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Band representations of space groups

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All the irreducible band representations of a space group are shown to be induced from a set of inequivalent relevant symmetry centers in the Wigner-Seitz cell. A connection is established between representations and band representations of space groups by using the Born—von Kármán boundary conditions. Continuity chords are used for proving the equivalency theorem which enables one to distinguish between equivalent and inequivalent band representations. As examples we consider a one-dimensional crystal and the D_{6h}^4 space group for a hexagonal close-packed structure.

I. INTRODUCTION

In solids one interchangeably uses extended and localized functions. The extended or the Bloch functions were first introduced in the classical paper by Bloch[1] and they have been since widely used in solid-state physics. In the same paper Bloch discussed also the localized functions (atomic orbitals) but their use during the years has been much less widespread. The localized orbitals when orthonormalized on different sites of the Bravais lattice are known in solids as Wannier functions.[2]

Conventionally, band-structure calculations have been carried out by using Bloch functions $\psi_{nk}(\vec{r})$. They are specified by a band index n and the quasimomentum $\vec{k}$. In the symmetry specification of Bloch functions an important role is played by the irreducible representations of space groups.[3,4] Each $\psi_{nk}(\vec{r})$ is assigned a wave vector $\vec{k}$ which defines the behavior of the Bloch function under translations. The additional symmetry is defined by all those point-group elements that commute with the translations on the space of functions ψ_k for the given wave vector $\vec{k}$. In this symmetry specification the translations play a primary role and they define the extended nature of the Bloch functions.

An alternative approach to band calculations is based on localized orbitals.[5–8] In this approach one specifies the symmetry of the localized orbitals by means of the point symmetry of the space group. Such a specification assigns a symmetry label to the localized orbitals and correspondingly to the band of the solid as a whole entity. Unlike the Bloch functions' approach where the symmetry is specified at each point $\vec{k}$ in the Brillouin zone the approach by localized functions leads to a global symmetry label for a band in a solid. In a fundamental paper by Des Cloizeaux[9] it was shown how Bloch functions belonging to a given band can be expanded in symmetry-adapted Wannier functions corresponding to the same band. More recently, the symmetry type of a band via localized orbitals has been used in a number of band-calculation schemes in solids.[10–13]

Despite the fact that Bloch and Wannier functions can interchangeably be used for spanning a given band of a solid there is nevertheless a fundamental difference between them: The Bloch functions are eigenfunctions of the Schrödinger equation for an electron in a periodic potential while the Wannier functions are not. One of the consequences of this difference is in the level of the application of group theory to these two kinds of functions. The Bloch functions being eigenfunctions of the Schrödinger equation fit well into the general framework of representation theory.[14]

This is not the case with the Wannier functions or the localized orbitals to which the usual representation theory is not applicable. In a recent series of papers[15,16] it was shown that the symmetry of localized orbitals can be described by band representations of space groups. Unlike usual representations that correspond to a single energy of the eigenvalue equation, band representations correspond to bands of energy. This makes the band representations suitable for specifying symmetry types of localized orbitals and correspondingly of bands as whole entities in solids.

In this paper the band-space concept is used for defining bases of band representations. A band space is a set of f-localized orbitals which define at each point in the Brillouin-zone f-independent Bloch functions. Each band representation is shown to be equivalent to its canonical form. The latter is used in order to prove that all the irreducible band representations of a space group are induced from a set of inequivalent relevant-symmetry centers in the Wigner-Seitz cell. In general, not all such irreducible band representations are inequivalent. A connection is established between representations and band representations of a space group by using the Born—von Kármán boundary conditions. Continuity chords are used for proving the equivalency theorem, which serves as a criterion for distinguishing between equivalent and inequivalent band representations. As examples we consider a one-dimensional crystal and the hexagonal close-packed structure (D_{6h}^4).

II. BAND SPACE

One of the most striking features of the energy spectrum in solids is its band structure. The concept of a band was first introduced by Bloch[1] and has since been widely used in solids. In describing physical phenomena one usually focuses attention on an isolated band which can be either simple or composite.[9,10] A band is simple if there is one Bloch state corresponding to each quasimomentum $\vec{k}$ in the Brillouin zone. If there is a number of Bloch states, say f, for each point $\vec{k}$, then the band is called composite. Correspondingly, the space spanned by all the Bloch functions when $\vec{k}$ varies in the whole Brillouin zone is called the $\vec{f}$-branch band space.[16] There is much freedom in choosing the functions that span the band space. The Bloch functions $\psi_{nk}(\vec{r})$ constitute only one possible choice. Alternatively, one can choose another set of functions $\varphi_{sk}(\vec{r})$ defined by the following transformation:

$$\varphi_{sk}(\vec{r})=\sum_{s'=1}^{f} T_{s's}(\vec{k})\psi_{s'k}(\vec{r}) \ . \quad (1)$$

These functions will also span the same band space if $T(\vec{k})$ is a nonsingular matrix at each $\vec{k}$ in the Brillouin zone. Clearly, the new functions $\varphi_{sk}(\vec{r})$ preserve the index $\vec{k}$, meaning that they are eigenfunctions of the translation operators on the Bravais lattice. This also means that like the Bloch functions, the functions $\varphi_{sk}(\vec{r})$ are of extended nature.

An alternative definition of a band space can be given by using localized orbitals. Let $a_i(\vec{r})$, $i=1,\ldots,f$ be f-square-integrable linearly independent functions and let us build out of them f-Bloch-type functions $\varphi_{ik}(\vec{r})$:

$$\varphi_{ik}(\vec{r})=\Omega^{-1/2}\sum_{m}\exp(i\vec{k}\cdot\vec{R}_m)a_i(\vec{r}-\vec{R}_m) \ . \quad (2)$$

Ω is the reciprocal-lattice unit cell volume. The $fa_i(\vec{r})$ orbitals form an f-branch band space if at no point $\vec{k}$ in the Brillouin zone can one construct a vanishing linear combination

$$\sum_{i=1}^{f}\alpha_i(\vec{k})\varphi_{ik}(\vec{r})=0 \ . \quad (3)$$

Here $\alpha_i(\vec{k})$ are arbitrary $\vec{k}$-dependent functions. The condition expressing the impossibility of building relation (3) insures that there are f-independent Bloch functions (2) at each point $\vec{k}$ in the Brillouin zone. The $fa_i(\vec{r})$, $i=1,\ldots,f$ orbitals span therefore an f-branch band space in very much the same way as the Bloch functions $\psi_{nk}(\vec{r})$ in the previous definition. There is, however, a significant difference between the two definitions of a band space. The one based on the extended (Bloch) functions $\psi_{nk}(\vec{r})$ is local in $\vec{k}$ space. In this definition we assign f Bloch functions to each point k in the Brillouin zone. A connection between the functions $\psi_{nk}(\vec{r})$ at different points $\vec{k}$ is achieved by demanding that they belong to a given energy range via the Schrödinger equation that they satisfy. The continuity of the energy range introduces some continuity on the wave functions $\psi_{nk}(\vec{r})$ as functions of $\vec{k}$. On the other hand, the band-space definition based on the localized orbitals $a_i(\vec{r})$ is local in $\vec{r}$ space. Each such orbital leads directly, according to relation (2), to Bloch-type functions $\varphi_{ik}(\vec{r})$ in the whole Brillouin zone. This means that the connection between the functions $\varphi_{ik}(\vec{r})$ for different $\vec{k}$'s follows from the fact that all of them are built from the same orbital $a_i(\vec{r})$. The continuity properties of $\varphi_{ik}(\vec{r})$ as a function of $\vec{k}$ is fully defined by the orbital $a_i(\vec{r})$. In this definition of the band space the energy spectrum of the solid doesn't appear at all. This might seem as a disadvantage. However, since one is free to choose the $a_i(\vec{r})$ completely arbitrarily this approach enables one to find all those band spaces that can, in principle, be built from localized orbitals. For this reason, the band-space definition based on localized orbitals turns out to be useful in the construction of band representations of space groups.

