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

In what follows we give a classification of all irreducible-induced representations of point groups. Among them we shall also obtain the irreducible representations. From Theorem 1, we know the results for Abelian point groups. We shall prove that we can extend it to all 2 or 3 dimensional point groups, but some of the obtained representations might be equivalent.
Theorem 2. The irreducible-induced representations of 2 or 3 dimensional point groups are induced representations from one dimensional representations of maximal subgroups. We know it for Abelian groups. Outside the five cubic groups, the non-Abelian point groups have irreducible representations of dimension 1 or 2. (We shall refer to it as property I_a). Moreover, each such point group P has an Abelian maximal subgroup A of index 2. Indeed $P \leq D_{n\text{h}}$ with $n = 3, 4$ or 6.

Define $A_P = P \cap C_{n\text{h}}$ (since $D_{n\text{h}}/C_{n\text{h}} = Z_2$, $P/A_P = Z_2$). Let

$\gamma_P^{(\alpha)}$ be a two-dimensional irreducible representation of $P$. $\text{Res}_{A_P}^{P}(\alpha) = \gamma_A^{(\alpha_1)} + \gamma_A^{(\alpha_2)}$ and by Frobenius reciprocity

$\text{Ind}_{A_P}^{P}(\gamma_A^{(\alpha_1)}) = \text{Ind}_{A_P}^{P}(\gamma_A^{(\alpha_2)}) = \gamma_P^{(\alpha)}$. 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 $|P|/|M|$ 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 $\leq 3$.

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

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 $T_d$ have maximal subgroups with two-dimensional irreducible representations. For the other, induction from a 2-dimensional representation of a subgroup 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 $O \sim T_c$. 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

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

When the $\psi(\vec{r})$ are square integrable functions, Rel. (52) defines a linear action of $G$ on the Hilbert space $L^2(\mathbb{R}^3)$. 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 $\mathbb{R}^3$ (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 $L^2(\mathbb{R}^3)$. 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 $O^7_h$ 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 $\psi_j^{(w,\rho)}(\vec{r})$, $j = 1, 2, ..., p$ 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).

$$\gamma(\omega)\psi_j^{(w,\rho)}(\vec{r}) = \sum_{j'=1}^{p} D_j^{(\rho)}(\gamma)\psi_{j'}^{(w,\rho)}(\vec{r})$$  \hspace{1cm} (53)

where $\gamma(\omega)$ 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 $O$.

$$\gamma_m^* \psi_j^{(w,\rho)}(\vec{r}) = \sum_{j'=1}^{p} D_j^{(\rho)}(\gamma)\psi_{j'}^{(w,\rho)}(\vec{r}-\vec{R})$$  \hspace{1cm} (54)

A band representation is the induced representation $\text{Ind}_G^G(\gamma(\rho))$. The basis of this induced representation is
\[ \psi_j^{(w_1, \rho)} (\mathbf{r}) = \psi_j^{(w_2, \rho)} (\mathbf{r}) , \quad \psi_j^{(w_2, \rho)} (\mathbf{r}) = (\mathbf{a}_2 | v(\mathbf{a}_2)) \psi_j^{(w_1, \rho)} (\mathbf{r}), \ldots, \]

\[ \psi_j^{(w_m, \rho)} (\mathbf{r}) = (\mathbf{a}_m | v(\mathbf{a}_m)) \psi_j^{(w_1, \rho)} (\mathbf{r}) \]

plus all those functions that are obtained by applying to (55) all the translations of \( T \). In Rel. (55) \((\mathbf{a}_s | v(\mathbf{a}_s))\) 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 acquires 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 \( Q_4^f \), 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)).

$$
\psi_{jk}(\vec{r}) = \sum_{n} \exp(ik_{n}\vec{R}_{n})\psi_{j}(\vec{r}-\vec{R}_{n}),
$$

(56)

where $s = 1,2,\ldots,m$ labels the vectors in the star, and $j = 1,2,\ldots,p$ labels the functions in the representation $\gamma^{(\rho)}$. It is easy to check that the quasi-Bloch functions (56) form bases for finite-dimensional representations of $G$.

