Continuity chords of bands in solids: The diamond structure

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(Received 24 November 1980)

The concept of a continuity chord is defined for denoting all those Bloch states at different symmetry points in the Brillouin zone that by symmetry and continuity can, in principle, belong to one band of a solid. The continuity chords for different bands are derived on the basis of band representations of space groups. A specific example of the diamond group O_h^7 is considered in detail and the continuity chords are calculated for all the possible symmetry types of bands for this group.

I. INTRODUCTION

Irreducible representations of space groups serve as a useful tool for labeling the Bloch states at different symmetry points $\vec{k}$ in the Brillouin zone.[1] This symmetry labeling is so popular that it has developed into a language among solid-state physicists. It is hard today to dissociate the description of bands in solids from the sets of letters Γ, L, X, and so on, that are used for labeling of the different symmetry points in the Brillouin zone. Each such letter is assigned a subscript, like Γ_1, Γ_2, that specifies the particular representation at the given point. This symmetry specification is local in $\vec{k}$ space in that it assigns labels at different k points separately. Connections between symmetry labels at different points in the Brillouin zone are achieved by compatibility[2] or connectivity relations[3] which are based on both symmetry and continuity arguments. However, because of its local character in $\vec{k}$ space this symmetry labeling doesn't specify a band globally, as one whole entity. In particular, the local k-space specification of Bloch states does not answer the important question of whether or not some sets of states, say Γ_i, L_j, $X_k X_l$, and so on, can in principle, belong to one band in a solid.

In a recent paper[4] it was shown that global symmetry properties of a band can be defined by means of band representations of space groups. Unlike usual representations which are built on Bloch functions and correspond to a single energy, band representations are built on localized orbitals and they correspond to a band of energies. A band representation is labeled by a symmetry center $\vec{q}$ in the Wigner-Seitz cell and by the representation index l of the point group of G_q, the symmetry group of the vector $\vec{q}$. The indices $\vec{q}$ and l together define a symmetry label for a band in a solid.

Band representations provide a symmetry connection between extended functions (in particular, Bloch functions) and localized orbitals (in particular, Wannier functions) for a given band. Such a connection was first considered in a series of papers on molecular orbital theory[5] and soon afterwards it was extended to solids.[6,7] Later this symmetry connection was considered in a fundamental paper by Des Cloizeaux[8] who has shown how to construct symmetry adapted sets of Wannier functions by forming linear combinations of eigenfunctions with preassigned symmetry. A similar approach is adopted in other papers[9–11] where, as a rule, the Wannier functions are defined as linear combinations of Bloch functions. There is a difficulty that arises in following this approach which was already mentioned above. This difficulty is connected with the local in k-space symmetry specification of Bloch functions. The framework of such a local specification is suited for Bloch functions which correspond to a single energy but is not suited for localized orbitals which correspond to a band of energies.[6,7,12] In the local k-space approach to the problem there is no symmetry index for a band as a whole entity. In Ref. 4 the process is inverted and one first specifies the symmetry of the localized orbitals via band representations of the space group. These representations specify from the very beginning symmetries of bands as whole entities. Having the band representations one can find the symmetries of the corresponding Bloch states at different points in the Brillouin zone.

In this paper it is shown how to find all those Bloch states Γ_i, L_j, $X_k X_l$, and so on, that can, in principle, belong to one particular band of a solid. This is done by first finding the irreducible-band representations of the space group which give the symmetry types or the symmetry labels $(\vec{q},l)$ for the bands of the solid. The band representations are then reduced at each point in the Brillouin zone (at Γ, L, X, and so on) into the usual irreducible representations of the space group. By doing so we obtain the possible sets of states Γ_i, L_j, X_kX_l, and so on, that belong to a given band in a solid and that are labeled by a band index $(\vec{q},l)$. It turns out that the labels $\vec{q}$ and l carry the global information about the symmetry of a band as a whole in a solid. In particular, it can be shown that this symmetry band label $(\vec{q},l)$ defines a set of local symmetries in k space of the Bloch states Γ_i, L_j, X_kX_l, and so on, at different symmetry points in the Brillouin zone. Such a set of symmetry points belonging to a symmetry type $(\vec{q},l)$ of a band will be called the continuity chord. This term comes to point out that only some very particular symmetries in k space can appear for a band with a given symmetry label $(\vec{q},l)$. The continuity chord is closely related to compatibility[2] and connectivity[3] relations in band theory which are derived from symmetry and continuity arguments. It will be shown in this paper that by having a symmetry band label $(\vec{q},l)$ it becomes possible to find the continuity chord of the band or to list all the irreducible representations Γ_i, L_j, X_kX_l, and so on, at different points in the Brillouin zone that are related to one another in a continuous formation of a band. An explicit example is considered for the diamond-structure space group O_h^7. The results for the sets of different symmetry points or the continuity chords belonging to a band with a given symmetry type are listed in Tables V and VII.

