible to prove by using the arguments of Part 2 (Part 1 is inapplicable because the space groups cannot have an Abelian point group) that the representations (q,ρ) and $D^{(q')}$ are inequivalent. However, in all those cases when $G_{r''}$ is an isotropy group, it turns out that it is also an invariant subgroup of G_r. If one collects all the conditions that $G_{r''}$ has to satisfy : 1) it is an isotropy group, 2) an invariant subgroup of a maximal isotropy group G_r and 3) from representation γ'' of $G_{r''}$ a multi-dimensional representation of G_r can be induced then one ends up with the following list of groups for $G_{r''}$:

$$C_4(D_4)\ ,\ C_{2v}(D_{2d})\ ,\ C_3(D_3)\ ,\ C_6(D_6) \tag{81}$$

where in the parentheses the maximal subgroup G_r is listed. For $G_{r''}$ belonging to this list of groups it can be checked by using the International X-Ray Tables [13] that $G_{r''}$ is also a subgroup of another maximal isotropy group, say $G_{r'}$. We have $G_{r''} = G_r \cap G_{r'}$. Since in all possible cases when $\gamma^{(\rho)}$ was not inducible from a representation of an isotropy subgroup $G_{r''}$ of G_r, the band representations $D^{(q,\rho)}$ and $D^{(q')}$ were inequivalent, it follows that when they are equivalent one necessarily has $G_{r''} = G_r \cap G_{r'}$ and both $\gamma^{(\rho)}$ and γ' are inducible from γ'' of $G_{r''}$. The latter is then an isotropy group by itself. This completes the proof of our criterion.

Before outlining the consequences of the criterion let us consider the possibility of the appearance of equivalent band representations when inducing from different irreducible representations of a single maximal isotropy group G_r. In this context the concept of polar (and non-polar) point groups is relevant. A point group is polar if it leaves a non-zero vector invariant. Otherwise it is non-polar. There are 22 non-polar point groups (See Table 1).

Lemma 4. When a non polar group G_r is an isotropy group, then $N_G(G_r) = G_r$ i.e. it is equal to its normalizer.

We remark that the points of the normalizer orbit $N_G(G_r)\cdot\vec{r}$ have all the same isotropy group G_r. Let $\vec{r}' \neq \vec{r}$ be one of them and $\vec{r}(\lambda) = \vec{r}'+(1-\lambda)\vec{r}$, the set of points $(\lambda \in \mathbb{R})$ of the straight line $\vec{r}\,\vec{r}'$. Then $G_r\cdot\vec{r}(\lambda) = \vec{r}(\lambda)$, so G_r is a polar group.

The remark which follows equation (33) can be extended to the present case : Irreducible representations of G_r which do not belong to the same orbit of $N(G_r)$ on $\hat{G}_r$, induce inequivalent representations of G.

To find the exceptional equivalence of two band representations induced from two different unireps $\gamma^{(\rho)}_{G_r}$ and $\gamma^{(\rho')}_{G_r}$ of the same G_r, one has to consider only the 10 polar G_r's and a non trivial action of $N(G_r)$ on $\hat{G}_r$. This action is always trivial if $\hat{G}_r = 1$ or Z_2 that is for $G_1 = 1$, C_2, C_s. Since the group $G_r\cdot C_G(G_r)$ (where $C_G(G_r)$ is the centralizer of G_r in G) acts trivially on $\hat{G}_r$, the action of $N(G_r)$ is effective through the quotient $N_G(G_r)\,/\,(G_r\cdot C_G(G_r)) = Q_r$. From the group law of G (See Rel. (7)) :

$$(1,\vec{t})(\beta,\vec{v}(\beta))(1,\vec{t})^{-1} = (\beta,(I-\beta)\vec{t}+\vec{v}(\beta)) \tag{82}$$

we note that if a translation $\vec{t}$ is in $N_G(G_r)$, it is $\in C_G(G_r)$ so

$$Q_r \sim Q'_r = N_P(P_r)/(P_r\cdot C_P(P_r)) \tag{83}$$

(because one can divide the numerator and denominator of Q_r by $N_G(G_r) \cap T$). We can easily compute an upper limit of Q'_r :

(84)

P_r	C_3	C_{3v}	C_6	C_{6v}	C_{2v}	C_4	C_{4v}
$N_P(P_r) < D_{6h}$						D_{4h}	
$Q'_r <$	Z_2	1	Z_2	1	Z_2	Z_2	1

Since $Q'_r < Z_2$, these exceptional equivalences occur at most for pairs of representations $\gamma^{(\rho)}_{G_r}$, $\gamma^{(\rho')}_{G_r}$ at the same site. A direct computation yields easily that if $\vec{r} = \vec{r}'$ and $G_r = G_{r'} = \{(\beta,\vec{v}(\beta)+\vec{t}_\beta)\}$ then $\vec{t}'-\vec{t} \in \bigcap_{\beta \in P_r} \mathrm{Ker}(I-\beta)$ that is $\vec{r}$ and $\vec{r}'$ are on the axis left invariant by $G_r = C_{2v}$ or C_n , $n = 3,4,6$. Moreover the element of the normalizer $N_G(G_r)$ which acts non trivially on $\hat{G}_r$ must transform this axis into itself without fixed points (if there is one fixed point, the axis does not belong to a closed stratum, and all points cannot be fixed!) so they are either glide reflection through plane containing the axis for $G_r = C_n$, $n = 3,4,6$ or helicoidal rotation $(\beta_4,\vec{v}(\beta))$ (β_4 of order $4, \vec{v}(\beta)$ parallel to this axis) for $G_r = C_{2v}$. Hence, to find this exceptional equivalence of irreducible band representations induced by inequivalent unireps of G_r for the same site $\vec{r}$, we have to search among the 44 space groups with closed strata of dimension 1 : They have to be non-Abelian, non-symmorphic, have a maximal isotropy group either C_{2v} and a corresponding helicoidal rotation $(\beta_4,\vec{v}(\beta))$, or C_n , $n = 3,4,6$ and a corresponding glide reflection. These exceptional equivalences occur only in 10 space groups for 15 such pairs. They are listed in Table 10. (See Rel. (81)).

From the above discussion it should be clear that the overwhelming majority of band representations induced from irreducible representations of maximal isotropy subgroups are inequivalent irreducible-band representations. However, as was already pointed out exceptions to this rule exist. Thus, form the criterion it follows that two band representations (q,ρ) and $D^{(q')}$ induced from $\gamma^{(\rho)}$ (irreducible representation) and γ' of maximal isotropy groups G_r and G'_r correspondingly are equivalent if and only if $\gamma^{(\rho)}$ and γ' are by themselves induced from a representation γ'' of $G_{r''} = G_r \cap G_{r'}$. With this in mind it is simple to find the equivalent band representations corresponding to $\vec{r}' \neq \vec{r}$. In looking for them one has to consider only multidimensional representations $\gamma^{(\rho)}$ because one-dimensional one cannot be induced representations.

Also we have to consider only the cases when G_r has an isotropy subgroup $G_{r''}$ out of which $\gamma^{(\rho)}$ can be induced. With these restrictions it is easy to find the full list of all equivalent band representations $D^{(q')}$ to the band representations (q,ρ) induced from irreducible representations $\gamma^{(\rho)}$ of maximal isotropy groups. It might turn out that some of the band representations $D^{(q')}$ will be inducible from reducible representations γ' of $G_{r'}$. In the latter case (q,ρ) (and also $D^{(q')}$) is a reducible band representation. If (q,ρ) is equivalent to $D^{(q')}$ which is induced from irreducible representations only (γ' has then a superscript and is denoted $\gamma^{(\ell')}$) then (q,ρ) is an irreducible-band representation. If we add to this the information we derived about equivalent band representations steming from representations of a single maximal isotropy group, then we arrive at the full list of equivalent band representations given in Table 10. We call them exceptional band representations. With this list at hand one can deduce a full list of the inequivalent irreducible-band representations of all space groups.