What is, however, more interesting is that the $p \times m$ quasi-Bloch functions in (56) for a fixed $k$ form a basis for a representation of $G_{\hat{k}}$, in general, a reducible one. Indeed, let $(\beta|\hat{v}(\beta))$ be an element of $G_{\hat{k}}$. For any element of $G$ one can write [11]

$$
(\beta|\hat{v}(\beta))(\alpha_{m}|\hat{v}(\alpha_{m})) = (\alpha_{n}|\hat{v}(\alpha_{n}))(\gamma|\hat{v}(\gamma))
$$

(57)

where the elements $(\alpha_{s}|\hat{v}(\alpha_{s}))$ appear in the decomposition (13) and $(\gamma|\hat{v}(\gamma))$ is an element of $G_{\hat{w}}$ up to a Bravais lattice vector. By using Rel. (54), (56) and (57) and the fact that $\beta_{\hat{k}} = \hat{k}$ up to a vector of the reciprocal lattice, we find

$$
(\beta|\hat{v}(\beta))\psi_{jk}(\vec{r}) = \exp(-i\vec{k}_{n}\cdot\vec{q})\sum_{j' = 1}^{p} \psi_{j'}(\gamma)\psi_{j'}(\vec{r})
$$

(58)

Rel. (58) defines a $pm \times pm$ matrix connecting Bloch-like functions for the vector $\hat{k}$. This means that the $pm$ functions $(\psi_{jk})$ (Rel. (56)) form a basis for a $pm$-dimensional representation of $G_{\hat{k}}$. 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 \( \exp(-i \cdot a_k \cdot R_n^{(\gamma)}(\gamma \cdot \hat{v}(\gamma))) \cdot D^{(\cdot)}(\gamma) \), where \( \gamma \) 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 \( (q, \rho) \). The result we
have is that by forming linear combinations (Rel. (56)) of the basis functions
\( \psi_j^{(q, \rho)}(\mathbf{r}) \) for the band representation \( (q, \rho) \), the latter reduces into finite-
dimensional representations of \( G_k \). The difference between the quasi-Bloch
functions \( \psi_{jk}^{(q, \rho)}(\mathbf{r}) \) in Rel. (56) and the Bloch functions \( \psi_{nk}(\mathbf{r}) \)
is that the latter are also eigenfunctions of the Hamiltonian. Correspondingly, \( \psi_{nk}(\mathbf{r}) \)
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 \( \chi^{(q, \rho)}(\mathbf{r}) \) of the \( k \)-component
\( D^{(q, \rho)}(k) \) in (58). The reason for this is that to the character \( \chi^{(q, \rho)}(\mathbf{r}) \)
only those block matrices contribute which are on the diagonal of \( D^{(q, \rho)}(k) \).
Thus, for finding the character \( \chi^{(q, \rho)}(\mathbf{r}) \) of the element \( (\beta | \hat{v}(\gamma)) \) in
Rel. (58) we have to check for which \( (\alpha_{\mathbf{r}} | \hat{v}(\alpha_{\mathbf{r}})) \) Rel. (57) becomes

\[
(\beta | \hat{v}(\beta)) (\alpha_{\mathbf{r}} | \hat{v}(\alpha_{\mathbf{r}})) = (\alpha_{\mathbf{r}} | \hat{v}(\alpha_{\mathbf{r}})) (\gamma | \hat{v}(\gamma))
\]  

(59)

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

\[
(\beta | \hat{v}(\beta)) \psi_{jk}^{(q, \rho)}(\mathbf{r}) = \exp(-i \cdot a_k \cdot R_n^{(\beta)}(\beta \cdot \hat{v}(\beta))) \cdot \sum_{j'=1}^{p} D^{(\rho)}_{j'j}(\gamma) \psi_{jk}^{(q, \rho)}(\mathbf{r})
\]  

(60)

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

\[
\chi^{(q, \rho)}(\beta \cdot \hat{v}(\beta)) = \sum_{n} \exp(-i \cdot a_k \cdot R_n^{(\beta)}(\hat{v}(\beta))) \cdot \chi^{(\rho)}(n) (\alpha_{n}^{-1} \beta \cdot \alpha_{n})
\]  