III. BAND REPRESENTATIONS OF SPACE GROUPS

According to the definition, a band space contains an infinite set of functions (for an infinite crystal). This is seen either from the fact that the number of Bloch states in the Brillouin zone is infinite or from the fact that there is an infinite set of localized orbitals corresponding to different sites $\vec{R}_m$ in the Bravais lattice. It turns out that by using the concept of band representations[15] it becomes possible to list the symmetries of all those band spaces that can, in principle, span actual bands in solids. Let us review the main concepts of Ref. 15 in the framework of band spaces.

The definition of a band representation can conveniently be given in the kq representation.[17] Let G be a space group with elements $(\alpha \mid \vec{t}\,)$, α being a point-group element and $\vec{t}$ a translation.[4] Although G is assumed to be a space group the results in this paper can straightforwardly be extended to double-[18] and magnetic-space groups.[19] By definition the functions $a_i(\vec{k},\vec{q})$, $i=1,\ldots,f$ of a band space form a basis for a band representation if

$$(\alpha \mid \vec{t}\,)a_i(\vec{k},\vec{q})=\sum_{i'=1}^{f} D_{i'i}[(\alpha \mid \vec{t}\,),\vec{k}]a_{i'}(\vec{k},\vec{q})\ . \tag{4}$$

The matrix D in (4) is k dependent and nonsingular at each $\vec{k}$ in the Brillouin zone. In the kq representation the band representation in relation (4) appears with an f-dimensional matrix $D(\vec{k})$. However, since $\vec{k}$ is a variable the band representation is actually infinite dimensional.

If the functions $a_s'(\vec{k},\vec{q})$ form a new basis of the band space then the equivalent band representation D' will be given by the matrices

$$D'[(\alpha \mid \vec{t}\,),\vec{k}]=T^{-1}(\vec{k})D[(\alpha \mid \vec{t}\,),\vec{k}]T(\alpha^{-1}\vec{k})\ . \tag{5}$$

In the matrix on the right the vector $\vec{k}$ is replaced by $\alpha^{-1}\vec{k}$. The band representation $D[(\alpha \mid \vec{t}\,),\vec{k}]$ is reducible if a matrix $T(\vec{k})$ exists for which all the matrices in (5) assume a quasidiagonal form. If such a matrix T does not exist then $D[(\alpha \mid \vec{t}\,),\vec{k}]$ is called an irreducible band representation.

In general, the matrices of the band representations are nonunitary. However, if the basis is chosen to be orthonormal,

$$\Omega \int a_s^*(\vec{k},\vec{q})a_{s'}(\vec{k},\vec{q})d\vec{q}=\delta_{ss'}\ , \tag{6}$$

then, as can be checked, the band representation satisfies a unitarity condition

$$\Omega^{-1}\int d\vec{k}\,D^{\dagger}[(\alpha \mid \vec{t}\,),\vec{k}]D[(\alpha \mid \vec{t}\,),\vec{k}]=E\ . \tag{7}$$

In (7) E is a unit matrix. The basis functions $a_s(\vec{k},\vec{q})$ satisfying relation (6) are the Wannier functions of the problem.[2]

In the construction of band representations of space groups it is convenient to work with the concepts of a symmetry center $\vec{q}$ in the Wigner-Seitz cell and the corresponding symmetry group G_q. For each quasicoordinate $\vec{q}$ in the Wigner-Seitz cell[20] we define a symmetry group G_q with the element $(\gamma \mid \vec{c}\,)$ that leave $\vec{q}$ invariant:

$$(\gamma \mid \vec{c}\,)\vec{q}=\vec{q}+\vec{R}_q^{(\gamma \mid \vec{c}\,)}\ . \tag{8}$$

Here $\vec{R}_q^{(\gamma \mid \vec{c}\,)}$ is a Bravais-lattice vector depending on both the center $\vec{q}$ and the group element $(\gamma \mid \vec{c}\,)$.

In relation (8) the point-group element γ is assumed to be written with respect to the origin of the crystal. When written with respect to the symmetry center $\vec{q}$, the same element will become γ_q [page 15, Ref. (21)]:

$$\gamma_q=(E \mid \bar{\vec{q}}\,)\gamma(E \mid \vec{q}\,)=(\gamma \mid \vec{c}-\vec{R}_q^{(\gamma \mid \vec{c}\,)})\ , \tag{9}$$

where E is the unit element of the point group. What relation (9) shows is that around the symmetry center $\vec{q}$ the point-group elements of G_q appear with primitive translations. Together with a symmetry center $\vec{q}$ we define its star. This can be done as follows. The space group G can be decomposed into cosets with respect to its subgroup G_q:

$$G=G_q+(\alpha_2 \mid \vec{a}_2)G_q+\cdots+(\alpha_s \mid \vec{a}_s)G_q\ , \tag{10}$$

where $(\alpha_i \mid \vec{a}_i)$ are elements not belonging to G_q and representing different cosets. With the decomposition (10) in mind the star of $\vec{q}$ is defined as containing the following vectors:

$$\vec{q},\vec{q}_2=(\alpha_2 \mid \vec{a}_2)\vec{q},\ldots,\vec{q}_s=(\alpha_s \mid \vec{a}_s)\vec{q}\ . \tag{11}$$

The construction of band representations of a space group G can be carried out in the following way.[15] Let $G_{q'}$ by a subgroup of G corresponding to the symmetry center $\vec{q}\,'$ (we use the prime in order to distinguish the symmetry center $\vec{q}\,'$ from the quasicoordinate $\vec{q}$ of the kq representation). As was already mentioned above, the point group elements of $G_{q'}$ appear with primitive translations when written with respect to the center $\vec{q}\,'$ itself [relation (9)]. We denote by $g_{q'}$ the point group of $G_{q'}$ and let $D^{(l)}(\gamma)$, $l=1,\ldots,m$ be the irreducible representations of $g_{q'}$. One can check (see Appendix) that the correspondence

$$(\gamma \mid \vec{c}\,):D^{(q',l)}[(\gamma \mid \vec{c}\,),\vec{k}]=\exp(-i\vec{k}\cdot\vec{R}_{q'}^{(\gamma \mid \vec{c}\,)})D^{(l)}(\gamma)\ , \tag{12}$$

defines a band representation of the space group $G_{q'}$. The Bravais-lattice vector $\vec{R}_{q'}^{(\gamma \mid \vec{c}\,)}$ is given in relation (8).

The dependence on the symmetry center $\vec{q}\,'$ in the band representation (12) appear in the exponential factor $\exp(-i\vec{k}\cdot\vec{R}_{q'}^{(\gamma|\vec{c})})$. In Table I we list these factors for the symmetry centers[22] $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$ of the space group D_{6h}^4. We shall call (12) the canonical form of a band representation. It is clear that if we apply the transformation (5) to the canonical form (12) we will obtain a band representation which will no longer have the form of a k-dependent exponent multiplied by a k-independent matrix. We shall return to this problem later.

Having a band representation of $G_{q'}$ it is a simple matter to induce a band representation of the full space group G. Thus, if the functions $C_{iq'}^{(l)}(\vec{k},\vec{q})$ with $i=1,\ldots,r$ form a basis for a band representation of $G_{q'}$ then it is clear that the set of rxs functions

$$C_{iq'}^{(l)}\ ,\ C_{iq_2'}^{(l)}=(\alpha_2\,|\,\vec{a}_2)C_{iq'}^{(l)},\ \ldots\ ,\ C_{iq_s'}^{(l)}=(\alpha_s\,|\,\vec{a}_s)C_{iq'}^{(l)} \tag{13}$$

form a basis for a band representation of G. This band representation can be written down in very much the same way as in the induction process of usual representations of space groups. The following relation holds for an arbitrary element $(\alpha\,|\,\vec{a})$ of G^4:

$$(\alpha\,|\,\vec{a})(\alpha_m\,|\,\vec{a}_m)=(\alpha_n\,|\,\vec{a}_n)(\gamma'\,|\,\vec{c}\,')\ , \tag{14}$$

where $(\alpha_m\,|\,\vec{a}_m)$ are the elements in the decomposition (10) and $(\gamma'\,|\,\vec{c}\,')$ belongs to $G_{q'}$. With the notation in (13) the induced band representation of the space group G assumes the form

$$(\alpha\,|\,\vec{a})C_{iq_m'}^{(l)}=\sum_{j=1}^{r}D_{ji}^{(q',l)}[(\gamma'\,|\,\vec{c}\,'),\alpha^{-1}\vec{k}]C_{jq_n'}^{(l)}\ . \tag{15}$$

This relation defines the matrix $D^{(q'^*,l)}[(\alpha\,|\,\vec{a}),\vec{k}]$ of the induced band representation corresponding to the element $(\alpha\,|\,\vec{a})$. In correspondence with formula (12), formula (15) will be called the canonical form of a band representation of the whole space group. Band representations in their canonical form are of much importance because as is shown below any band representation of a space group can be brought to the canonical form by the transformation (5).