In conclusion of this section let us list the statistics of the exceptional band representations (Table 10). As was already mentioned above there are 15 pairs of equivalent band representations at the same site in the following 10 space groups

$$101,103,105,108,130,137,138,158,159,161 \qquad (85)$$

At different sites there are 35 pairs of equivalent irreducible-induced representations in the following 25 space groups

$$\left.\begin{array}{l} 89,97,111,115,119,121,125,126,129,134 \\ 137,141,149,150,155,162,163,177,182, \\ 208,210,212,213,214,223 \end{array}\right\} \qquad (86)$$

and finally, there are 37 reducible-band representations induced from irreducible representations of maximal isotropy groups in the following 24 space groups

$$\left.\begin{array}{l}124,131,132,139,140,163,165,167,188,190\\192,193,207,208,210,211,215,222,223,224\\226,228,229,230.\end{array}\right\} \quad (87)$$

VII. Irreducible Band-Representations of Space Groups in 2 Dimensions.

Space groups in 2 dimensions are much simpler than the ones in 3 dimensions and for the former it is quite straightforward to calculate the k-component characters of all the irreducible-band representations (See Formula (61)). Having these characters one easily finds (by using Formula (62)) the continuity chords of the irreducible-band representations. This material is summarized in Table 11. One of the very interesting results is that all band representations of 2-dimensional space groups induced from irreducible representations of maximal isotropy groups are irreducible-band representations. The only case where we have equivalent band representations is for the non-symmetric square space group p4gm : the irreducible-band representation $(b^*,3)$ and $(b^*,4)$ which are induced from the irreducible representations 3 and 4 of the isotropy group C_{2v} for the symmetry center $\vec{b} = (\frac{a}{2},0)$ turn out to be equivalent. All the other irreducible-band representations of 2D space groups are inequivalent. There are altogether 131 inequivalent irreducible-band representations for 2-dimensional space groups.

We include the results for the space groups in 2-Dimensions both for didactic reasons and because of their potential use in surface physics [20].

VII. Summary.

The structure and classification of band representations of space groups is investigated in this paper. It is shown that band representations are induced representations from finite order isotropy groups in the physical space of the crystal. This fact creates an elegant framework for dealing with band representations by employing the concepts of strata and their little groups. In this framework band representations are specified by a pair of indices $(\vec{q},\rho)$ where $\vec{q}$ is the Wyckoff position (or symmetry center in the Wigner-Seitz cell) and ρ denotes an irreducible representation $\gamma^{(\rho)}$ of the isotropy group G_r. This is to be compared with irreducible representations of space groups which are also specified by a pair of indeces $(\vec{k},m)$ where $\vec{k}$ is a symmetry point in the inverse space (the Brillouin zone) with its isotropy group G_k and m denotes an irreducible representation Γ_m of G_k. The irreducible representations of space groups are also induced representations and are finite-dimensional. Band representations, on the other hand, are infinite-dimensional and are therefore reducible. The infinite-dimensionality of band representations is in agreement with the physical fact that energy bands in solids contain an infinite number of energy levels. The band representations are equivalent if they contain the same irreducible representations of the space group or the same continuity chords. The elementary building blocks of band representations are the irreducible-band representations. The latter, by definition, cannot be written as a direct sum of band representations induced from representations of a given isotropy group. From the point of view of physics, irreducible-band representations correspond to isolated energy bands. In general, they play an important role in the classification of band representations. A simple Theorem is proven in the paper showing that all irreducible-band representations of a space group are obtained by induction from the irreducible representations of its maximal isotropy subgroups. The latter are symmetry groups of closed strata and they are listed in the

International Tables for X-Ray Crystallography. Closed strata acquire therefore the very special significance that only they have to be considered when constructing irreducible-band representations of space groups. It turns out that the overwhelming majority of band representations induced from irreducible representations of maximal isotropy groups (corresponding to close strata) are inequivalent irreducible-band representations. There are very few exceptions to this rule. Thus, for space groups in two dimensions the only exception is that in the square group p4gm the band representations (b,3) and (b,4) (b is the Wyckoff position [13] and the numbers 3 and 4 label the irreducible representations of the isotropy group $G_b = C_{2v}$, See Ref.[15]) are equivalent. In two dimensions the induction from irreducible representations of maximal isotropy groups leads exclusively to irreducible-band representations. For space groups in 3 dimensions it is proven in the paper that equivalent band representations can be obtained when inducing from different irreducible representations of maximal isotropy groups listed in Rel. (81). There are actually very few such equivalent band representations (See Table 10). Concerning the equivalency of band representations induced from non-conjugate maximal isotropy groups, the following criterion is proven in the paper : a sufficient and necessary condition for two band representations $(\vec{q},\rho)$ and $(\vec{q}',\rho')$ to be equivalent is for the representations $\gamma^{(\rho)}$ and $\gamma^{(\rho')}$ of the isotropy groups G_r and $G_{r'}$ to be induced from a single representation. This is a very useful criterion and for any space group it is easy to check whether one obtains equivalent band representations. It might happen that a band representation $(\vec{q},\rho)$ induced from an irreducible representation $\gamma^{(\rho)}$ of G_r is equivalent to a reducible band representation, e.g. $(\vec{q}',\rho')$ which is induced from a reducible representation γ of $G_{r'}$. In this case we say that an irreducible representation of a maximal isotropy group induces a reducible-band representation. Such cases are exceptional and a full list of them is given in Table 10. For example, this never happens when the induction is from one-dimensional representations of maximal isotropy groups. In the latter case one induces irreducible-band representations only. Equipped with the list of the exceptional equivalent band representations (Table 10) it is easy to find all the inequivalent irreducible-band representations of any space group. For this we find the maximal isotropy groups (corresponding to closed strata) from the International Tables [13] for the particular space group and check whether any of them appear in Table 10. For example, for the diamond structure group O_h^7 none of its maximal isotropy groups appear in Table 10 (See Table 4). What this means is that the irreducible representations of T_d (for the closed strata a and b) and of D_{3d} (for the closed strata c and d) induce inequivalent and irreducible-band representations, altogether 22 in number [5] (10 from T_d and 12 from D_{3d}). The same situation prevails for the hexagonal close-packed structures with the symmetry D_{6h}^4 . The Wyckoff position a has the symmetry D_{3d} while the positions b-d have the symmetry D_{3h} . This space group has 24 inequivalent irreducible-band representations [4]. As an example of a space group with exceptional band representations let us consider the tetragonal group D_{4h}^2 (this is the first space group that has reducible-band representations among the ones induced from closed strata, See Table 10). From the International Tables [13] we find the following closed strata : a and c with D_4-symmetry, b and d with C_{4h}-symmetry, e with C_{2h}-symmetry and f with D_2-symmetry. From the irreducible representations of these groups we induce 34 band representations (See Ref.[15]for irreducible representations of point gorups). From Table 10 we find that the band representations $D_4(a,5)$ (induced from the irreducible representation # 5 of the point group D_4) and $C_{4h}(b,3+7)$ (induced from the reducible representation 3+7 of the point group C_{4h}) are equivalent and the same is true for $D_4(c,5)$ and $C_{4h}(d,3+7)$. From Table 10 it also follows that $D_4(a,5)$ and $C_{4h}(b,3+7)$ are both equivalent to the band representation $C_4(g,3)$ (induced from the representation # 3 of the point group C_4). This is in agreement with the criterion according to which if two band representations induced from different closed strata are equivalent then they are induced from a third stratum (an open one). The band representations $D_4(a,5)$ and $D_4(c,5)$ are therefore reducible-band representations. With this in mind we find that the space group D_{4h}^2 has 32 inequivalent irreducible-band representations.