(61)
where the summation is over all those \( n \) for which \( \alpha_n^{-1} \beta_n \) 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 \( \chi(q^*(\gamma \rho)) \) of the irreducible representation \( \gamma(\rho) \) of \( G_w \) are the phases \( \exp(-ik \cdot \vec{R}(\beta \bar{v}(\beta))) \)

The latter are easily found and, for example, in Ref. (5) they are listed for all the closed strata of \( O^7_h \). 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 \( O^7_h \). 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 \( Ind_G^{G_k}(\gamma \mu) \), where \( \gamma \mu \) 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, \( n^{(q^*, \rho)}_{\mu}(k) \), the irreducible representation \( \gamma \mu \) of \( G_k \) with the character \( \chi^{(k, \mu)}(\gamma \mu) \) is contained in the band representation \( D(q^*, \rho) \). This is given by the elementary formula from the algebra of characters [2]:

\[
n^{(q^*, \rho)}_{\mu}(k) = \frac{1}{|G_k|} \sum_{(\beta \bar{v}(\beta))} \chi_k^{(q^*, \rho)}(\beta \bar{v}(\beta)) \chi^{(k, \mu)^*}(\beta \bar{v}(\beta))
\]

(62)
where \(|g_k|\) is the order of \(G_k T\) and the summation is over the representative elements in the decomposition of \(G_k\) with respect to the translation group \(T\)

\[
G_k = T + (\beta_2 |v(\beta_2)|T + \ldots + (\beta_j |v(\beta_j)|T
\]

(63)

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

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

Having in mind that the character \(\chi_k(q^*, \rho)\) identifies the band representation, one should also be able to use it in the reduction process of a reducible band representation into irreducible-band representations. Thus, given a band representation, \(D\), and its \(k\)-component character \(\chi_k\), one can immediately check whether \(D\) is a reducible band representation by comparing \(\chi_k\) with the list of the characters \(\chi_k(q^*, \rho)\) of all the irreducible-band representations of the given space group. If \(\chi_k\) equals to one of the \(\chi_k(q^*, \rho)\), then it belongs
to an irreducible-band representation. Otherwise D is a reducible-band representation. For finding which of the $\chi_{k}^{(q_{\rho}, p)}$ are contained in $\chi_{k}$ (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 $k$ of finite-dimensional representations of the space group. This feature of going from infinite-dimensional matrices to finite-dimensional ones (of small dimension, in general) by utilizing eigenfunctions of the translation group (Bloch-like functions) is encountered in many problems in solid state physics. It is well known, that in solids one can alternately use either localized orbitals (Wannier function), or extended functions (Bloch functions). Let us show that a similar situation exists also for band representations and that the latter can be defined by employing directly quasi-Bloch functions. Like in the original definition, we start with an irreducible representation $\gamma^{(\rho)}$ of the isotropy group $G_{r}$ of the Wyckoff position $\vec{r}$. (Since $\vec{r}$ appears in the wave function we shall use instead the notations $G_{\omega}$ and $\vec{v}$). This representation and its basis function $\psi_{j}^{(\omega_{\rho})}(\vec{r})$, $j = 1, 2, \ldots, p$ are given by Rels. (53) and (54). By using the decomposition ($G = T \cdot P$)

$$G = G_{q} + (\alpha_{1} \mid \vec{v}(\alpha_{1}) \rangle G_{q} + \ldots + (\alpha_{m} \mid \vec{v}(\alpha_{m}) \rangle G_{q}$$  (64)

one can define the functions $\psi_{j}^{(\omega_{\rho})}(\vec{r})$ for $j = 1, \ldots, p$
and \( s = 1, \ldots, m \) (See Rel. (55)). For those localized orbitals we define the quasi-Bloch functions \( \psi_{j\mathbf{k}, \mathbf{r}}(\mathbf{r}) \) (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 \( G_{\mathbf{k}} \) (See Rel. (58)). Clearly, this representation (of dimension \( mp \)) is, in general, a reducible representation of \( G_{\mathbf{k}} \). Having a representation of \( G_{\mathbf{k}} \) one can employ the usual induction method for inducing a representation of the full space group. By going through this process for each \( \mathbf{k} \) in the Brillouin zone we obtain a direct integral (over \( \mathbf{k} \)) of finite-dimensional representation of \( G \). They together form the band representation of \( G \) for the fixed couple of indices \((q, \rho)\). In other words, by fixing \((q, \mathbf{k})\) we define the set of \( mp \) Bloch functions (Rel. (56)). They form a basis of a representation of \( G_{\mathbf{k}} \). From this representation of \( G_{\mathbf{k}} \) we induce a representation of \( G \). This process has to be repeated for the continuum of \( \mathbf{k} \)-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 \( \mathbf{k} \)-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 \( \mathbf{kq} \)-representation [4,5]. Given a wave function \( \psi(\mathbf{r}) \) in the \( \mathbf{r} \)-representation, its \( \mathbf{kq} \)-representation \( C(\mathbf{k}, \mathbf{q}) \) is