Having established a process for constructing band representations the next question to ask is how to construct all of them. This question can be solved by introducing the concept of relevant symmetry centers. We shall do it by first defining the equivalency of symmetry centers. Two symmetry centers $\vec{q}_1$ and $\vec{q}_2$ are called equivalent if their groups coincide, $G_{q_1}=G_{q_2}$, and if their factor systems $\exp(-i\vec{k}\cdot\vec{R}_{q_1}^{(\gamma|\vec{c})})$ and $\exp(-i\vec{k}\cdot\vec{R}_{q_2}^{(\gamma|\vec{c})})$ are equivalent, meaning that

$$\begin{aligned}\exp(-i\vec{k}\cdot\vec{R}_{q_2}^{(\gamma|\vec{c})})&=\exp(-i\vec{k}\cdot\vec{R})\\&\quad\times\exp(-i\vec{k}\cdot\vec{R}_{q_1}^{(\gamma|\vec{c})})\\&\quad\times\exp(i\gamma^{-1}\vec{k}\cdot\vec{R})\ ,\end{aligned} \tag{16}$$

where $\vec{R}$ is a Bravais-lattice vector, and $(\gamma\,|\,\vec{c})$ are the elements of G_{q_1} [see relation (5) with $T(\vec{k})=\exp(i\vec{k}\cdot\vec{R})$]. The simplest case of equivalency is when $\vec{q}_2$ differs from $\vec{q}_1$ by a Bravais-lattice vector $\vec{R}$, $\vec{q}_2=\vec{q}_1+\vec{R}$. In this case, $G_{q_2}=G_{q_1}$ and relation (16) can be easily checked to hold. However, we can have symmetry centers $\vec{q}_1$ and $\vec{q}_2$ that are equivalent [$G_{q_1}=G_{q_2}$ and relation (16) is satisfied], but the centers themselves do not differ by a Bravais-lattice vector. An example are the symmetry centers $q_e=(0,0,z)$ and $q_{e2}(0,0,\bar{z})$ of D_{6h}^4 (see Ref. 22) with the same symmetry group C_{3v} and identical factor systems $\exp(-i\vec{k}\cdot\vec{R}^{(\gamma|\vec{c})})$ (they equal 1 for both centers). These two symmetry centers are therefore equivalent according to the above definition despite the fact that they differ by the vector $(0,0,2z)$. In constructing band representations, equivalent symmetry centers will, clearly, lead to equivalent band representations.

Next, let us define the concept of subequivalency. $\vec{q}_2$ with the symmetry G_{q_2} is subequivalent to $\vec{q}_1$, with the symmetry G_{q_1} if G_{q_2} is a subgroup of G_{q_1} and if on all elements $(\gamma\,|\,\vec{c})$ of G_{q_2} the phase factors satisfy the equivalency condition (16). Thus, $\vec{q}_e=(0,0,z)$ with the symmetry group C_{3v}, is subequivalent to $\vec{q}_a=(0,0,0)$ with the symmetry D_{3d}, because C_{3v} is a subgroup of D_{3d} (see Ref. 22) and on C_{3v} these two centers have identical factor systems. In general, a given symmetry center $\vec{q}$ can be subequivalent to a number of symmetry centers $\vec{q}_1,\vec{q}_2,\ldots,\vec{q}_r$. Thus, it can be checked that the above considered symmetry center $\vec{q}_e=(0,0,z)$ of D_{6h}^4 is subequivalent to all the following centers: $\vec{q}_a=(0,0,0)$, $\vec{q}_{a2}=(0,0,c/2)$, $\vec{q}_b=(0,0,c/4)$, $\vec{q}_{b2}=(0,0,\bar{c}/4)$. In particular, a general symmetry center $\vec{q}$ with translational symmetry only is clearly subequivalent to all the other symmetry centers in the Wigner-Seitz cell. If in constructing band representations of a given space group one considers all the symmetry centers $\vec{q}_1,\vec{q}_2,\ldots,\vec{q}_r$ to which $\vec{q}\,'$ is subequivalent, then there should be no need to consider also $\vec{q}\,'$. The reason for this is as follows. $G_{q'}$ is a subgroup of

TABLE I. Phase factors $\exp(-i\vec{k}\cdot\vec{R}_q^{(\gamma|\vec{c})})$ for the relevant symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, $\vec{q}_d$, and their stars. Hexagonal coordinate axes are used (Refs. 21 and 22). The letter C denotes a rotation, the subscript gives the order of rotation and the superscript the rotation axis. Thus, C_2^3 is a rotation by $2\pi/3$ around the axis 3 (Ref. 21). The letter S denotes a rotation with a reflection in the plane perpendicular to the rotation axis; the subscript and the superscript have the same meaning as for C. The letter σ denotes a reflection in a plane; the superscript gives the direction of the plane. Thus, σ^{xy} is a reflection perpendicular to the axis (xy). I is the inversion. The elements of the group C_{3v} $(E, C_3^z, C_3^{2z}, \sigma^{xy}, \sigma^x, \sigma^y)$ and IC_{3v} are pure point-group elements. On the other hand, all the elements $\sigma^z C_{3v}$ and $\sigma_2^z C_{3v}$ appear with the partial translation $(0,0,c/2)$ (Ref. 21). $\xi=\exp(ik_xa)$, $\eta=\exp(ik_ya)$, $\zeta=\exp(ik_zc)$.

					$\exp(-i\vec{k}\cdot\vec{R}_q^{(\gamma\|\vec{c})})$							
D_{3d} \ $\vec{q}$	E	C_3^z	C_3^{2z}	σ^{xy}	σ^x	σ^y	I	S_6^z	S_6^{5z}	C_2^{xy}	C_2^x	C_2^y
$\vec{q}_a=(0,0,0)$	1	1	1	1	1	1	1	1	1	1	1	1
$\vec{q}_{a2}=(0,0,c/2)$	1	1	1	1	1	1	ζ	ζ	ζ	ζ	ζ	ζ
D_{3h} \ $\vec{q}$	E	C_3^z	C_3^{2z}	σ^{xy}	σ^x	σ^y	σ^z	S_3^z	S_3^{2z}	C_2^3	C_2^1	C_2^2
$\vec{q}_b=(0,0,c/4)$	1	1	1	1	1	1	1	1	1	1	1	1
$\vec{q}_{b2}=(0,0,\bar{c}/4)$	1	1	1	1	1	1	ζ^*	ζ^*	ζ^*	ζ^*	ζ^*	ζ^*
$\vec{q}_c=(a/3,\bar{a}/3,c/4)$	1	$\xi^{1/2}\eta^*$	$\xi\eta^{*1/2}$	1	$\xi\eta^{*1/2}$	$\xi^{1/2}\eta^*$	1	$\xi^{1/2}\eta^*$	$\xi\eta^{*1/2}$	1	$\xi^{1/2}\eta^*$	$\xi\eta^{*1/2}$
$\vec{q}_{c2}=(\bar{a}/3,a/3,\bar{c}/4)$	1	$\xi^{*1/2}\eta$	$\xi^*\eta^{1/2}$	1	$\xi^*\eta^{1/2}$	$\xi^{*1/2}\eta$	ζ^*	$\eta(\xi^{1/2}\zeta)^*$	$\eta^{1/2}(\xi\zeta)^*$	ζ^*	$\eta(\xi^{1/2}\zeta)^*$	$\eta^{1/2}(\xi\zeta)^*$
$\vec{q}_d=(a/3,\bar{a}/3,\bar{c}/4)$	1	$\xi^{1/2}\eta^*$	$\xi\eta^{*1/2}$	1	$\xi\eta^{*1/2}$	$\xi^{1/2}\eta^*$	ζ^*	$\xi^{1/2}(\eta\zeta)^*$	$\xi(\eta^{1/2}\zeta)^*$	ζ^*	$\xi^{1/2}(\eta\zeta)^*$	$\xi(\eta^{1/2}\zeta)^*$
$\vec{q}_{d2}=(\bar{a}/3,a/3,c/4)$	1	$\xi^{*1/2}\eta$	$\xi^*\eta^{1/2}$	1	$\xi^*\eta^{1/2}$	$\xi^{*1/2}\eta$	1	$\xi^{*1/2}\eta$	$\xi^*\eta^{1/2}$	1	$\xi^{*1/2}\eta$	$\xi^*\eta^{1/2}$

all the groups $G_{q_1}, G_{q_2}, \ldots, G_{q_r}$.