Table 10 enables one therefore to find all the inequivalent irreducible-band representations of space groups.

Appendix : Quasi-Bloch Functions and the Mackey Double Coset Method.

In reducing band representations into irreducible representations of space groups much use was made in the paper of formula (61). The latter was obtained by using the concept of quasi-Bloch functions (Rel. (56)) which lead to the reduction of the infinite-dimensional band representations into finite-dimensional representations of the isotropy groups G_k for the vectors $\vec{k}$ in the Brillouin zone. Formula (61) gives the character $\chi_k^{(q^*,\rho)}$ of the k-component of the band representation induced from the ρ-representation of the isotropy group G_q ($\vec{q}$ is the position in the Wigner-Seitz cell that corresponds to the symmetry center $\vec{r}$ with the isotropy groups G_r ; the connection between G_q and G_r is explained in Section II A). Having the k-component character $\chi_k^{(q^*,\rho)}$ it is easy to find how many times (multiplicity) an irreducible representation $D^{(k,\mu)}$ of G_k is contained in the band representation $D^{(q^*,\rho)}$ (See Formula (62)). An alternative method for calculating this multiplicity was given in the paper (Formula (46)) by using Mackey's double coset expansion (Rel.(43)). The latter method is of very general nature and can be applied each time when we have an induced representation $\mathrm{Ind}_H^G \gamma_H^{(\rho)}$ of the group G from an irreducible representation $\gamma_H^{(\rho)}$ of its subgroup and we are asking for the multiplicity of the induced representation $\mathrm{Ind}_K^G \gamma_K^{(\alpha)}$ of G from an irreducible representation $\gamma_K^{(\alpha)}$ of another subgroup K of G . However, in applying the double coset method one encounters, in general, a decomposition of the group G into double cosets with respect to H and K (Rel. (43)). As a rule, this double coset decomposition is not entirely elementary and it is for this reason that we have prefered the reduction method based on the quasi-Bloch functions (Formula (61)). It should be pointed out that in some cases the double coset expansion reduces to an expansion into single cosets and then the Mackey method becomes very simple. An example of such cases is when $\vec{k} = 0$, because then $G_k = G$ (in the notations of Section II B , $K = G_k = G$) and the general formula for multiplicities (Formula (44)) goes over into the simple expression (46). A more general example for the double coset expansion to reduce to an expansion in single ones is when G_k is an invariant subgroup of the space group G. This is so because the $Hs\,G_k$ (we replace K by G_k in Formula (43)) can be rewritten as $HG_k s'$. Also from the invariance property of G_k it follows that HG_k is a subgroup of G and expansion (43) turns therefore into a decomposition in single coset with respect to the subgroup HG_k of G.

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Point Group P	Dimension d of stratum
C_1	3
C_s	2
C_2, C_3, C_4, C_6 $C_{2v}, C_{3v}, C_{4v}, C_{6v}$	1
The 22 other point groups	0

Table 1. Dimension d of the stratum corresponding to isotropy groups G_r isomorphic to the point group P . The ten point groups which are isotropy groups of a stratum of dimension > 0 (i.e. with non-isolated points) are called polar groups : they leave at least one non-zero vector invariant in their vector representations. The 22 others are called non-polar.

Dimension of Closed Strata	Number of Space Groups	Dimension of Closed Strata	Number of Space Groups
0	104	1 and 2	6
1	61	0 and 2	2
2	5	0 and 1	38
3	13	0,1 and 2	1

Table 2. Statistics of Dimensions of Closed Strata of Space Groups in 3 Dimensions.

Number of Group	International Symbol	Dimension of Stratum	Number of Strata	Little Group	Number of Group	International Symbol	Dimension of Stratum	Number of Strata	Little Group
1	P1	3	1	1	57	Pbcm	0	2	$\bar{1}$
4	$P2_1$	3	1	1			1	1	2
7	Pb	3	1	1					
9	Bb	3	1	1			2	1	m
19	$P2_12_12_1$	3	1	1	194	$P6_3/mmc$	0	1	$\bar{3}m$
29	$Pca2_1$	3	1	1					
33	$Pna2_1$	3	1	1			0	3	$\bar{6}m2$
76	$P4_1$	3	1	1	221	Pm3m	0	2	m3m
78	$P4_3$	3	1	1			0	2	4/mmm
144	$P3_1$	3	1	1	225	Fm3m	0	2	m3m
145	$P3_2$	3	1	1			0	1	$\bar{4}3m$
169	$P6_1$	3	1	1			0	1	mmm
170	$P6_5$	3	1	1	227	Fd3m	0	2	$\bar{4}3m$
6	Pm	2	2	m			0	2	$\bar{3}m$
8	Bm	2	1	m	229	Im3m	0	1	m3m
26	$Pmc2_1$	2	2	m			0	1	4/mmm
31	$Pmn2_1$	2	1	m			0	1	$\bar{3}m$
36	$Cmc2_1$	2	1	m			0	1	$\bar{4}2m$

Table 3. Examples of closed strata with their little groups. On the left, in the upper part space groups are listed with 3-dimensional closed strata only. On the left, in the lower part, the same for 2-dimensional closed strata. On the right, in the upper part the space group (# 57) is listed as an exceptional group having 0-, 1- and 2-dimensional closed strata. On the right in lower part some space groups with 0-dimensional closed strata are listed.

Symmetry center $\vec{q}$	Little Group
$\vec{r}_a = (000)$	$T_d = G_a$
$\vec{r}_b = (\frac{a}{2} 00)$	$(E\|\frac{a}{2} 00) T_d (E\|\frac{\bar{a}}{2} 00) = G_b$
$\vec{r}_c = (\frac{a}{8} \frac{a}{8} \frac{a}{8})$	$D_{3d}^{(xyz)} = G_c$
$\vec{r}_d = (\frac{a}{8} \frac{a}{8} \frac{3\bar{a}}{8})$	$(E\|00 \frac{\bar{a}}{2}) D_{3d}^{(xyz)} (E\|00 \frac{a}{2}) = G_d$

Table 4. Symmetry centers $\vec{r}$ of closed strata with their little groups G_r for the diamond structure space group O_h^7.

O_h

O	1	1 + 6
	2	2 + 7
	3	3 + 8
	4	5 + 10
	5	4 + 9
T_d	1	1 + 7
	2	2 + 6
	3	3 + 8
	4	4 + 10
	5	5 + 9
T_h	1	1 + 2
	2	3
	3	3
	4	4 + 5
	5	6 + 7
	6	8
	7	8
	8	9 + 10
D_{4h}	1	1 + 3
	2	5
	3	2 + 3
	4	4
	5	4 + 5
	6	6 + 8
	7	10
	8	7 + 8
	9	9
	10	9 + 10
D_{3d}	1	1 + 4
	2	2 + 5
	3	3 + 4 + 5
	4	7 + 10
	5	6 + 9
	6	8 + 9 + 10

O

T	1	1 + 2
	2	3
	3	3
	4	4 + 5
D_4	1	1 + 3
	2	4
	3	2 + 3
	4	5
	5	4 + 5
D_3	1	1 + 5
	2	2 + 4
	3	3 + 4 + 5

T_d

T	1	1 + 2
	2	3
	3	3
	4	4 + 5
D_{2d}	1	1 + 3
	2	5
	3	2 + 3
	4	4
	5	4 + 5
C_{3v}	1	1 + 4
	2	2 + 5
	3	3 + 4 + 5