\[
C(\mathbf{k}, \mathbf{q}) = \frac{1}{\Omega} \sum_{n} \exp(i\mathbf{k} \cdot \mathbf{R}_n) \psi(\mathbf{r} - \mathbf{R}_n) \tag{65}
\]

where \( \mathbf{k} \) and \( \mathbf{q} \) are the quasi-momentum and the quasi-coordinate correspondingly, and \( \Omega \) is the volume of a unit cell of the reciprocal lattice. The action of a space group element \( (\alpha|\psi(\alpha)) \) on \( C(\mathbf{k}, \mathbf{q}) \) is as follows [4].
\[(a | \overrightarrow{\nu}(\alpha)) \ C(\overrightarrow{k}, \overrightarrow{q}) = C(\alpha^{-1} \overrightarrow{k}, (\alpha | \overrightarrow{\nu}(\alpha))^{-1} \overrightarrow{q}) \] (66)

If we define the \( C_{j}^{(w, \rho)}(\overrightarrow{k}, \overrightarrow{q}) \) functions for the localized orbitals \( \psi_{j}^{(w, \rho)}(\overrightarrow{r}) \) (Rel. (55)) then the following is clear: on one hand, the basis \( C_{j}^{(w, \rho)}(\overrightarrow{k}, \overrightarrow{q}) \) 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 \((\beta | \overrightarrow{\nu}(\beta))\) of \( G_{k} \) the functions \( C_{j}^{(w, \rho)}(\overrightarrow{k}, \overrightarrow{q}) \) transform exactly like Bloch functions for a given \( \overrightarrow{k} \) (this follows from Rel. (66); one should also pay attention to the fact that under a pure translation \((E | \overrightarrow{R}_{m})\) any \( C(\overrightarrow{k}, \overrightarrow{q}) \) goes into \( \exp(-i \overrightarrow{k} \cdot \overrightarrow{R}_{m}) \ C(\overrightarrow{k}, \overrightarrow{q}) \). 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 $\chi_k$ of its k-component (Formula 61). In particular, this means that two band representations $(q,\rho)$ and $(q',\rho')$ (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:

$$\chi_k^{(q,\rho)}(\beta|\vec{v}(\beta)) = \chi_k^{(q',\rho')} (\beta|\vec{v}(\beta))$$  \hspace{1cm} (67)

for all elements $(\beta|\vec{v}(\beta))$ $(\ell\ell' = \ell')$ 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 $(q,\rho)$ and $(q',\rho')$ are inequivalent. This fact will extensively be used in verifying the inequivalency of band representations. It was already pointed out that for finding the irreducible-band representations of a space group it is sufficient to consider the induction from irreducible representations of maximal isotropy groups only. However, two things might happen. First, some of the band representations induced in such a way might turn out to be reducible-band representations [17]. Second, among the irreducible-band representations induced from irreducible representations of maximal isotropy groups some might be equivalent. In order to find all the inequivalent irreducible-band representations of a space group the following procedure will be used: We construct all the band representations for all the closed strata and we exclude the above-mentioned two kinds:

1) the reducible-band representations and 2) the equivalent ones. It turns out that there are relatively few band representations that are induced from maximal
isotropy groups and that belong to these two kinds of band representations. In what follows we shall call them the exceptional ones. Since relatively few are exceptional it is not hard to tabulate them. Knowing this list and knowing that all irreducible-band representations are induced from irreducible representations of maximal isotropy groups one can deduce the full list of all the inequivalent irreducible-band representations.