The induction of band representations from $G_{q'}$ for the whole group G can therefore be carried out by first constructing from $G_{q'}$ band representations for the set of the groups $G_{q_1}, G_{q_2}, \ldots, G_{q_r}$. However, since any of the groups of this set and $G_{q'}$ have identical factor systems [up to equivalency, see relation (16)] this means that the irreducible band representations that can be induced from $G_{q'}$ are all contained among the irreducible band representations (12) of $G_{q_1}, G_{q_2}, \ldots, G_{q_r}$ for the symmetry centers $\vec{q}_1, \vec{q}_2, \ldots, \vec{q}_r$, correspondingly. As a consequence of this the subequivalent center $\vec{q}\,'$ can be discarded in the construction process of the irreducible band representations for a given space group. A center $\vec{q}_a$ that is not subequivalent to any other center will be called a relevant symmetry center. An important property of a relevant symmetry center $\vec{q}_a$ is that any band representation induced from it by formulas (12) and (15) is irreducible. This can be seen in the following way.

We denote by $D^{(q_a,l)}$ [see formula (12)] an irreducible band representation of G_a (the symmetry group of $\vec{q}_a$) and correspondingly by $D^{(q_a^*,l)}$ the band representation of the whole space group G which is induced from the center $\vec{q}_a$ according to relation (15). We show that if $\vec{q}_a$ is a relevant symmetry center then $D^{(q_a^*,l)}$ is irreducible. Assume the opposite and let $D^{(q_a^*,l)}$ be reducible into, say, two band representations of G. When considered on the subgroup G_a only, each of these two band representations have to contain, by the reciprocity theorem of Frobenius[23] the band representation $D^{(q_a,l)}$. One should therefore be able to distinguish between different sets of functions that on G_a behave in the same way. This can only be done if the basis functions for the representation $D^{(q_a^*,l)}$ can be labeled with respect to a symmetry center $\vec{q}_a'$ to which $\vec{q}_a$ is subequivalent. We arrive at a contradiction because by the assumption $\vec{q}_a$ is a relevant symmetry center. This proves that each relevant symmetry center $\vec{q}_a$ induces, by formulas (12) and (15), an irreducible band representation of the space group.

Let us denote by $\vec{q}_1, \vec{q}_2, \ldots, \vec{q}_p$ all the inequivalent relevant symmetry centers of the space group. This is usually a small number of symmetry centers. Thus, for the group D_{6h}^4 there are four such centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$ (see Table I). From what was said above it is clear that for constructing all the irreducible band representations of a space group it is sufficient to consider in the induction process only the relevant symmetry centers.

Because of the space-group symmetry of a solid, each symmetry center $\vec{q}$ appears actually as an infinite lattice of centers.[9,15] One can say that the symmetry of the basis functions for a band representation is specified with respect to a whole lattice of symmetry centers. $\vec{q}$ gives the origin of this lattice and the star of $\vec{q}$ gives the type of the lattice. We can call it the q lattice of symmetry centers. If $\vec{q}$ is a relevant symmetry center then it induces irreducible band representations. Since each irreducible band representation defines the symmetry type of a band one should expect a q lattice of a relevant symmetry center to be an invariant property of the band.[15] Such a q lattice should, in principal, be possible to determine if the information about the band becomes accessible.

We have shown that all the irreducible band representations of a space group in their canonical form can be induced from the full set of inequivalent relevant symmetry centers. In order to prove that this exhausts all the irreducible band representations one still has to prove that any irreducible band representation of a space group can be written in the canonical form. This can be proven in the following way. Let $C_1(\vec{k},\vec{q})$, $C_2(\vec{k},\vec{q}), \ldots, C_f(\vec{k},\vec{q})$ be a basis for an irreducible representation $D[(\alpha \mid \vec{a}),\vec{k}]$ of G. In general, these functions will have some symmetry. What this means is that it is possible to choose a center $\vec{q}_a$ with highest possible symmetry G_a ($\vec{q}_a$ is a relevant symmetry center) around which a subset of the functions, say, $C'_{1q_a}(\vec{k},\vec{q})$, $C'_{2q_a}(\vec{k},\vec{q}), \ldots, C'_{mq_a}(\vec{k},\vec{q})$ with $m \leq f$ form a basis for a representation of the point group g_a (the point group of G_a). These primed functions will, obviously, lead to an irreducible band representation of G_a [see relation (12)]. They can then be used for constructing the functions (13) and correspondingly for inducing the band representation in the form (15). Clearly, when the functions in $C_1(\vec{k},\vec{q}), C_2(\vec{k},\vec{q}), \ldots, C_f(\vec{k},\vec{q})$ have no symmetry, this is a particular case of G_a (when there is no symmetry, G_a is the translation group itself). The conclusion is, that any irreducible band representation $D[(\alpha \mid \vec{a}),\vec{k}]$ of a space group G can be written in the canonical form (15). This completes the proof that the induction process [formulas (12) and (15)] from all the inequivalent relevant symmetry centers leads to all the irreducible band representations of a space group. It may, however, happen that some of these irreducible band representations will be equivalent. In Sec. V an equivalency criterion is proven which enables one to distinguish between equivalent and inequivalent band representations.

In conclusion of this section we point out that the construction of band representations of a space group G are significantly simplified when $G_{q'}$ is an invariant subgroup of G. In this case, relation (14) for the elements of $G_{q'}$ assumes the form

$$(\gamma \mid \vec{c})(\alpha_m \mid \vec{a}_m)=(\alpha_m \mid \vec{a}_m)(\gamma' \mid \vec{c}\,') , \qquad (17)$$

where $(\gamma \mid \vec{c})$ and $(\gamma' \mid \vec{c}\,')$ are elements of $G_{q'}$. From (17) it follows that $G_{q'}$ is also the symmetry group of any of the vectors of the star of $\vec{q}\,'$. This can be seen in the following way. Let $\vec{q}\,'_m=(\alpha_m \mid \vec{a}_m)\vec{q}\,'$ be the mth vector of the star of $\vec{q}\,'$. Then the symmetry elements of the group of $\vec{q}\,'_m$ are

$$(\alpha_m \mid \vec{t}_m)(\gamma \mid \vec{c})(\alpha_m \mid \vec{a}_m)^{-1} . \qquad (18)$$

From relation (17) it follows that all the elements of relation (18) belong to $G_{q'}$. The latter is therefore the symmetry group of all the vectors of the star of $\vec{q}\,'$. Having this in mind we can look at relation (12) as defining irreducible band representations of the group $G_{q'}$ for different vectors $\vec{q}\,'_m$ in the star. If all $\vec{q}\,'_m$ are inequivalent then they will, in general, define different irreducible band representations of $G_{q'}$. From relation (17) it also follows that the matrices $D^{(q'^*,l)}$ for any band representation that is induced according to formula (15) will have a quasidiagonal form for the elements of $G_{q'}$. Formula (15) for the elements of $G_{q'}$ will be

$$(\gamma \mid \vec{c})C^{(l)}_{iq'_m}=\exp(-i\vec{k}\cdot\vec{R}^{(\gamma\mid\vec{c})}_{q'_m})\sum_j D^{(l)}_{ji}(\gamma')C^{(l)}_{jq'_m} , \qquad (19)$$

where γ' is defined by relation (17). Formula (19) turns out to be very useful for constructing irreducible band representations because very often the symmetry groups of relevant symmetry centers are invariant subgroups of the space group. Thus, this is the case for the relevant symmetry centers of D^4_{6h}.