T_h

T	1	1 + 5
	2	2 + 6
	3	3 + 7
	4	4 + 8
D_{2h}	1	1 + 2 + 3
	2	4
	3	4
	4	4
	5	5 + 6 + 7
	6	8
	7	8
	8	8
C_{3i}	1	1 + 4
	2	2 + 4
	3	3 + 4
	4	5 + 8
	5	6 + 8
	6	7 + 8

T

D_2	1	1 + 2 + 3
	2	4
	3	4
	4	4
C_3	1	1 + 4
	2	2 + 4
	3	3 + 4

D_{4h}

C_{4h}	1	1 + 2
	2	3 + 4
	3	5
	4	5
	5	6 + 7
	6	8 + 9
	7	10
	8	10
D_4	1	1 + 6
	2	2 + 7
	3	3 + 8
	4	4 + 9
	5	5 + 10
C_{4v}	1	1 + 7
	2	2 + 6
	3	3 + 9
	4	4 + 8
	5	5 + 10
D_{2h}	1	1 + 3
	2	5
	3	5
	4	2 + 4
	5	6 + 8
	6	10
	7	10
	8	7 + 9
D'_{2h}	1	1 + 4
	2	5
	3	5
	4	2 + 3
	5	6 + 9
	6	10
	7	10
	8	7 + 8
D_{2d}	1	1 + 8
	2	2 + 9
	3	3 + 6
	4	4 + 7
	5	5 + 10
D'_{2d}	1	1 + 9
	2	2 + 8
	3	4 + 6
	4	3 + 7
	5	5 + 10

D_4

C_4	1	1 + 2
	2	3 + 4
	3	5
	4	5
D_2	1	1 + 3
	2	5
	3	5
	4	2 + 4
D'_2	1	1 + 4
	2	5
	3	5
	4	2 + 3

D_{2d}

S_4	1	1 + 2
	2	3 + 4
	3	5
	4	5
D_2	1	1 + 3
	2	5
	3	5
	4	2 + 4
C_{2v}	1	1 + 4
	2	5
	3	2 + 3
	4	5

C_{4v}

C_4	1	1 + 2
	2	3 + 4
	3	5
	4	5
C_{2v}	1	1 + 3
	2	5
	3	2 + 4
	4	5
C'_{2v}	1	1 + 4
	2	5
	3	2 + 3
	4	5

D_{6h}

C_{6h}	1	1 + 2
	2	9 + 10
	3	6
	4	6
	5	11
	6	11
	7	7 + 8
	8	3 + 4
	9	12
	10	12
	11	5
	12	5
D_6	1	1 + 7
	2	2 + 8
	3	3 + 9
	4	4 + 10
	5	5 + 11
	6	6 + 12
C_{6v}	1	1 + 8
	2	2 + 7
	3	3 + 10
	4	4 + 9
	5	5 + 11
	6	6 + 12
D_{3h}	1	1 + 9
	2	2 + 10
	3	6 + 11
	4	3 + 7
	5	4 + 8
	6	5 + 12
D'_{3h}	1	1 + 10
	2	2 + 9
	3	6 + 11
	4	4 + 7
	5	3 + 8
	6	5 + 12
D_{3d}	1	1 + 3
	2	2 + 4
	3	5 + 6
	4	8 + 10
	5	7 + 9
	6	11 + 12
D'_{3d}	1	1 + 4
	2	2 + 3
	3	5 + 6
	4	8 + 9
	5	7 + 10
	6	11 + 12
D_{2h}	1	1 + 6
	2	3 + 5
	3	4 + 5
	4	2 + 6
	5	7 + 12
	6	9 + 11
	7	10 + 11
	8	8 + 12

D_6

C_6	1	1 + 2
	2	3 + 4
	3	6
	4	6
	5	5
	6	5
D_3	1	1 + 3
	2	2 + 4
	3	5 + 6
D'_3	1	1 + 4
	2	2 + 3
	3	5 + 6
D_2	1	1 + 6
	2	3 + 5
	3	4 + 5
	4	2 + 6

C_{6v}

C_6	1	1 +2
	2	3 + 4
	3	6
	4	6
	5	5
	6	5
C_{3v}	1	1 + 3
	2	2 + 4
	3	5 + 6
C'_{3v}	1	1 + 4
	2	2 + 3
	3	5 + 6
C_{2v}	1	1 + 6
	2	3 + 5
	3	2 + 6
	4	4 + 5

D_{3h}

C_{3h}	1	1 + 2
	2	3
	3	3
	4	4 + 5
	5	6
	6	6
D_3	1	1 + 4
	2	2 + 5
	3	3 + 6
C_{3v}	1	1 + 5
	2	2 + 4
	3	3 + 6
C_{2v}	1	1 + 3
	2	2 + 3
	3	4 + 6
	4	5 + 6

D_{3d}

S_6	1	1 + 2
	2	3
	3	3
	4	4 + 5
	5	6
	6	6
D_3	1	1 + 4
	2	2 + 5
	3	3 + 6
C'_{3v}	1	1 + 4
	2	2 + 5
	3	3 + 6
C_{2h}	1	1 + 3
	2	2 + 3
	3	5 + 6
	4	4 + 6

D_3

C_3	1	1 + 2
	2	3
	3	3
C_2	1	1 + 3
	2	2 + 3

C_{3v}

C_3	1	1 + 2
	2	3
	3	3
C_s	1	1 + 3
	2	2 + 3

D_{2h}

C^z_{2h}	1	1 + 4
	2	2 + 3
	3	5 + 8
	4	6 + 7
C_i	1	1 + 2 + 3 + 4
	2	5 + 6 + 7 + 8

D_2

C^z_2	1	1 + 4
	2	2 + 3
C^x_2	1	1 + 2
	2	3 + 4

C_{2v}

C_2	1	1 + 3
	2	2 + 4

Table 5. Induced representations of Point Groups. On top we list the group for which the representations are induced. In the column on the right-hand side the groups are listed from which we induce the representations. The numbers label the representations of the point groups according to Ref. 15. The induced representations are listed by their contents of irreducible representations of the particular group. Consider as an example the cubic group O_h . When inducing from representation 1 of O we obtain an induced representation of O_h which contains the irreducible representations 1 and 6 of the latter.

INDUCTION from T	INDUCED REPS of T_d	INDUCTION from D_{2d}	INDUCED REPS of T_d	INDUCTION from C_{3v}	INDUCED REPS of T_d	IRREDUCIBLE INDUCED REPS of T_d
$\gamma^{(1)}$	$\gamma^{(1)}+\gamma^{(2)}$	$\gamma^{(1)}$	$\gamma^{(1)}+\gamma^{(3)}$	$\gamma^{(1)}$	$\gamma^{(1)}+\gamma^{(4)}$	$\gamma^{(1)}+\gamma^{(2)}$, $\gamma^{(3)}$
$\gamma^{(2)}$	$\gamma^{(3)}$	$\gamma^{(2)}$	$\gamma^{(2)}+\gamma^{(3)}$	$\gamma^{(2)}$	$\gamma^{(2)}+\gamma^{(5)}$	$\gamma^{(1)}+\gamma^{(3)}$
$\gamma^{(3)}$	$\gamma^{(3)}$	$\gamma^{(3)}$	$\gamma^{(4)}$	$\gamma^{(3)}$	$\gamma^{(3)}+\gamma^{(4)}+\gamma^{(5)}$	$\gamma^{(2)}+\gamma^{(3)}$
$\gamma^{(4)}$	$\underline{\gamma^{(4)}+\gamma^{(5)}}$	$\gamma^{(4)}$	$\gamma^{(5)}$			$\gamma^{(1)}+\gamma^{(4)}$
		$\gamma^{(5)}$	$\underline{\gamma^{(4)}+\gamma^{(5)}}$			$\gamma^{(2)}+\gamma^{(5)}$
						$\gamma^{(4)},\gamma^{(5)}$