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

Let \((q, \rho)\) 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 \(\gamma'\) of a non-conjugate maximal isotropy group \(G_{r'}\) to be equivalent to \((q, \rho)\) is for a subgroup \(G'' = G_r \cap G_{r'}\) (where \(G_r \cap G_{r'}\) is the intersection of \(G_r\) and \(G_{r'}\)) to exist such that both \(\gamma^{(\rho)}\) and \(\gamma'\) are induced representations from a representation \(\gamma''\) of \(G''\).

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 \( \gamma'' \) 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 \( \gamma^{(p)} \) and \( \gamma' \) are not induced from a single representation \( \gamma'' \) then \( (q,\rho) \) and \( D^{(q')} \) are inequivalent. From here it will follow that when \( (q,\rho) \) and \( D^{(q')} \) are equivalent they are necessarily induced from \( \gamma'' \). 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 \( \alpha_n \) commute with \( \beta \), Formula (61) will assume the following form

\[
\chi_k^{(q,\rho)}(\beta|\nu(\beta)) = \chi^{(\rho)}(\beta) \Sigma_n \exp(-i k \cdot R^{(\beta)}|q_n \nu(\beta))
\]  

(68)

Here \( \chi^{(\rho)}(\beta) \) is a character for a one-dimensional representation of the point group of \( G_r \) (since \( G_r \) is assumed to be Abelian, all its irreducible representations are one-dimensional). Formula (68) shows that the character \( \chi_k \) of the induced representation is zero for elements not belonging to \( G_r \) and it is
given by $\chi^{(p)}(\beta)$ multiplied by a sum of the phase factors when $\beta$ 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

$$\chi^{(q',p)}_k(\beta | v(\beta)) = \chi^{(q')}_k(\beta | v(\beta))$$  \hspace{1cm} (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 $q' \neq q$. 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 $r' = 0$. Then the stars of $r'$ and $r$ in the Wigner-Seitz cell will be (See decomposition (13))

$$\mathbf{q}' = 0, \mathbf{v}(\alpha_2), \ldots, \mathbf{v}(\alpha_m)$$  \hspace{1cm} (70)$$

$$\mathbf{q}, (\alpha_2 | \mathbf{v}(\alpha_2))\mathbf{q}, \ldots, (\alpha_m | \mathbf{v}(\alpha_m))\mathbf{q}$$  \hspace{1cm} (71)$$

The sum in Rel. (68) will correspondingly become: for $q' = 0$ (we denote it by $\Sigma_0$)

$$\Sigma_0 = \Sigma \exp(-ik \cdot \mathbf{v}(\alpha_n))$$  \hspace{1cm} (72)$$
and for $q$

$$\Sigma \exp(-ik \cdot \mathbf{R}^{q_n})$$  \hspace{1cm} (73)$$

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

$$\Sigma \exp(-ik \cdot \mathbf{R}^{n}) = \exp(-ik \cdot \mathbf{R}^{q_n}) \Sigma \exp(-ik \cdot [\mathbf{R}^{q_n} - \mathbf{R}^{q}])$$  \hspace{1cm} (74)$$

One can see that
\[ \tilde{R}_{Qn}^{\beta} - \tilde{R}_{Q}^{\beta} = \tilde{R}_{Q}^{\beta}(\alpha_n^v) + \alpha_n \tilde{R}_{Q}^{\beta} - \tilde{R}_{Q}^{\beta} \]

where we have explicitly used the fact that \( \beta \) and \( \alpha_n \) commute (\( P \) is abelian).

With the aid of Expression (75), Rel. (74) becomes

\[ \sum_n \exp(-i\vec{k} \cdot \tilde{R}_{Qn}^{\beta}) = \exp(-i\vec{k} \cdot \tilde{R}_{Q}^{\beta}) \exp(-i[\alpha_n^{-1} \vec{k} - \vec{k}] \cdot \tilde{R}_{Q}^{\beta}) \sum_o \]

(76)

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

\[ \alpha_n^{-1} \vec{k} - \vec{k} = \vec{k} \]

(77)

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

\[ \sum_n \exp(-i\vec{k} \cdot \tilde{R}_{Qn}^{\beta}) = \exp(-i\vec{k} \cdot \tilde{R}_{Q}^{\beta}) \sum_o \]