II. IRREDUCIBLE-BAND REPRESENTATIONS OF O_h^7

Let G be a space group and let G_q be the group of the symmetry center $\vec{q}$ in the Wigner-Seitz cell.[1] By definition[4] to G_q all those elements $(\gamma\,|\,\vec{c})$ of G belong for which

$$(\gamma\,|\,\vec{c})\vec{q}=\gamma\vec{q}+\vec{c}=\vec{q}+\vec{R}_q^{(\gamma|\vec{c})}\ , \tag{1}$$

where $\vec{R}_q^{(\gamma|\vec{c})}$ is a Bravais lattice vector. Equation (1) can also be interpreted as a definition of a set of Bravais lattice vectors. For a given symmetry center $\vec{q}$ these vectors vary as a function of the space-group elements $(\gamma\,|\,\vec{c})$. The different symmetry centers $\vec{q}$ and the corresponding sets of Bravais lattice vectors $\vec{R}_q^{(\gamma|\vec{c})}$ have been used in the past in establishing symmetry connections between Wannier and Bloch functions.[6,8,10,13] The significance of $\vec{q}$ and $\vec{R}_q^{(\gamma|\vec{c})}$ in the construction of band representations is discussed below.

As examples we list in Tables I and II symmetry centers $\vec{q}$ with their symmetry groups G_q for the diamond space group O_h^7. Together with each symmetry center $\vec{q}$, its star is also listed. The latter is defined in the following way.[4] In general, the group G_q is a subgroup of G. One can decompose G with respect to G_q as

$$G=G_q+(\alpha_2\,|\,\vec{a}_2)G_q+\cdots+(\alpha_f\,|\,\vec{a}_f)G_q\ , \tag{2}$$

where $(\alpha_2\,|\,\vec{a}_2),\ldots,(\alpha_f\,|\,\vec{a}_f)$ do not belong to G_q and they define the different cosets. Given the decomposition (2) we can assign a star to each vector $\vec{q}$ which together with $\vec{q}$ contains the vectors

$$\vec{q}^{\,(2)}=(\alpha_2\,|\,\vec{a}_2)\vec{q},\ \ldots,\ \vec{q}^{\,(f)}=(\alpha_f\,|\,\vec{a}_f)\vec{q}\ .$$

In Table I we list the symmetry centers $\vec{q}_a=(0,0,0)$ and $\vec{q}_b=(a/2,0,0)$ with the symmetry T_d and their stars. Information on the symmetry centers in the Wigner-Seitz cell can be found in the International Tables.[14] For the centers $\vec{q}_a$ and $\vec{q}_b$ the decomposition (2) takes on the form

$$O_h^7=T_d+(I\,|\,a/4,a/4,a/4)T_d\ , \tag{3}$$

where T_d is the space group with the point symmetry T_d and $(I\,|\,a/4,a/4,a/4)$ is the inversion element I accompanied by a translation $(a/4,a/4,a/4)$. Equation (3) shows explicitly that the group O_h^7 is nonsymmorphic.[15] By definition the star of the vector $\vec{q}_a$ contains also

$$\begin{aligned}\vec{q}_a^{\,(2)}&=(I\,|\,a/4,a/4,a/4)\vec{q}_a\\&=(a/4,a/4,a/4)\ .\end{aligned}$$

Similarly, the star of the center $\vec{q}_b$ contains the vector

$$\begin{aligned}\vec{q}_b^{\,(2)}&=(I\,|\,a/4,a/4,a/4)\vec{q}_b\\&=(\bar{a}/4,a/4,a/4)\ .\end{aligned}$$

In Table II we list the same information for the symmetry centers $\vec{q}_c=(a/8,a/8,a/8)$ and $\vec{q}_d=(a/8,a/8,3a/8)$ with the symmetry D_{3d}. Equation (2) assumes the form

$$\begin{aligned}O_h^7=D_{3d}&+(C_4^z\,|\,a/4,a/4,a/4)D_{3d}+C_2^zD_{3d}\\&+(C_4^{3z}\,|\,a/4,a/4,a/4)D_{3d}\ ,\end{aligned} \tag{4}$$