IV. EXAMPLE

As an example we consider the construction of irreducible band representations for the space group D^4_{6h} of the hexagonal close-packed structure. We have already mentioned that this group has four inequivalent relevant symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$ (Table I). The symmetry of $\vec{q}_a$ is D_{3d} (the space group with the point-group symmetry D_{3d}), while the remaining three centers have the symmetry D_{3h}. We can first use formula (12) for constructing the irreducible band representations of the subgroups D_{3d} and D_{3h}. Since each of the point groups D_{3d} and D_{3h} has six irreducible representations (we shall label them from 1 to 6 as in Ref. 21), formula (12) will give six irreducible band representations for each of the mentioned relevant symmetry centers. With their aid and by using formulas (14) and (15) we can find the irreducible band representations of the space group D^4_{6h}. We obtain altogether 24 irreducible band representations of D^4_{6h}: Each of the point groups D_{3d} and D_{3h} has four one-dimensional representations and two two-dimensional ones; the induction method [formula (15)] will lead to 16 two-dimensional band representations and eight four-dimensional ones. For the explicit construction of the band representations one can use the simplified formula (19) because both D_{3d} and D_{3h} are invariant subgroups of D^4_{6h}. Let us demonstrate the construction process on the example of the symmetry center $\vec{q}_a=(0,0,0)$. For this center the decomposition (15) will be

$$D^4_{6h}=D_{3d}+\left(C^z_2 \,\middle|\, 0,0,\frac{c}{2}\right)D_{3d} . \qquad (20)$$

For being able to use formula (19) we need the multiplication table for the point-group elements of relation (17). In this case the table is very simple because C^z_2 commutes with all the elements of D_{3d} (the same is also correct with respect to the group D_{3h} of the other relevant symmetry centers in Table I). What this means is that for all the elements of D_{3d} (or equally for D_{3h}) $\gamma'=\gamma$ in formula (19). Having the irreducible representations of the point groups D_{3d} (and D_{3h}) and the information of Table I we find the matrices $D^{(q^*_a,l)}$ (also for the other invariant symmetry centers) for the elements of D_{3d} (or D_{3h}). For the elements not belonging to D_{3d} (or D_{3h}) the diagonal elements of $D^{(q^*_a,l)}$ are zero. This follows from the multiplication rule (14) for an invariant subgroup. We shall label the irreducible band representations of D^4_{6h} by (a,l), (b,l), (c,l), and (d,l) with $l=1,2,\ldots,6$. The labels a, b, c, and d replace the star labels $\vec{q}^*_a$, $\vec{q}^*_b$, etc. The induction process leads therefore to 24 irreducible band representations. The question that remains to be answered is whether or not all these band representations are inequivalent. This is answered affirmatively in the next section.

V. CONNECTION WITH USUAL REPRESENTATIONS AND CONTINUITY CHORDS

Up to now the band representations were written as finite-dimensional k-dependent matrices in the kq representation. It was pointed out that because of $\vec{k}$ being a variable the representations are actually infinite dimensional in the sense of usual representations. We show in this section that they can be made finite dimensional by using the Born—von Kármán cyclic boundary conditions as is usually done in the representation theory of space groups.[4,20] This can be achieved by putting periodic conditions on the wave function $\psi(\vec{r})$:

$$\psi(\vec{r}+2N\vec{a}_i)=\psi(\vec{r}) , \tag{21}$$

where $\vec{a}_i$ are the unit vectors of the Bravais lattice ($i=1,2,3$) and N is any large integer. The factor 2 is used for convenience so that the lattice can be considered in a symmetric way around the origin. With the condition (21), the translation group will have $(2N)^3$ elements and correspondingly the band representations will become finite dimensional in the sense of usual representations.

As an example let us consider a one-dimensional crystal with inversion symmetry.[9] The space group C_i of this crystal contains the unit element E, the inversion I and $2N$ translations ma, $m=0,\pm 1,\ldots,\pm(N-1), N$, where a is the lattice constant. As was shown in Ref. 9 this group has $N+3$ classes: $N+1$ classes of pure translations $(ma, -ma)$ $m=0,1,\ldots,N$, one class for each m and two classes containing the inversion $(I\mid 2ma)$, $(I\mid(2m+1)a)$ with m assuming any possible value. There are two relevant symmetry centers $q_a=0$ and $q_b=a/2$, both with the symmetry C_i. The band representations corresponding to these symmetry centers are given according to formula (12) with the phase factors in Table II. There are four irreducible band representations, two for each symmetry center. In the second half of Table II we list the irreducible representations of C_i. Having applied condition (21), these band representations will be $2N$ dimensional when considered as usual representations. The basis functions of these representations can be labeled in the following way:

$$C_{mq'}^{(l)}(k,q)=\exp(-ikma)C_{q'}^{(l)}(k,q) , \tag{22}$$

where m labels the site, and it can assume the values $m=0,\pm 1,\ldots,\pm(N-1), N$, q' the symmetry center, and l the irreducible representations of the point group C_i (see Table II). When the boundary condition (21) is applied, k in (22) assumes $2N$ discrete values $k=\pi/(Na)r$ where $r=0,\pm 1,\ldots,\pm(N-1), N$. Among the functions (22) there are two ($m=0$, N) that go into themselves (up to $\pm$) under inversion.

TABLE II. The upper part gives the phase factors for the relevant symmetry centers q_a and q_b for the one-dimensional crystal. The lower part gives the irreducible representations of $C_i(E,I)$. I is the inversion $\xi=\exp(ika)$.

q \ C_i	E	I
$q_a=0$	1	1
$q_b=a/2$	1	ξ
1	1	1
2	1	-1

Having this in mind it is a simple matter to write the characters of the band representations for the relevant centers q_a and q_b (see Table III). These band representations are clearly reducible and they can be reduced into the irreducible representations of C_i. The latter are well known.[4] They are specified by a k vector and a representation index of the point-group symmetry. For the group C_i, $k=0$ (Γ point) and $k=\pi/a$ (X point), possess the fully symmetry C_i and the corresponding one-dimensional representations are given in Table II. For $k=0$ we denote them by Γ_1, Γ_2, and for $k=\pi/a$ by X_1, X_2 (in Table II they are labeled by 1 and 2). For a general point k, the irreducible representations of C_i are two dimensional (they are denoted by $D^{(k)}$). Table IV shows how the band representations of C_i for q_a and q_b which are denoted by (a,l) and (b,l), $l=1,2$, reduce into the irreducible representations of C_i. Thus, $(a,1)$ con-

TABLE III. Band representations as finite-dimensional representations of the space group C_i for a one-dimensional crystal. $2N$ is the number of unit cells, $m=0,\pm 1,\ldots,\pm(N-1), N$. E is the unit element and I is the inversion. (a,l) and (b,l) with $l=1,2$ denote the irreducible band representations. q is a center without symmetry.

	E	$(I\mid 2ma)$	$(I\mid(2m+1)a)$	$(E\mid ma)$, $m\neq 0$
$(a,1)$	$2N$	2	0	0
$(a,2)$	$2N$	-2	0	0
$(b,1)$	$2N$	0	2	0
$(b,2)$	$2N$	0	-2	0
$(q,1)$	$4N$	0	0	0

TABLE IV. Continuity chords for the band representations of C_i for a one-dimensional crystal. k is a general point in the Brillouin zone and $D^{(k)}$ is the two-dimensional representation for this point. All the other notations are like in Fig. 1 and Table III.