(78)

Since there is always a \( \beta \) for which \( \tilde{R}_{Q}^{\beta} \neq 0 \) (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

\[ \sum_n \exp(-i\vec{k} \cdot \tilde{R}_{Qn}^{\beta}) \neq \sum_o \]

(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 \( k = 0 \) in the Brillouin zone the quasi-Bloch functions \( \psi_{j_n} \) in Rel. (56) form a basis for an induced representation of the point group \( G_{k=0} \) 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 \( k \) for which \( G_r \) is a subgroup of \( G_k \). Clearly, when \( k = 0 \), \( G_r \) is always a subgroup of \( G_{k=0} \) and it follows that the character formula (61) for \( k = 0 \) will give the character of the induced representation of \( G_{k=0} \) from the representation \( \gamma^{(\rho)} \) of \( G_r \) (See also Formula (32)):

\[
\chi_{0}^{(q,\rho)}(\beta | \nu(\beta)) = \sum_{\alpha} \chi^{(\rho)}(\alpha^{-1}_n \beta \alpha_n) \quad (80)
\]

where again the summation is on all those \( n \) for which \( \alpha^{-1}_n \beta \alpha_n \) 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 \( (q,\rho) \) 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 \( \gamma' \) 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 \((q,\rho)\) and \( D(q') \) are also non-equivalent and the proof of part 2 for these cases is finished. When \( \gamma(\rho) \) and \( \gamma' \) 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 \( k \neq 0 \) (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 \( \exp(-i \mathbf{k} \cdot \mathbf{R}^{(q)}(\beta)) \) in Rel. (61) for the induction from the groups \( G_r \) and \( G_r' \) (for some \( \beta \) belonging to the intersections \( G_r \cap G_r' \)) and correspondingly Rel. (67) will not hold for \( k \neq 0 \). 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 \( \gamma' \) 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 \( \gamma'' \) 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 \( (q, \rho) \) 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 \( \gamma'' \) of \( G_r'' \) a multidimensional representation of \( G_r \) can be induced then one ends up with the following list of groups for \( G_r'' \):

\[
C_4(D_4), \quad C_{2v}(D_{2d}), \quad C_3(D_3), \quad C_6(D_6)
\]  

(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 \( \gamma' \) are inducible from \( \gamma'' \) of \( G_r'' \). The latter is then an isotropy group by itself. This completes the proof of our criterion.

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

**Lemma 4.** When a non-polar group \( G_r \) is an isotropy group, then \( N_G(G_r) = G_r \)
i.e. it is equal to its normalizer.
We remark that the points of the normalizer orbit $N_G(G_r) \cdot \vec{r}$ have all the same isotropy group $G_r$. Let $\vec{r}' \neq \vec{r}$ be one of them and $\vec{r}(\lambda) = \lambda \vec{r}' + (1-\lambda) \vec{r}$, the set of points ($\lambda \in \mathbb{R}$) of the straight line $\vec{r} \vec{r}'$. Then $G_r \cdot \vec{r}(\lambda) = \vec{r}(\lambda)$, so $G_r$ is a polar group.

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

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

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

(82)

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

$$Q_r \sim Q_r' = N_{P_r}(P_r)/(P_r \cdot C_{P_r}(P_r))$$

(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 $Q_r'$:

$$
\begin{array}{c|c|c|c|c|c|c|c|c}
 P_r & C_3 & C_{3v} & C_6 & C_{6v} & C_{2v} & C_4 & C_{4v} \\
\hline
 N_{P_r} < D_{6h} & & & & & D_{4h} \\
\hline
 Q_r' < Z_2 & 1 & Z_2 & 1 & Z_2 & Z_2 & 1 \\
\end{array}
$$