Table 6. Induced representations from maximal subgroups and irreducible-induced representation of T_d . The underlined induced representations are reducible-induced. Thus,

$$\mathrm{Ind}_T^{T_d}\,\gamma_T^{(4)} = \gamma_{T_d}^{(4)} + \gamma_{T_d}^{(5)} = \mathrm{Ind}_{D_{2d}}^{T_d}(\gamma_{D_{2d}}^{(3)} + \gamma_{D_{2d}}^{(4)})$$

$$\mathrm{Ind}_{C_{3v}}^{T_d}\,\gamma_{C_{3v}}^{(3)} = \gamma_{T_d}^{(3)} + \gamma_{T_d}^{(4)} + \gamma_{T_d}^{(5)} = \mathrm{Ind}_T^{T_d}(\gamma_T^{(3)} + \gamma_T^{(4)}$$

INDUCTION from C_{3v}	BAND REPS of T_d	INDUCTION from C_{2v}	BAND REPS of T_d
$\gamma^{(1)}$	$\gamma^{(1)}+\gamma^{(4)}$	$\gamma^{(1)}$	$\gamma^{(1)}+\gamma^{(3)}+\gamma^{(4)}$
$\gamma^{(2)}$	$\gamma^{(2)}+\gamma^{(5)}$	$\gamma^{(2)}$	$\gamma^{(4)}+\gamma^{(5)}$
$\gamma^{(3)}$	$\gamma^{(3)}+\gamma^{(4)}+\gamma^{(5)}$	$\gamma^{(3)}$	$\gamma^{(2)}+\gamma^{(3)}+\gamma^{(5)}$
		$\gamma^{(4)}$	$\gamma^{(4)}+\gamma^{(5)}$

Table 7. Band representations from maximal isotropy subgroups of T_d. They are all irreducible-band representations. Two of them are equivalent $\mathrm{Ind}_{C_{2v}}^{T_d} \gamma_{C_{2v}}^{(2)} \sim \mathrm{Ind}_{C_{2v}}^{T_d} \gamma_{C_{2v}}^{(4)}$.

	a	b		a	b					Number of Groups	a	b
O_h	10	20	D_{4h}	10	30	C_4, S_4	4	2	Cu	5	32	54
O, T_d	5	8	D_4, C_{4v}, D_{2d}	5	7	C_3	3	1	Hex	7	54	101
T_h	8	13	D_3, C_{3v}	3	4	D_{2h}	8	12	Trig.	5	21	33
T	4	5	C_{6h}	12	22	D_2, C_{2v}, C_{2h}	4	6	Tatr.	7	41	67
D_{6h}	12	40	C_6, S_6, C_{3h}	6	5	C_2, C_s, C_i	2	1	Orth.	3	16	24
D_6, C_{6v} D_{3d}, D_{3h}	6	12	C_{4h}	8	12	C_1	1		Mon.	3	8	8
									Tric.	2	3	1

<u>Table 8</u>. Statistics of Irreducible and Irreducible-Induced Representations of Crystallographic point groups in 3 dimensions; a) Inequivalent Irreducible Representations; b) Inequivalent Irreducible-Induced Representations.

Table 9

$\chi \backslash \alpha$	E	C_3^{xyz}	C_3^{2xyz}	$C_3^{\bar{x}yz}$	$C_3^{2\bar{x}yz}$	$C_3^{x\bar{y}z}$	$C_3^{2x\bar{y}z}$
$\chi^{(a^*;1)}(\alpha,\vec{k})$	2	2	2	$1+\delta\varepsilon$	$1+\gamma\varepsilon$	$1+\delta\gamma$	$1+\delta\varepsilon$
$\chi^{(b^*;1)}(\alpha,\vec{k})$	2	$\delta\gamma^*+\delta^*\gamma$	$\delta\varepsilon^*+\delta^*\varepsilon$	$\delta\gamma^*+\gamma\varepsilon$	$\delta\varepsilon+\delta^*\varepsilon$	$1+\delta\gamma$	$1+\delta\gamma$

$\chi \backslash \alpha$	$C_3^{xy\bar{z}}$	$C_3^{2xy\bar{z}}$	C_2^{x}	C_2^{y}	C_2^{z}	σ^{xy}	$\sigma^{\bar{x}y}$
$\chi^{(a^*;1)}(\alpha,\vec{k})$	$1+\gamma\varepsilon$	$1+\delta\gamma$	$1+\gamma\varepsilon$	$1+\delta\varepsilon$	$1+\delta\gamma$	$1+\delta\gamma$	2
$\chi^{(b^*;1)}(\alpha,\vec{k})$	$\delta\gamma+\delta^*\varepsilon$	$\delta\varepsilon^*+\gamma\varepsilon$	$1+\gamma\varepsilon$	$\delta^2+\delta^*\varepsilon$	$\delta^2+\delta^*\gamma$	$1+\delta\varepsilon$	$\delta\gamma^*+\delta^*\gamma$

$\chi \backslash \alpha$	σ^{xz}	$\sigma^{\bar{x}z}$	σ^{yz}	$\sigma^{\bar{y}z}$	S_4^{x}	S_4^{3x}	S_4^{y}
$\chi^{(a^*;1)}(\alpha,\vec{k})$	$1+\delta\varepsilon$	2	$1+\gamma\varepsilon$	2	$1+\delta\gamma$	$1+\delta\varepsilon$	$1+\gamma\varepsilon$
$\chi^{(b^*;1)}(\alpha,\vec{k})$	$1+\delta\varepsilon$	$\gamma\varepsilon^*+\delta^*\varepsilon$	$1+\gamma\varepsilon$	2	$\delta^2+\delta^*\gamma$	$\delta^2+\delta^*\varepsilon$	$\delta\varepsilon+\delta^*\gamma$

$\chi \backslash \alpha$	S_4^{3y}	S_4^{z}	S_4^{3z}
$\chi^{(a^*;1)}(\alpha,\vec{k})$	$1+\delta\gamma$	$1+\delta\varepsilon$	$1+\gamma\varepsilon$
$\chi^{(b^*;1)}(\alpha,\vec{k})$	$\delta\varepsilon^*+\gamma\varepsilon$	$\delta\gamma^*+\gamma\varepsilon$	$\delta\gamma+\delta^*\varepsilon$

$\chi \backslash \alpha$	E	C_3^{xyz}	C_3^{2xyz}	$C_2^{\bar{x}y}$	$C_2^{\bar{x}z}$	$C_2^{\bar{y}z}$	I
$\chi^{(c^*;1)}(\alpha,\vec{k})$	4	1	1	$1+\delta^*\gamma^*$	$1+\delta\varepsilon$	$1+\gamma\varepsilon$	$1+\gamma\varepsilon+$ $+\delta^*\gamma^*+\delta\varepsilon$
$\chi^{(d^*;1)}(\alpha,\vec{k})$	4	$\delta\varepsilon^*$	$\gamma\varepsilon^*$	$(\varepsilon^*)^2+(\delta\gamma\varepsilon^2)^*$	$1+\delta^*\varepsilon^*$	$1+\gamma^*\varepsilon^*$	$(\varepsilon^*)^2+\gamma\varepsilon^*+$ $+(\delta\gamma\varepsilon^2)^*+\delta\varepsilon^*$

$\chi \backslash \alpha$	S_6^{xyz}	S_6^{5xyz}	$\sigma^{\bar{x}y}$	$\sigma^{\bar{x}z}$	$\sigma^{\bar{y}z}$	$C_3^{2x\bar{y}z}$	C_3^{xyz}
$\chi^{(c^*;1)}(\alpha,\vec{k})$	1	1	2	2	$2\gamma\varepsilon^*$	$\delta\varepsilon$	$\delta\gamma$
$\chi^{(d^*;1)}(\alpha,\vec{k})$	$\delta^*\varepsilon^*$	$\gamma^*\varepsilon^*$	2	$2\delta\varepsilon^*$	$2\gamma\varepsilon^*$	$\delta\gamma$	$\delta\varepsilon^*$

Table 9 (Cont.)

