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.

<u>Theorem 2</u>. 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 . $\text{Res}_A^P \gamma_P^{(\alpha)} = \gamma_A^{(\alpha_1)} + \gamma_A^{(\alpha_2)}$

and by Frobenius reciprocity $\text{Ind}_A^P \gamma_A^{(\alpha_1)} = \text{Ind}_A^P \gamma_A^{(\alpha_2)} = \gamma_P^{(\alpha)}$. 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, $\text{Ind}_M^P \gamma_M^{(\rho)}$ is a direct sum

of $\dfrac{|P|}{|M|}$ 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, $\text{Ind}_H^C \gamma_H^{(a)}$ 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 representation
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

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

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

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)).

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

where s = 1,2,...,m labels the vectors in the star, and j = 1,2,...,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 × 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 × 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 represen-

tations 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 repre-

sentation, 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 represen-tation. 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-dimensiona ones (of small dimension, in general) by utilizing eigenfunctions of the trans-lation 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 $\psi_j^{(w,\rho)}(\vec{r})$, $j = 1,2,...,p$ are given by Rels. (53) and (54). By using the decomposition $(G_q = T.P)$

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

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

and $s = 1,...,m$ (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 represen- tations 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 :

Part 1. 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

$$\chi_k^{(q,\rho)}(\beta|\vec{v}(\beta)) = \chi^{(\rho)}(\beta) \sum_n \exp(-i\vec{k}\cdot\vec{R}_{q_n}^{(\beta|v(\beta))}) \tag{68}$$

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 represen-

tations 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))

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

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

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

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

and for $\vec{q}$

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

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

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

One can see that

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

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

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

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

$$\alpha_n^{-1}\vec{k}-\vec{k} = \vec{K} \qquad (77)$$

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

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

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

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

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 $\exp(-i\vec{k}\cdot\vec{R}_{q_n}^{(\vec{\beta}|v(\beta))})$ 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 $\underline{\text{same}}$ isotropy group G_r . Let $\vec{r}' \neq \vec{r}$ be one of them and $\vec{r}(\lambda) = \lambda \vec{r}' + (1-\lambda)\vec{r}$, 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 $\gamma_{G_r}^{(\rho)}$ and $\gamma_{G_r}^{(\rho')}$ 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' :

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

$$(84)$$

Since $Q_r' < Z_2$, these exceptional equivalences occur at most for pairs of

representations $\gamma_{G_r}^{(\rho)}$, $\gamma_{G_r}^{(\rho')}$ 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 $\vec{r}' - \vec{r} \in \bigcap_{\beta \in P_r} Ker(I - \beta)$

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

$$101,103,105,108,130,137,138,158,159,161 \tag{85}$$

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

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

and finally, there are 37 reducible-band representations induced from irreducible

representations of maximal isotropy groups in the following 24 space groups

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

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. <u>Summary</u>.

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.