	$(a,1)$	$(2,a)$	$(b,1)$	$(b,2)$	$(q,1)$
Γ	Γ_1	Γ_2	Γ_1	Γ_2	$\Gamma_1\Gamma_2$
X	X_1	X_2	X_2	X_1	X_1X_2
k	$(N-1)D^{(k)}$	$(N-1)D^{(k)}$	$(N-1)D^{(k)}$	$(N-1)D^{(k)}$	$2(N-1)D^{(k)}$

tains once Γ_1, once X_1, and $(N-1)$ times the representation $D^{(k)}$. The dimensionality of all of them together is $2N$ which is the same as of $(a,1)$. It is seen for Table IV that each irreducible band representation contains Bloch states with well-defined symmetries, e.g., Γ_i, X_j, at different symmetry points in the Brillouin zone. For different irreducible band representations the sets Γ_i, X_j are different. What this means is that each irreducible band representation leads to Bloch states with well-specified symmetries at different k points. The set Γ_i, X_j of Bloch states at different points in the Brillouin zone corresponding to a given band representation is called the continuity chord.[24] In Fig. 1 we plot the possible four bands with their continuity chords for the four different band representations (a,i), (b,i), $i=1,2$. The conclusion is that a one-dimensional crystal with the symmetry C_i can have bands belonging to one of the four symmetry types as given in Table IV or Fig. 1.

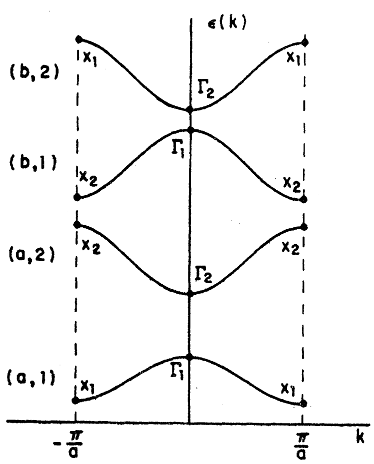

FIG. 1. Symmetry types of bands for a one-dimensional crystal with an inversion symmetry. Γ_1 and Γ_2 are even and odd Bloch states correspondingly at $k=0$; X_1, X_2 are the same at $k=\pi/a$. (a,l) and (b,l) with $l=1,2$ labels the band representations.

This is in full agreement with previous work.[9,25]

It is possible to construct other band representations of C_i. However, they will necessarily be reducible. Thus, consider a general point q, differing from q_a and q_b. For such a symmetry center, q and $Iq=-q$ belong to the same star. The band representation induced from q has a character $\chi^{(q,1)}$ given in the last line of Table III. It is easy to see that $\chi^{(q,1)}$ can be written either as a sum $\chi^{(q,1)}=\chi^{(a,1)}+\chi^{(a,2)}$ or $\chi^{(q,1)}=\chi^{(b,1)}+\chi^{(b,2)}$. This might look strange that a given reducible band representation can be split into irreducible band representations in different ways. However, as representations go $\chi^{(a,1)}$, $\chi^{(a,2)}$, $\chi^{(b,1)}$, and $\chi^{(b,2)}$ are by themselves reducible (they are irreducible only as band representations on a basis of localized orbitals). Having this in mind, the above reduction of $\chi^{(q,1)}$ will no longer be surprising because as a representation $\chi^{(q,1)}$ contains all the irreducible representations that are contained in both $\chi^{(a)}$ and $\chi^{(b)}$ (see Table IV).

In a similar way one could apply the boundary conditions (21) to the hexagonal close-packed structure (D_{6h}^4) and find the finite-dimensional irreducible band representations. For large N this may become rather tedious. However, since we are interested in finding the continuity chords of a band corresponding to a given band representation, this can directly be obtained from the information about the band representation in the kq representation and there is no need to construct explicitly the finite-dimensional band representations. Let us consider the question of finding the continuity chords in more detail. They not only define the symmetry of the band but they are also important in the equivalency criterion which is derived below.

Having the irreducible band representations of a space group one can determine the symmetries of a band at different points in the Brillouin zone. This is what we call the continuity chord of a band and it is given by a set Γ_i, L_j, X_kX, . . . , of irreducible representations for symmetry groups G_k at different points $\vec{k}$ in the Brillouin zone. By definition[4] all those elements $(\beta \mid \vec{b})$ of the space group G belong to G_k for which

$$\beta\vec{k}=\vec{k}+\vec{K}\ , \tag{23}$$

where $\vec{K}$ is a vector of the reciprocal lattice. For finding the continuity chord of a band we shall use the fact that any band representation of G when considered for a fixed $\vec{k}$ becomes a representation of G_k. This can be shown in the following way. Let $D^{(q^*,l)}[(\alpha \mid \vec{t}\,),\vec{k}]$ be a band representation of G. Then, by definition the matrix corresponding to $(\alpha_2 \mid \vec{t}_2)(\alpha_1 \mid \vec{t}_1)$ is

$$D^{(q^*,l)}[(\alpha_2 \mid \vec{t}_2)(\alpha_1 \mid \vec{t}_1),\vec{k}] = D^{(q^*,l)}[(\alpha_2 \mid \vec{t}_2),\vec{k}]D^{(q^*,l)}[(\alpha_1 \mid \vec{t}_1),\alpha_2^{-1}\vec{k}]\ , \tag{24}$$

where in the last matrix $\alpha_2^{-1}\vec{k}$ appears, showing that $\vec{k}$ is a variable. For the elements of G_k, relation (24) will assume the usual form of a multiplication rule for a representation. This follows from relation (23) for the elements of G_k and the fact that the band-representation matrices $D[(\alpha \mid \vec{t}\,),\vec{k}]$ are periodic in $\vec{k}$ with the periodicity of the reciprocal-lattice vectors. It therefore follows that each band representation of a space group G when considered for a fixed $\vec{k}$ becomes a representation of G_k. The latter is, in general, reducible. In order to find the continuity chord of a band we start with an irreducible band representation $(\vec{q},l)$ of the space group [relation (15)] and for each $\vec{k}$ we find the representation $D^{(k)}$ of G_k that is given by the same formula (15). Having found $D^{(k)}$ we reduce it and this gives us the set of the irreducible representations of G_k at the point $\vec{k}$ in the Brillouin zone. By going through with this process over all the symmetry points in the Brillouin zone we find the continuity chord of the band $(\vec{q},l)$. The connection of the band-representation matrices $D[(\alpha \mid \vec{a}),\vec{k}]$ and the corresponding matrices $D^{(k)}$ of the usual representations is a simple consequence of the connection between the localized $a(\vec{k},\vec{q})$ and the extended functions.

With the above remarks in mind it becomes a simple matter to use the information of Table I in order to find the continuity chords for the irreducible band representations of D_{6h}^4. As an example let us consider the point $H=(4\pi/3a,0,c)$ in the Brillouin zone.[21] The symmetry group G_k of this point is D_{3h}. The irreducible representations of G_k are given in Table V (upper part). In the same table we list also the characters of the representations $\chi_H^{(q,l)}$ of G_k that are obtained from the band representations of D_{6h}^4 at the point H. At this point $\xi=\exp[i(4\pi)/3]$, $\eta=1$, $\zeta=-1$ (see Table I). In obtaining the characters χ_H we just have to add the two lines for each symmetry center in Table I and to multiply the result by the corresponding character of the irreducible representation of D_{3d} (for the symmetry center $\vec{q}_a$) or of D_{3h} (for the symmetry centers $\vec{q}_b$, $\vec{q}_c$, $\vec{q}_d$). Each of the groups D_{3d} and D_{3h} have six irreducible representations which we label from 1 to 6 according to Ref. 21. Correspondingly the band representations of D_{6h}^4 are labeled by (a,l), (b,l), (c,l), and (d,l), $l=1,\ldots,6$.

TABLE V. The upper part gives the irreducible representations for the symmetry point in the Brillouin zone $H=(4\pi/3a,0,\pi/c)$ (Ref. 21). The lower part gives the characters $\chi_H^{(q,l)}$ of the representations of G_k (the symmetry group of H) that are obtained from the band representations (a,l), (b,l), (c,l), and (d,l), $l=1,2,\ldots,6$. a, b, c, and d denote the symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$. l denotes the irreducible representations of the groups D_{3d} and D_{3h}. The symmetry elements are like in Table I.