χ \ α	C_2^{xy}	C_2^{xz}	$S_6^{5x\bar{y}z}$	$S_6^{x\bar{y}z}$	σ^{xy}	σ^{xz}	$C_3^{\bar{x}yz}$	$C_3^{2\bar{x}yz}$
$\chi^{(c;1)}(\alpha,\vec{k})$	$\delta^*\varepsilon+\gamma^*\varepsilon$	$\delta^*\gamma+\delta^*\gamma^*$	$\delta^*\gamma$	$\delta^*\varepsilon$	$2\delta\gamma$	$1+\delta\varepsilon$	1	1
$\chi^{(d;1)}(\alpha,\vec{k})$	$\delta^*\varepsilon^*+\gamma^*\varepsilon^*$	$\gamma\varepsilon^*+\gamma^*\varepsilon$	$\delta^*\varepsilon^*$	1	$2\delta\gamma$	$1+\delta^*\varepsilon^*$	$\delta^*\varepsilon^*$	$\gamma^*\varepsilon^*$

χ \ α	C_2^{yz}	$S_6^{\bar{x}yz}$	$S_6^{5\bar{x}yz}$	σ^{yz}	$C^{2xy\bar{z}}$	$C_3^{xy\bar{z}}$	$S_6^{5xy\bar{z}}$	$S_6^{xy\bar{z}}$	Other
$\chi^{(c;1)}(\alpha,\vec{k})$	$\delta^*\gamma^*+\delta\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$1+\gamma\varepsilon$	$\delta\gamma$	$\gamma\varepsilon$	$\gamma^*\varepsilon$	$\delta\gamma^*$	0
$\chi^{(d;1)}(\alpha,\vec{k})$	$\delta^*\varepsilon^*+\delta\varepsilon^*$	$\gamma^*\varepsilon^*$	$\delta^*\varepsilon^*$	$1+\gamma^*\varepsilon^*$	$\delta\varepsilon^*$	$\delta\gamma$	1	$\gamma^*\varepsilon^*$	0

Table 9. Characters of the k-components of all the irreducible band representations for the diamond structure space group O_h^7. a,b,c,d are the different symmetry centers of the closed strata. The characters are listed for the band representation that is induced from the unit representation of the little group. All other characters are obtained according to the formula

$\chi^{(r,\rho)}(\alpha,\vec{k}) = \chi^{(r,1)}(\alpha) \times D^{(\rho)}(\alpha)$. For r = a,b, ρ = 1,2,3,4,5 ; for r = c,d , ρ = 1,2,3,4,5,6. $\delta = \exp(\frac{i}{2} k_x a)$; $\gamma = \exp(\frac{i}{2} k_y a)$; $\varepsilon = \exp(\frac{i}{2} k_z a)$.

SPACE GROUPS	EQUIVALENT BAND REPRESENTATIONS		
89 D_4^1	$D_4(a,5)$	$D_4(b,5)$	$C_4(g,3)$
	$D_4(c,5)$	$D_4(d,5)$	$C_4(h,3)$
97 D_4^9	$D_4(a,5)$	$D_4(b,5)$	$C_4(e,3)$
101 C_{4v}^3	$C_{2v}(a,2)$	$C_{2v}(a,4)$	
	$C_{2v}(b,2)$	$C_{2v}(b,4)$	
103 C_{4v}^5	$C_4(a,3)$	$C_4(a,4)$	
	$C_4(b,3)$	$C_4(b,4)$	
105 C_{4v}^7	$C_{2v}(a,2)$	$C_{2v}(a,4)$	
	$C_{2v}(b,2)$	$C_{2v}(b,4)$	
108 C_{4v}^{10}	$C_4(a,3)$	$C_4(a,4)$	
111 D_{2d}^1	$D_{2d}(a,5)$	$D_{2d}(c,5)$	$C_{2v}(g,2)$
	$D_{2d}(b,5)$	$D_{2d}(d,5)$	$C_{2v}(h,2)$
115 D_{2d}^5	$D_{2d}(a,5)$	$D_{2d}(d,5)$	$C_{2v}(e,2)$
	$D_{2d}(b,5)$	$D_{2d}(c,5)$	$C_{2v}(f,2)$
119 D_{2d}^9	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
	$D_{2d}(c,5)$	$D_{2d}(d,5)$	$C_{2v}(f,2)$
121 D_{2d}^{11}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
124 D_{4h}^2	$D_4(a,5)$	$C_{4h}(b,3+7)$	$C_4(g,3)$
	$D_4(c,5)$	$C_{4h}(d,3+7)$	$C_4(h,3)$
125 D_{4h}^3	$D_4(a,5)$	$D_4(b,5)$	$C_4(g,3)$
	$D_{2d}(c,5)$	$D_{2d}(d,5)$	$C_{2v}(h,2)$
126 D_{4h}^4	$D_4(a,5)$	$D_4(b,5)$	$C_4(e,3)$
129 D_{4h}^7	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(f,2)$
130 D_{4h}^8	$C_4(c,3)$	$C_4(c,4)$	
131 D_{4h}^9	$D_{2d}(e,5)$	$D_{2h}(a,2+7)$	$C_{2v}(g,2)$
	$D_{2d}(f,5)$	$D_{2h}(b,2+7)$	$C_{2v}(h,2)$
132 D_{4h}^{10}	$D_{2d}(b,5)$	$D_{2h}(a,2+7)$	$C_{2v}(g,2)$

SPACE GROUPS	EQUIVALENT BAND REPRESENTATIONS		
	$D_{2d}(d,5)$	$D_{2h}(c,2+7)$	$C_{2v}(h,2)$
134 D_{4h}^{12}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(g,2)$
137 D_{4h}^{15}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(d,2)$
	$C_{2v}(d,2)$	$C_{2v}(d,4)$	
138 D_{4h}^{16}	$C_{2v}(e,2)$	$C_{2v}(e,4)$	
139 D_{4h}^{17}	$D_{2d}(d,5)$	$D_{2h}(c,2+7)$	$C_{2v}(g,2)$
140 D_{4h}^{18}	$D_4(a,5)$	$C_{4h}(c,3+7)$	$C_4(f,3)$
	$D_{2d}(b,5)$	$D_{2h}(d,2+7)$	$C_{2v}(g,2)$
141 D_{4h}^{19}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
149 D_3^1	$D_3(a,3)$	$D_3(b,3)$	$C_3(g,2)$
	$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$
	$D_3(e,3)$	$D_3(f,3)$	$C_3(i,2)$
150 D_3^2	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
155 D_3^7	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
158 C_{3v}^3	$C_3(a,2)$	$C_3(a,3)$	
	$C_3(b,2)$	$C_3(b,3)$	
	$C_3(c,2)$	$C_3(c,3)$	
159 C_{3v}^4	$C_3(a,2)$	$C_3(a,3)$	
161 C_{3v}^6	$C_3(a,2)$	$C_3(a,3)$	
162 D_{3d}^1	$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$
163 D_{3d}^2	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(e,2)$
	$D_3(c,3)$	$D_3(d,3)$	$C_3(f,2)$
165 D_{3d}^4	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(c,2)$
167 D_{3d}^6	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(c,2)$
177 D_6^1	$D_6(a,5)$	$D_6(b,5)$	$C_6(e,3)$
	$D_6(a,b)$	$D_6(b,6)$	$C_6(e,5)$
	$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$