TABLE I. Phase factors $\exp(i\vec{k}\cdot\vec{R}_q^{\gamma})$ for the symmetry centers $\vec{q}_a, \vec{q}_b$, and their stars. Their symmetry group is T_d. The letter C denotes a rotation, the subscript gives the order of rotation, and the superscript the rotation axis. Thus, C_3^{xyz} is a rotation by $2\pi/3$ around the axis (xyz). 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). $\delta=\exp(ik_xa/2)$, $\gamma=\exp(-ik_ya/2)$, $\epsilon=\exp(-ik_za/2)$.

		$\exp(i\vec{k}\cdot\vec{R}_q^{\gamma})$											
$\vec{q}$	γ	E	C_3^{xyz}	C_3^{2xyz}	$C_3^{\bar{x}yz}$	$C_3^{2\bar{x}yz}$	$C_3^{x\bar{y}z}$	$C_3^{2x\bar{y}z}$	$C_3^{xy\bar{z}}$	$C_3^{2xy\bar{z}}$	C_2^{x}	C_2^{y}	C_2^{z}
$\vec{q}_a=(0,0,0)$		1	1	1	1	1	1	1	1	1	1	1	1
$\vec{q}_a^{(2)}=(a/4,a/4,a/4)$		1	1	1	$\delta\epsilon$	$\gamma\epsilon$	$\delta\gamma$	$\delta\epsilon$	$\gamma\epsilon$	$\delta\gamma$	$\gamma\epsilon$	$\delta\epsilon$	$\delta\gamma$
$\vec{q}_b=(a/2,0,0)$		1	$\delta\gamma^*$	$\delta\epsilon^*$	$\delta\gamma^*$	$\delta\epsilon$	$\delta\gamma$	$\delta\gamma$	$\delta\gamma$	$\delta\epsilon^*$	1	δ^2	δ^2
$\vec{q}_b^{(2)}=(\bar{a}/4,a/4,a/4)$		1	$\delta^*\gamma$	$\delta^*\epsilon$	$\gamma\epsilon$	$\delta^*\epsilon$	1	1	$\delta^*\epsilon$	$\gamma\epsilon$	$\gamma\epsilon$	$\delta^*\epsilon$	$\delta^*\gamma$

$\vec{q}$	γ	σ^{xy}	$\sigma^{\bar{x}y}$	σ^{xz}	$\sigma^{\bar{x}z}$	σ^{yz}	$\sigma^{\bar{y}z}$	S_4^{x}	S_4^{3x}	S_4^{y}	S_4^{3y}	S_4^{z}	S_4^{3z}
$\vec{q}_a=(0,0,0)$		1	1	1	1	1	1	1	1	1	1	1	1
$\vec{q}_a^{(2)}=(a/4,a/4,a/4)$		$\delta\gamma$	1	$\delta\epsilon$	1	$\gamma\epsilon$	1	$\delta\gamma$	$\delta\epsilon$	$\gamma\epsilon$	$\delta\gamma$	$\delta\epsilon$	$\gamma\epsilon$
$\vec{q}_b=(a/2,0,0)$		$\delta\epsilon$	$\delta\gamma^*$	$\delta\epsilon$	$\gamma\epsilon^*$	1	1	δ^2	δ^2	$\delta\epsilon$	$\delta\epsilon^*$	$\delta\gamma^*$	$\delta\gamma$
$\vec{q}_b^{(2)}=(\bar{a}/4,a/4,a/4)$		1	$\delta^*\gamma$	1	$\delta^*\epsilon$	$\gamma\epsilon$	1	$\delta^*\gamma$	$\delta^*\epsilon$	$\delta^*\gamma$	$\gamma\epsilon$	$\gamma\epsilon$	$\delta^*\epsilon$

TABLE II. Phase factors $\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma|\vec{c})})$ for the symmetry centers $\vec{q}_c$, $\vec{q}_d$, and their stars. Their symmetry group is D_{3d}. I is the inversion. All the other symbols have the same meaning as in Table I.