H	E	$2C_3^z$	S_3^z	S_3^{2z}	Other elements
H_1	2	2	0	0	
H_2	2	-1	$i\sqrt{3}$	$-i\sqrt{3}$	0
H_3	2	-1	$-i\sqrt{3}$	$i\sqrt{3}$	
$\chi_H^{(a,1)}=\chi_H^{(a,2)}=\chi_H^{(a,4)}=\chi_H^{(a,5)}=\chi_H^{(b,1)}=\chi_H^{(b,2)}=\chi_H^{(b,3)}=\chi_H^{(b,4)}$	2	2	0	0	
$\chi_H^{(a,3)}=\chi_H^{(a,6)}=\chi_H^{(b,3)}=\chi_H^{(b,6)}$	4	-2	0	0	
$\chi_H^{(c,1)}=\chi_H^{(c,2)}=\chi_H^{(d,4)}=\chi_H^{(d,5)}$	2	-1	$i\sqrt{3}$	$-i\sqrt{3}$	
$\chi_H^{(c,3)}=\chi_H^{(d,6)}$	4	1	$-i\sqrt{3}$	$i\sqrt{3}$	
$\chi_H^{(c,4)}=\chi_H^{(c,5)}=\chi_H^{(d,1)}=\chi_H^{(d,2)}$	2	-1	$-i\sqrt{3}$	$i\sqrt{3}$	
$\chi_H^{(c,6)}=\chi_H^{(d,3)}$	4	1	$i\sqrt{3}$	$-i\sqrt{3}$	

In Table V the characters $\chi_H^{(a,l)}$ are given only for those elements for which the characters of the representations of G_H do not vanish. From Table V it is easy to find how the irreducible band representations of D_{6h}^4 split at the point H of the Brillouin zone. Thus, $\chi_H^{(a,1)}=\chi^{(H_1)}$. Also $\chi_H^{(a,3)}=\chi^{(H_2)}+\chi^{(H_3)}$, and so on. We have carried out this process for all the symmetry points in the Brillouin zone. In Tables VI and VII, a list is given of the continuity chords for all the irreducible band representations of D_{6h}^4. As is seen from the tables, the continuity chords for all 24 irreducible band representations of the space group D_{6h}^4 are different. What this means is that all the irreducible band representations that are induced from the relevant symmetry centers of D_{6h}^4 lead to different continuity chords. This is, in general, not true for other space groups. Thus, it might happen that some of the irreducible band representations that are induced by formula (15) from inequivalent relevant symmetry centers will lead to identical continuity chords. An example, are the $(a,3)$ and $(b,3)$ band representations for the diamond structure.[24] In solids with the D_{6h}^4 symmetry this does not happen and as Tables VI and VII show all the irreducible band representations corresponding to the relevant symmetry centers lead to different continuity chords.

An important connection exists between band representations and their continuity chords. We have already shown that each band representation defines a continuity chord. One can actually prove the following statement: (1) two equivalent band representations lead to identical continuity chords, and (2) two band representations leading to identical continuity chords are equivalent. The first part of this statement follows directly from the definiton of equivalent band representations [relation (15)]. In finding continuity chords for a particular $\vec{k}$ vector we employ elements $(\beta\,|\,\vec{b})$ which belong to the group of $\vec{k}$, G_k. But for these elements relation (37) holds, and the matrix in relation (5) will become

$$D'[(\beta\,|\,\vec{b}),\vec{k}]=T^{-1}(\vec{k})D[(\beta\,|\,\vec{b}),\vec{k}]T(\vec{k})\,, \qquad (25)$$

where D' is equivalent to the representation D. We see therefore that the band representation $D[(\alpha\,|\,\vec{a}),\vec{k}]$ and the equivalent band representation of relation (5) lead to equivalent representations [relation (25)] of G_k at each point in the Brillouin zone. This also means that equivalent band representations lead to identical continuity chords, because from relation (25) it follows that $D[(\beta\,|\,\vec{b}),\vec{k}]$ and $D'[(\beta\,|\,\vec{b}),\vec{k}]$ have the same characters.

Let us now prove the second part of the statement: if two band representations $D[(\alpha\,|\,\vec{a}),\vec{k}]$ and $D'[(\alpha\,|\,\vec{a}),\vec{k}]$ lead to identical continuity

TABLE VI. Continuity chords for the band representations (a,l), $l=1,2,\ldots,6$. a and l are as in Table V. The notations for the symmetry points in the Brillouin zone follow Ref. 21.

	$(a,1)$	$(a,2)$	$(a,3)$	$(a,4)$	$(a,5)$	$(a,6)$
Γ	$\Gamma_1\Gamma_2$	$\Gamma_2\Gamma_4$	$\Gamma_5\Gamma_6$	$\Gamma_8\Gamma_{10}$	$\Gamma_7\Gamma_9$	$\Gamma_{11}\Gamma_{12}$
Δ	$\Delta_1\Delta_3$	$\Delta_2\Delta_4$	$\Delta_5\Delta_6$	$\Delta_1\Delta_3$	$\Delta_2\Delta_4$	$\Delta_5\Delta_6$
Σ	$\Sigma_1\Sigma_2$	$\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2$	$\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3\Sigma_4$
T	T_1T_3	T_2T_4	$T_1T_2T_3T_4$	T_2T_4	T_1T_3	$T_1T_2T_3T_4$
N	N_1N_2	N_1N_2	$2N_12N_2$	N_1N_2	N_1N_2	$2N_12N_2$
Ξ	$\Xi_1\Xi_2$	$\Xi_1\Xi_2$	$2\Xi_12\Xi_2$	$\Xi_1\Xi_2$	$\Xi_1\Xi_2$	$2\Xi_12\Xi_2$
A	A_1	A_2	A_3	A_1	A_2	A_3
K	K_1K_4	K_2K_5	K_3K_6	K_2K_5	K_1K_4	K_3K_6
H	H_1	H_1	H_2H_3	H_1	H_1	H_2H_3
M	M_1M_3	M_2M_4	$M_1M_2M_3M_4$	M_6M_8	M_5M_7	$M_5M_6M_7M_8$
L	L_1	L_2	L_1L_2	L_1	L_2	L_1L_2
P	P_1P_2	P_1P_2	P_3	P_1P_2	P_1P_2	P_3
U	U_1U_2	U_3U_4	$U_1U_2U_3U_4$	U_1U_2	U_3U_4	$U_1U_2U_3U_4$
T'	$T'_1T'_3$	$T'_2T'_4$	$T'_1T'_2T'_3T'_4$	$T'_2T'_4$	$T'_1T'_3$	$T'_1T'_2T'_3T'_4$
S'	S'_1	S'_1	$2S'_1$	S'_1	S'_1	$2S'_1$
C	C_1C_2	C_1C_2	$2C_12C_2$	C_1C_2	C_1C_2	$2C_12C_2$
S	S_1	S_1	$2S_1$	S_1	S_1	$2S_1$
R	R_1R_2	R_3R_4	$R_1R_2R_3R_4$	R_1R_2	R_3R_4	$R_1R_2R_3R_4$
B	B_1B_2	B_1B_2	$2B_12B_2$	B_1B_2	B_1B_2	$2B_12B_2$

TABLE VII. Continuity chords for the band representations (b,l), (c,l), and (d,l), $l=1,2,\ldots,6$. b, c, d, and l are as in Table V. The notations for the symmetry points in the Brillouin zone follow Ref. 21.