SPACE GROUPS	EQUIVALENT BAND REPRESENTATIONS		
182 D_6^6	D_3(a,3)	D_3(b,3)	C_3(e,2)
	D_3(c,3)	D_3(d,3)	C_3(f,2)
188 D_{3h}^2	D_3(a,3)	C_{3h}(b,2+5)	C_3(g,2)
	D_3(c,3)	C_{3h}(d,2+5)	C_3(h,2)
	D_3(e,3)	C_{3h}(f,2+5)	C_3(i,2)
190 D_{3h}^4	D_3(a,3)	C_{3h}(b,2+5)	C_3(e,2)
192 D_{6h}^2	D_6(a,5)	C_{6h}(b,5+11)	C_6(e,5)
	D_6(a,6)	C_{6h}(b,3+9)	C_6(e,3)
	D_3(c,3)	C_{3h}(d,2+5)	C_3(h,2)
193 D_{6h}^3	D_3(d,3)	C_{3h}(c,2+5)	C_3(h,2)
207 O^1	D_4(c,5)	O(b,4+5)	C_4(f,3)
208 O^2	D_3(b,3)	T(a,2+4)	C_3(g,2)
	D_3(c,3)	T(a,2+4)	C_3(g,2)
	D_3(b,3)	D_3(c,3)	C_3(g,2)
210 O^4	D_3(c,3)	T(a,2+4)	C_3(e,2)
	D_3(d,3)	T(a,2+4)	C_3(e,2)
	D_3(c,3)	D_3(d,3)	C_3(e,2)
211 O^5	D_3(c,3)	O(a,3+4+5)	C_3(f,2)
212 O^6	D_3(a,3)	D_3(b,3)	C_3(c,2)
213 O^7	D_3(a,3)	D_3(b,3)	C_3(c,2)
214 O^8	D_3(a,3)	D_3(b,3)	C_3(e,2)
215 T_d^1	D_{2d}(d,5)	T_d(a,4+5)	C_{2v}(f,2)
	D_{2d}(c,5)	T_d(b,4+5)	C_{2v}(g,2)
222 O_h^2	D_4(b,5)	O(a,4+5)	C_4(e,3)
223 O_h^3	D_{2d}(c,5)	D_{2h}(b,2+7)	C_{2v}(g,2)
	D_{2d}(d,5)	D_{2h}(b,2+7)	C_{2v}(h,2)
	D_{2d}(c,5)	D_{2d}(d,5)	C_{2v}(g,2)
	D_3(e,3)	T_h(a,2+7)	C_3(i,2)

SPACE GROUPS	EQUIVALENT BAND REPRESENTATIONS		
224 O_h^4	$D_{2d}(d,5)$	$T_d(a,4+5)$	$C_{2v}(g,2)$
226 O_h^6	$D_{2d}(c,5)$	$T_h(b,4+8)$	$C_{2v}(e,2)$
228 O_h^8	$D_3(b,3)$	$T(a,3+4)$	$C_3(e,2)$
229 O_h^9	$D_{2d}(d,5)$	$D_{4h}(b,5+10)$	$C_{2v}(g,2)$
230 O_h^{10}	$D_3(b,3)$	$C_{3i}(a,2+5)$	$C_3(e,2)$

Table 10. List of equivalent band representations (also called exceptional ones) induced by maximal finite subgroups. We give an example of using this Table (in addition to the examples in the Summary Section) : Space group 89 (D_4^1) . From Ref. 13 we learn that there exist six closed Wyckoff positions a,b,c,d,e,f. The band representations obtained from them are $D_4(a,i)$, $D_4(b,i)$, $D_4(c,i)$, $D_4(d,i)$, $D_2(e,j)$, $D_2(f,j)$ where i runs from 1 to 5 and j from 1 to 4 since D_4 has five irreducible representations and D_2 four. This leads to $4 \times 5 + 2 \times 4 = 28$ band representations. From the Table we see that there are two pairs of equivalent representations among them. They correspond to inductions from one-dimensional representations of a non-maximal isotropy group given in the third column. We are left with 28-2 = 26 non equivalent irreducible-band representations. When a band representation is equivalent to a direct sum of induced representations (first example appears for group 124) it is, of course, a reducible-band representation.

Table 11. Continuity Chords of Irreducible Band Representations for 2-Dimensional Space Groups. The symmetry points in the Brillouin zone and their symmetry groups are given in Table 12. The irreducible representaions for the non-symmorphic space groups are presented in Table 13.

OBLIQUE

p2 N°2

	(a,1)	(a,2)	(b,1)	(b,2)	(c,1)	(c,2)	(d,1)	(d,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_1	X_2	X_2	X_1	X_2	X_1
Y	Y_1	Y_2	Y_2	Y_1	Y_1	Y_2	Y_2	Y_1
R	R_1	R_2	R_2	R_1	R_2	R_1	R_1	R_2

RECTANGULAR

p1m1 N°3

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_2	X_1

p1g1 N°4

	(a,1)
Γ	$\Gamma_1\Gamma_2$
X	X_1X_2

c1m1 N°5*

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_2	X_1

* The symmetry center b $\frac{a}{2}$ y) is missing in Ref. 13.

p2mm N°6

	(a,1)	(a,2)	(a,3)	(a,4)	(b,1)	(b,2)	(b,3)	(b,4)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4
X	X_1	X_3	X_2	X_4	X_1	X_3	X_2	X_4
Y	Y_1	Y_3	Y_2	Y_4	Y_3	Y_1	Y_4	Y_2
R	R_1	R_3	R_2	R_4	R_3	R_1	R_4	R_2

	(c,1)	(c,2)	(c,3)	(c,4)	(d,1)	(d,2)	(d,3)	(d,4)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4
X	X_4	X_2	X_3	X_1	X_4	X_2	X_3	X_1
Y	Y_1	Y_3	Y_2	Y_4	Y_3	Y_1	Y_4	Y_2
R	R_4	R_2	R_3	R_1	R_2	R_4	R_1	R_3

p2mg N°7

	(a,1)	(a,2)	(b,1)	(b,2)	(c,1)	(c,2)
Γ	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$
X	X_1	X_1	X_1	X_1	X_1	X_1
Y	Y_1Y_2	Y_3Y_4	Y_3Y_4	Y_1Y_2	Y_1Y_3	Y_2Y_4
R	R_1	R_1	R_1	R_1	R_1	R_1

p2gg N°8

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$
X	X_1	X_1	X_1	X_1
Y	Y_1	Y_1	Y_1	Y_1
R	R_1R_2	R_3R_4	R_3R_4	R_1R_2

c2mm N°9

	(a,1)	(a,2)	(a,3)	(a,4)	(b,1)	(b,2)	(b,3)	(b,4)	(c,1)	(c,2)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$
X	X_1	X_3	X_2	X_4	X_1	X_3	X_2	X_4	X_3X_4	X_1X_2
R	R_1	R_2	R_1	R_2	R_2	R_1	R_2	R_1	R_1R_2	R_1R_2