							$\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma\|\vec{c})})$						
$\vec{q}$	γ	E	C_3^{xyz}	C_3^{2xyz}	$C_2^{\bar{x}y}$	$C_2^{\bar{x}z}$	$C_2^{\bar{y}z}$	I	S_6^{xyz}	S_6^{5xyz}	$\sigma^{\bar{x}y}$	$\sigma^{\bar{x}z}$	$\sigma^{\bar{y}z}$
$\vec{q}_c=(a/8,a/8,a/8)$		1	1	1	1	1	1	1	1	1	1	1	1
$\vec{q}_d=(a/8,a/8,3\bar{a}/8)$		1	$\delta\epsilon^*$	$\gamma\epsilon^*$	$(\epsilon^*)^2$	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	$(\epsilon^*)^2$	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	1	$\delta\epsilon^*$	$\gamma\epsilon^*$
$\vec{q}$	γ	E	$C_3^{2x\bar{y}z}$	$C_3^{x\bar{y}z}$	C_2^{xy}	C_2^{xz}	$C_2^{\bar{y}z}$	I	$S_6^{5x\bar{y}z}$	$S_6^{x\bar{y}z}$	σ^{xy}	σ^{xz}	$\sigma^{\bar{y}z}$
$\vec{q}_c^{(2)}=(a/8,3a/8,3a/8)$		1	$\delta\epsilon$	$\delta\gamma$	$\delta^*\epsilon$	$\delta^*\gamma$	$\gamma\epsilon$	$\gamma\epsilon$	$\delta^*\gamma$	$\delta^*\epsilon$	$\delta\gamma$	$\delta\epsilon$	1
$\vec{q}_d^{(2)}=(a/8,3a/8,\bar{a}/8)$		1	$\delta\gamma$	$\delta\epsilon^*$	$\delta^*\epsilon^*$	$\gamma\epsilon^*$	1	$\gamma\epsilon^*$	$\delta^*\epsilon^*$	1	$\delta\gamma$	1	$\gamma\epsilon^*$
$\vec{q}$	γ	E	$C_3^{\bar{x}yz}$	$C_3^{2\bar{x}yz}$	$C_2^{\bar{x}y}$	C_2^{yz}	C_2^{xz}	I	$S_6^{\bar{x}yz}$	$S_6^{5\bar{x}yz}$	$\sigma^{\bar{x}y}$	σ^{yz}	σ^{xz}
$\vec{q}_c^{(3)}=(\bar{a}/8,\bar{a}/8,a/8)$		1	1	1	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	1	1	1
$\vec{q}_d^{(3)}=(\bar{a}/8,\bar{a}/8,3\bar{a}/8)$		1	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	$(\delta\gamma\epsilon^2)^*$	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	$(\delta\gamma\epsilon^2)^*$	$\gamma^*\epsilon^*$	$\delta^*\epsilon^*$	1	$\gamma^*\epsilon^*$	$\delta^*\epsilon^*$
$\vec{q}$	γ	E	$C_3^{2xy\bar{z}}$	$C_3^{xy\bar{z}}$	C_2^{xy}	$C_2^{\bar{x}z}$	C_2^{yz}	I	$S_6^{5xy\bar{z}}$	$S_6^{xy\bar{z}}$	σ^{xy}	$\sigma^{\bar{x}z}$	σ^{yz}
$\vec{q}_c^{(4)}=(3a/8,a/8,3a/8)$		1	$\delta\gamma$	$\gamma\epsilon$	$\gamma^*\epsilon$	$\delta\epsilon$	$\delta\gamma^*$	$\delta\epsilon$	$\gamma^*\epsilon$	$\delta\gamma^*$	$\delta\gamma$	1	$\gamma\epsilon$
$\vec{q}_d^{(4)}=(3a/8,a/8,\bar{a}/8)$		1	$\delta\epsilon^*$	$\delta\gamma$	$\gamma^*\epsilon^*$	1	$\delta\epsilon^*$	$\delta\epsilon^*$	1	$\gamma^*\epsilon^*$	$\delta\gamma$	$\delta\epsilon^*$	1