	$(b,1)$ $(c,1)$ $(d,1)$	$(b,2)$ $(c,2)$ $(d,2)$	$(b,3)$ $(c,3)$ $(d,3)$	$(b,4)$ $(c,4)$ $(d,4)$	$(b,5)$ $(c,5)$ $(d,5)$	$(b,6)$ $(c,6)$ $(d,6)$
Γ	$\Gamma_1\Gamma_{10}$	$\Gamma_2\Gamma_9$	$\Gamma_6\Gamma_{11}$	$\Gamma_4\Gamma_7$	$\Gamma_3\Gamma_8$	$\Gamma_5\Gamma_{12}$
Δ	$\Delta_1\Delta_3$	$\Delta_2\Delta_4$	$\Delta_5\Delta_6$	$\Delta_2\Delta_4$	$\Delta_1\Delta_3$	$\Delta_5\Delta_6$
Σ	$2\Sigma_1$	$2\Sigma_4$	$2\Sigma_1 2\Sigma_4$	$2\Sigma_3$	$2\Sigma_2$	$2\Sigma_2 2\Sigma_3$
T	T_1T_4	T_1T_4	$2T_1 2T_4$	T_2T_3	T_2T_3	$2T_2 2T_3$
N	N_1N_2	N_1N_2	$2N_1 2N_2$	N_1N_2	N_1N_2	$2N_1 2N_2$
Ξ	$2\Xi_1$	$2\Xi_1$	$4\Xi_1$	$2\Xi_2$	$2\Xi_2$	$4\Xi_2$
A	A_1	A_2	A_3	A_2	A_1	A_3
$K(b)$	K_1K_2	K_1K_2	$2K_3$	K_4K_5	K_4K_5	$2K_6$
$K(c,d)$	K_3	K_3	$K_1K_2K_3$	K_6	K_6	$K_4K_5K_6$
$H(b)$	H_1	H_1	H_2H_3	H_1	H_1	H_2H_3
$H(c)$	H_2	H_2	H_1H_3	H_3	H_3	H_1H_2
$H(d)$	H_3	H_3	H_1H_2	H_2	H_2	H_1H_3
M	M_1M_6	M_4M_7	$M_1M_4M_6M_7$	M_2M_5	M_3M_8	$M_2M_3M_5M_8$
L	L_1	L_2	L_1L_2	L_2	L_1	L_1L_2
$P(b)$	P_1P_2	P_1P_2	$2P_3$	P_1P_2	P_1P_2	$2P_3$
$P(c,d)$	P_3	P_3	$P_1P_2P_3$	P_3	P_3	$P_1P_2P_3$
U	U_1U_2	U_3U_4	$U_1U_2U_3U_4$	U_3U_4	U_1U_2	$U_1U_2U_3U_4$
T'	$T'_1T'_4$	$T'_1T'_4$	$2T'_1 2T'_4$	$T'_2T'_3$	$T'_2T'_3$	$2T'_2 2T'_3$
S'	S'_1	S'_1	$2S'_1$	S'_1	S'_1	$2S'_1$
C	C_1C_2	C_1C_2	$2C_1 2C_2$	C_1C_2	C_1C_2	$2C_1 2C_2$
S	S_1	S_1	$2S_1$	S_1	S_1	$2S_1$
R	$2R_1$	$2R_4$	$2R_1 2R_4$	$2R_3$	$2R_2$	$2R_2 2R_3$
B	$2B_1$	$2B_1$	$4B_1$	$2B_2$	$2B_2$	$4B_2$

chords then it follows that they are equivalent:

$$D'[(\alpha\,|\,\vec{a}),\vec{k}]=T^{-1}(\vec{k})D[(\alpha\,|\,\vec{a}),\vec{k}] \times T(\alpha^{-1}\vec{k})\,. \tag{26}$$

Since D' and D have identical continuity chords this means that at each point $\vec{k}$ in the Brillouin zone we have to have the equivalency given by relation (25) for $(\beta\,|\,\vec{b})$ satisfying relation (23) (for the representations $D'[(\beta\,|\,\vec{b}),\vec{k}]$ and $D[(\beta\,|\,\vec{b}),\vec{k}]$ to contain the same irreducible representations of G_k, they have to be equivalent). Relation (25) defines the matrix $T(k)$ at each point in the Brillouin zone. This matrix can be used for transforming the basis of the band representation $D[(\alpha\,|\,\vec{a}),\vec{k}]$ to a primed basis. The latter will be the basis for the band representation $D'[(\alpha\,|\,\vec{a}),\vec{k}]$ and we obtain therefore relation (26). This completes the proof of the statement that two equivalent band representations have identical continuity chords and, vice versa, two band representations that have identical continuity chords are equivalent. A corollary of this statement is that if two band representations have different continuity chords then they are inequivalent. The statement together with the corollary can serve as a criterion for distinguishing between equivalent and inequivalent band representations. We can formulate the following equivalency theorem: Two equivalent band representations have identical continuity chords, two band representations with identical continuity chords are equivalent, and finally, two band representations with different continuity chords (for continuity chords to be different it is enough for them to differ at one point in the Brillouin zone) are inequivalent.

Having the equivalency theorem one can summarize the method for constructing all the irreducible and inequivalent band representations of a space group. One first constructs the band representations [according to formula (12)] for all the inequivalent relevant symmetry centers. For this one needs the phase factors (see Table I). Then by using formula (15) one induces the irreducible band representations of the space group. In general, not all of them will be inequivalent. The equivalency theorem can be used for finding out which of them, if any, are equivalent. For this one uses the knowledge about the continuity chords. Among the constructed band representations only those are equivalent whose continuity chords are identical. Thus, for the hexagonal close-packed structure (D_{6h}^4) all the continuity chords are different (see Tables VI and VII), and therefore for this space group all the inequivalent principal symmetry centers (see Table I) lead to inequivalent irreducible band representations.

VI. CONCLUSIONS

Irreducible representations of space groups label the symmetry of Bloch states by means of a quasimomentum $\vec{k}$ and a representation index n of the point symmetry of G_k. Irreducible band representations label the symmetry of localized states by means of the quasicoordinate $\vec{q}$ and a representation index l of the point-group symmetry of G_q. Being labeled by $\vec{k}$ a Bloch state is local in $\vec{k}$ space and therefore extensive in $\vec{r}$ space. On the other hand, the localized state in $\vec{r}$ space are labeled by $\vec{q}$ and they correspond to a whole band of states in $\vec{k}$ space. An irreducible representation of a space group corresponds to a single energy level. An irreducible band representation corresponds to a band of energies. It may happen that more than one irreducible representation corresponds to a single energy level without being a consequence of symmetry. This is called accidental degeneracy.[26] The same may happen with band representations, and more than one irreducible band representation may correspond to a given band. In analogy with usual representations this can be called accidental degeneracy in band representations.

APPENDIX

Let us check that the definition (12) in the text gives a band representation of $G_{q'}$. For this we assume a similar relation for the element $(\gamma' \mid \vec{c}\,')$. For the product we shall have

$$(\gamma \mid \vec{c}\,)(\gamma' \mid \vec{c}\,') = (\gamma\gamma' \mid \gamma\vec{c}\,' + \vec{c}\,'):\exp(-i\vec{k}\cdot\vec{R}_{q'}^{(\gamma\gamma' \mid \gamma\vec{c}\,'+\vec{c}\,)})D^{(l)}(\gamma\gamma') \,. \tag{A1}$$

On the other hand, from relation (17), it follows that

$$(\gamma \mid \vec{c}\,)(\gamma' \mid \vec{c}\,'):\exp(-i\vec{k}\cdot\vec{R}_{q'}^{(\gamma \mid \vec{c}\,)} - i\gamma^{-1}\vec{k}\cdot\vec{R}_{q'}^{(\gamma' \mid \vec{c}\,')})D^{(l)}(\gamma)D^{(l)}(\gamma') \,. \tag{A2}$$

We have to show therefore that the exponents on the right-hand sides of (A1) and (A2) are identical [by definition, $D^{(l)}(\gamma\gamma') = D^{(l)}(\gamma)D^{(l)}(\gamma')$]. Let us take the exponent of (A2):

$$\vec{k}\cdot\vec{R}_{q'}^{(\gamma \mid \vec{c}\,)} + \vec{k}\cdot\gamma\vec{R}_{q'}^{(\gamma' \mid \vec{c}\,')} = \vec{k}\cdot(\gamma\vec{q}\,' + \vec{c} - \vec{q}\,' + \gamma\gamma'\vec{q}\,' + \gamma\vec{c}\,' - \gamma\vec{q}\,') = \vec{k}\cdot\vec{R}_{q'}^{(\gamma\gamma' \mid \gamma\vec{c}\,'+\vec{c}\,)} \,. \tag{A3}$$

This coincides with the exponent in (A1). It therefore follows that relation (12) in the text defines a band representation.

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