<u>SQUARE</u>

p4 N°10

	(a,1)	(a,2)	(a,3)	(a,4)	(b,1)	(b,2)	(b,3)	(b,4)	(c,1)	(c,2)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$
R	R_1	R_3	R_2	R_4	R_3	R_1	R_4	R_2	R_2R_4	R_1R_3
X	X_1	X_1	X_3	X_2	X_2	X_2	X_1	X_1	X_1X_2	X_1X_2

p4mm N°11

	(a,1)	(a,2)	(a,3)	(a,4)	(a,5)	(b,1)	(b,2)	(b,3)	(b,4)	(b,5)	(c,1)	(c,2)	(c,3)	(c,4)
Γ	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$	Γ_5	Γ_5
R	R_1	R_2	R_3	R_4	R_5	R_4	R_3	R_2	R_1	R_5	R_5	R_5	R_2R_4	R_1R_3
X	X_1	X_2	X_1	X_2	X_3X_4	X_2	X_1	X_2	X_1	X_1X_2	X_1X_4	X_2X_3	X_2X_4	X_1X_3

p4gm N°12

	(a,1)	(a,2)	(a,3)	(a,4)	(b,1)	(b,2)	(b,3)	(b,4)
Γ	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	Γ_5	Γ_5	$\Gamma_1\Gamma_4$	Γ_5	$\Gamma_2\Gamma_3$	Γ_5
R	R_5	R_5	R_1R_2	R_3R_4	R_1R_3	R_5	R_2R_4	R_5
X	X_1	X_1	X_1	X_1	X_1	X_1	X_1	X_1

HEXAGONAL

p3 N°13

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)
Γ	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
M	M_1	M_2	M_3	M_3	M_1	M_2	M_2	M_3	M_1
N	N_1	N_2	N_3	N_2	N_3	N_1	N_3	N_1	N_2

p3m1 N°14

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)
Γ	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
M	M_1	M_2	M_3	M_3	M_1	M_2	M_2	M_3	M_1
N	N_1	N_2	N_3	N_2	N_3	N_1	N_3	N_1	N_2

p31m N°15

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)
Γ	Γ_1	Γ_2	Γ_3	$\Gamma_1\Gamma_2$	Γ_3	Γ_3
M	M_1	M_2	M_3	M_3	M_1M_2	M_3
N	N_1	N_2	N_3	N_3	N_3	N_1N_2

p6 N°16

	(a,1)	(a,2)	(a,3)	(a,4)	(a,5)	(a,6)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)
Γ	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	$\Gamma_1\Gamma_2$	$\Gamma_4\Gamma_5$	$\Gamma_3\Gamma_6$	$\Gamma_1\Gamma_3\Gamma_4$	$\Gamma_2\Gamma_5\Gamma_6$
M	M_1	M_1	M_3	M_2	M_2	M_3	M_2M_3	M_1M_3	M_1M_2	$M_1M_2M_3$	$M_1M_2M_3$
N	N_1	N_1	N_3	N_2	N_2	N_3	N_2N_3	N_1N_3	N_1N_2	$N_1N_2N_3$	$N_1N_2N_3$
X	X_1	X_2	X_1	X_1	X_2	X_2	X_1X_2	X_1X_2	X_1X_2	$X_1 2X_2$	$(2X_1)X_2$
Y	Y_1	Y_2	Y_1	Y_1	Y_2	Y_2	Y_1Y_2	Y_1Y_2	Y_1Y_2	$Y_1 2Y_2$	$(2Y_1)Y_2$
R	R_1	R_2	R_1	R_1	R_2	R_2	R_1R_2	R_1R_2	R_1R_2	$R_1 2R_2$	$(2R_1)R_2$

6mm N°17

	(a,1)	(a,2)	(a,3)	(a,4)	(a,5)	(a,6)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)	(c,4)
Γ	Γ_1	Γ_2	Γ_3	Γ_4	Γ_6	Γ_5	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$	$\Gamma_5\Gamma_6$	$\Gamma_1\Gamma_5$	$\Gamma_3\Gamma_6$	$\Gamma_2\Gamma_5$	$\Gamma_4\Gamma_6$
M	M_1	M_2	M_1	M_2	M_3	M_3	M_3	M_3	$M_1M_2M_3$	M_1M_3	M_2M_3	M_2M_3	M_1M_3
N	N_1	N_2	N_1	N_2	N_3	N_3	N_3	N_3	$N_1N_2N_3$	N_1N_3	N_2N_3	N_2N_3	N_1N_3
X	X_1	X_2	X_3	X_4	X_3X_4	X_1X_2	X_1X_3	X_2X_4	$X_1X_2X_3X_4$	$X_1X_3X_4$	$X_1X_2X_3$	$X_2X_3X_4$	$X_1X_2X_4$
Y	Y_1	Y_2	Y_3	Y_4	Y_3Y_4	Y_1Y_2	Y_1Y_3	Y_2Y_4	$Y_1Y_2Y_3Y_4$	$Y_1Y_3Y_4$	$Y_1Y_2Y_3$	$Y_2Y_3Y_4$	$Y_1Y_2Y_4$
R	R_1	R_2	R_3	R_4	R_3R_4	R_1R_2	R_1R_3	R_2R_4	$R_1R_2R_3R_4$	$R_1R_3R_4$	$R_1R_2R_3$	$R_2R_3R_4$	$R_1R_2R_4$

1. OBLIQUE

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_2
$X = \frac{\vec{K}_1}{2}$	C_2
$Y = \frac{\vec{K}_2}{2}$	C_2
$R = \frac{1}{2}(\vec{K}_1+\vec{K}_2)$	C_2

2. RECTANGULAR (SIMPLE)

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{2v}
$X = \frac{\vec{K}_1}{2}$	C_{2v}
$Y = \frac{\vec{K}_2}{2}$	C_{2v}
$R = \frac{1}{2}(\vec{K}_1+\vec{K}_2)$	C_{2v}

3. RECTANGULAR (CENTERED)

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{2v}
$Y = \frac{\vec{K}_2}{2}$	C_{2v}
$R = \frac{1}{2}(\vec{K}_1+\vec{K}_2)$	C_2

4. SQUARE

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{4v}
$R = \frac{1}{2}(\vec{K}_1+\vec{K}_2)$	C_{4v}
$X = \frac{\vec{K}_1}{2}$	C_{2v}

5. HEXAGONAL

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{6v}
$M = \frac{1}{3}(\vec{K}_1+\vec{K}_2)$	C_{3v}
$N = \frac{2}{3}(\vec{K}_1+\vec{K}_2)$	C_{3v}
$X = \frac{\vec{K}_1}{2}$	C_{2v}
$Y = \frac{\vec{K}_2}{2}$	C_{2v}
$R = \frac{1}{2}(\vec{K}_1+\vec{K}_2)$	C_{2v}

Table 12. Symmetry points in the Brillouin zone and their isotropy groups for 2-dimensional space groups.

1. RECTANGULAR

p1g1 (N°4) :

X	E	σ^x
X_1	1	δ
X_2	1	$-\delta$

$\delta = \exp(i \frac{k_y b}{2})$

p2mg (N°7) :

X,R	E	C_2	σ^x	σ^y
1	2		0	

Y like Γ

pgg (N°8) :

X,Y	E	C_2	σ^x	σ^y
1	2		0	

R	E	C_2	σ^x	σ^y
R_1	1	1	i	i
R_2	1	1	i	-i
R_3	1	-1	i	-i
R_4	1	-1	-i	i

2. SQUARE

p4gm (N°12) :

R	E	C_4	C_4^2	C_4^3	σ^{xy}	$\sigma^{\bar{x}y}$	σ^x	σ^y
R_1	1	i	-1	-i	1	-1	i	-i
R_2	1	i	-1	-i	-1	1	-i	i
R_3	1	-i	-1	i	+1	-1	-i	i
R_4	1	-i	-1	i	-1	1	i	-i
R_5	2	0	2	0	0	0	0	0

X	E	C_2	σ^x	σ^y
X_1	2		0	

Table 13. Irreducible representations of non-symmetric groups for points on the surface of the Brillouin zone.