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 the 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 $G \times M \xrightarrow{\varphi} M$ 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 $G_{g\cdot m} = gG_m g^{-1}$. 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 :

$$g\cdot(aH) = (ga)H \qquad (3)$$

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

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

or, in shorter notation,

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

(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

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

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 dimensions the 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 $F_m = G_{\vec{b}}$.

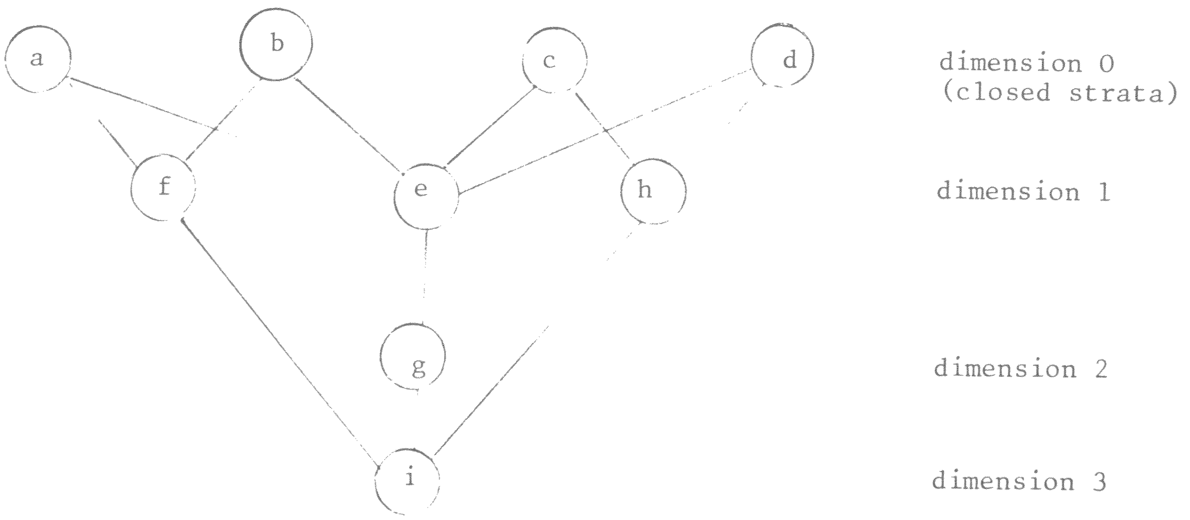
In general, an intersection of little groups is not a little group, but this is the case for finite groups [9] and the proof can be easily extended to space groups.

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)

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

where $(\gamma_i|v(\gamma_i))$, $i = 1,2,\dots,s$ 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))

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

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

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

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 $p \cdot s = I_{[G:H]}$ 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 $V_H^{(\alpha)}$: $h \rightsquigarrow D^{(\alpha)}(h)$; 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

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

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)

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

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

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

where (20) becomes : $h(g,g^{-1}m) = s_{g.m}^{-1}\ gs_m$. 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

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

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 $K \lhd G$) 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 Ker $\gamma_H^{(\alpha)}$. If $H \lhd G$ (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

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

where $G\cdot\gamma_H^{(\alpha)}$ is the G-orbit of $\gamma_H^{(\alpha)}$ in $\hat{H}$. In particular, when $H = 1 \lhd G$, 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

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

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. $\xi(g_1g_2) = \xi(g_2g_1)$ so $\xi(g_1g_2g_1^{-1}) = \xi(g_2)$ and $\bar{\xi}(g) = \xi(g^{-1})$ 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

<u>Frobenius reciprocity theorem</u> : 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 $A \lhd G$, 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

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

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

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

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) :

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

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

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

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

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

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

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

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, $\triangleleft$ reads invariant subgroups) :

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

Note that when c) is replaced by the weaker condition c') $G_i \triangleleft G_{i-1}$, 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.

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

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

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

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 $\text{Ind}_H^G(\gamma_H^{(\alpha)})$. 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