(84)
Since $Q'_{\mathbf{r}} < Z_2$, these exceptional equivalences occur at most for pairs of representations $\gamma^{(p)}_{G_{\mathbf{r}}}$, $\gamma^{(p')}_{G'_{\mathbf{r}}}$ at the same site. A direct computation yields easily that if $\mathbf{r} = \mathbf{r}'$ and $G_{\mathbf{r}} = G'_{\mathbf{r}} = \{ (\beta, \mathbf{v}(\beta) + \mathbf{r}_B) \}$ then $\tilde{\mathbf{r}}' - \tilde{\mathbf{r}} \in \bigcap_{\beta \in \mathbf{r}} \text{Ker}(I-\beta)$ that is $\mathbf{r}$ and $\mathbf{r}'$ are on the axis left invariant by $G_{\mathbf{r}} = C_{2\nu}$ or $C_n$, $n = 3, 4, 6$. Moreover the element of the normalizer $N_G(G_{\mathbf{r}})$ which acts non trivially on $\hat{G}_{\mathbf{r}}$ 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 $G_{\mathbf{r}} = C_n$, $n = 3, 4, 6$ or helicoidal rotation $(\beta_4, \mathbf{v}(\beta))$ $(\beta_4$ of order 4, $\mathbf{v}(\beta)$ parallel to this axis) for $G_{\mathbf{r}} = C_{2\nu}$. Hence, to find this exceptional equivalence of irreducible band representations induced by inequivalent unireps of $G_{\mathbf{r}}$ for the same site $\mathbf{r}$, 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 $C_{2\nu}$ and a corresponding helicoidal rotation $(\beta_4, \mathbf{v}(\beta))$, 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 $(q, \rho)$ and $D^{(q')}_{(\mathbf{r})}$ induced from $\gamma^{(p)}$ (irreducible representation) and $\gamma'$ of maximal isotropy groups $G_{\mathbf{r}}$ and $G'_{\mathbf{r}}$ correspondingly are equivalent if and only if $\gamma^{(p)}$ and $\gamma'$ are by themselves induced from a representation $\gamma''$ of $G_{\mathbf{r}''} = G_{\mathbf{r}} \cap G'_{\mathbf{r}}$. With this in mind it is simple to find the equivalent band representations corresponding to $\mathbf{r}' \neq \mathbf{r}$. In looking for them one has to consider only multidimensional representations $\gamma^{(p)}$ because one-dimensional one cannot be induced representations.
Also we have to consider only the cases when \( G_x \) has an isotropy subgroup \( G_x'' \), 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 \( (q,\rho) \) 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 \( \gamma' \) of \( G_x' \). In the latter case \( (q,\rho) \) (and also \( D(q') \)) is a reducible band representation.

If \( (q,\rho) \) is equivalent to \( D(q') \) which is induced from irreducible representations only (\( \gamma' \) has then a superscript and is denoted \( \gamma^{(\rho)} \)) then \( (q,\rho) \) is an irreducible-band representation. If we add to this the information we derived about equivalent band representations stemming 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

\[
101,103,105,108,130,137,138,158,159,161
\]

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

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

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

\[124, 131, 132, 139, 140, 163, 165, 167, 188, 190\]
\[192, 193, 207, 208, 210, 211, 215, 222, 223, 224\]
\[226, 228, 229, 230.\]
VII. Irreducible Band-Representations of Space Groups in 2 Dimensions.

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

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

The structure and classification of band representations of space groups is investigated in this paper. It is shown that band representations are induced representations from finite order isotropy groups in the physical space of the crystal. This fact creates an elegant framework for dealing with band representations by employing the concepts of strata and their little groups. In this framework band representations are specified by a pair of indices $(\mathbf{q}, \rho)$ where $\mathbf{q}$ is the Wyckoff position (or symmetry center in the Wigner-Seitz cell) and $\rho$ denotes an irreducible representation $\gamma^{(\rho)}$ of the isotropy group $G_{\mathbf{r}}$. This is to be compared with irreducible representations of space groups which are also specified by a pair of indices $(\mathbf{k}, m)$ where $\mathbf{k}$ is a symmetry point in the inverse space (the Brillouin zone) with its isotropy group $G_{\mathbf{k}}$ and $m$ denotes an irreducible representation $\Gamma_{m}$ of $G_{\mathbf{k}}$. 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 Ref. (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 $\Gamma_r$ and $\Gamma_{r'}$, 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 $\Gamma_r$ is equivalent to a reducible band representation, e.g. $(\vec{q'}, \rho')$ which is induced from a reducible representation $\gamma$ of $\Gamma_{r'}$. 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 groups). 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.