where D_{3d} denotes the space group with the point symmetry D_{3d} and C_4^z, C_2^z, and C_4^{3z} are rotations around the z axis by $\pi/2$, π, and $3\pi/2$, correspondingly. It should be pointed out that while for the centers $\vec{q}_a$ and $\vec{q}_b$ and their star vectors the symmetry group $\vec{G}_q$ is T_d and it is the same for all of them, the situation is different for the symmetry centers $\vec{q}_c$ and $\vec{q}_d$. In this case the symmetry group G_q is denoted by the same symbol D_{3d} but it is related to different symmetry axes as can be seen from Table II. Thus, for $\vec{q}_c$ and $\vec{q}_d$ the symmetry group is D_{3d}^{xyz}, while for $\vec{q}_c^{(2)}$ and $\vec{q}_d^{(2)}$ it is $D_{3d}^{x\bar{y}\bar{z}}$ and so on. (xyz) and $(x\bar{y}\bar{z})$ denote the threefold rotation axes. Details are given in Table II. The star of $\vec{q}_c$ contains also the vectors

$$\vec{q}_c^{(2)}=(C_4^z \mid a/4,a/4,a/4)\vec{q}_c =(a/8,3a/8,3a/8)\ ,$$

$$\vec{q}_c^{(3)}=C_2^z\vec{q}_c=(\bar{a}/8,\bar{a}/8,a/8)\ ,$$

$$\vec{q}_c^{(4)}=(C_4^{3z} \mid a/4,a/4,a/4)\vec{q}_c =(3a/8,a/8,3a/8)\ .$$

The star of $\vec{q}_d$ is found in the same way and is given in Table II. In Ref. 14, $\vec{q}_d =(5a/8,5a/8,5a/8)$. The symmetry center $\vec{q}_d$ in Table II is $(a/8,a/8,3\bar{a}/8)$ which differs from the one in Ref. 14 by the Bravais lattice vector $(\bar{a}/2,\bar{a}/2,\bar{a})$. We use here the fact that symmetry centers that differ by a Bravais lattice vector are equivalent.[4]

We turn now to the construction of the irreducible-band representations of the space group O_h^7. For doing this we construct first the irreducible-band representations $D^{(\vec{q},l)}[(\gamma \mid \vec{c}),\vec{k}]$ of the subgroups G_q of O_h^7 for different symmetry centers. They are obtained according to the following rule[7]:

$(\gamma \mid \vec{c})$:

$$D^{(\vec{q},l)}[(\gamma \mid \vec{c}),\vec{k}]=\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma \mid \vec{c})})D^{(l)}(\gamma)\ , \qquad (5)$$

where $D^{(l)}(\gamma)$ are the irreducible representations of the point theory of G_q (which is obtained by simply taking all the point-group elements of G_q without any translations) and $\vec{R}_q^{(\gamma \mid \vec{c})}$ are defined in Eq. (1). It should be pointed out that in its form (5) the band representations are written in the kq representation.[16] Since $\vec{k}$ is a variable the correspondence in (5) gives actually an infinite-dimensional representation. Only in its k-dependent form as a band representation, is (5) finite dimensional [it has then the dimensionality of $D^{(l)}(\gamma)$].

For O_h^7 we have mentioned above the symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$. The centers $\vec{q}_a$ and $\vec{q}_b$ have the same symmetry group which is T_d. In Table I we list the phase factors $\exp(i\vec{k}\cdot\vec{R}_q^{\gamma})$ of Eq. (5) corresponding to the sets of the Bravais lattice vectors $\vec{R}_a^{\gamma}=-\vec{q}_a+\gamma\vec{q}_a$ and $\vec{R}_b^{\gamma}=-\vec{q}_b+\gamma\vec{q}_b$ and accordingly also for the stars of $\vec{q}_a$ and $\vec{q}_b$. Table II contains the phase factors of Eq. (5) for the symmetry centers $\vec{q}_c$ and $\vec{q}_d$ and their stars.

Let us first consider in detail Eq. (5) for the symmetry centers $\vec{q}_a$ and $\vec{q}_b$. Their symmetry group is T_d and Eq. (5) gives four different irreducible-band representations of this space group for each irreducible representation $D^{(l)}(\gamma)$ of the point group T_d. Two band representations are obtained from the star of $\vec{q}_a$ and two from the star of $\vec{q}_b$. The phases in Eq. (5) can be interpreted in the following way. Let γ be an element of the space group around the origin of the crystal (it sometimes appears with a partial translation $\vec{c}$) and denote by γ_q the same element when related to the origin at $\vec{q}$. Then [see Eq. (1)]

$$\vec{\gamma}_q=(\epsilon \mid -\vec{q})\gamma(\epsilon \mid +\vec{q})=(\gamma \mid \vec{c}-\vec{R}_q^{(\gamma \mid \vec{c})})\ . \qquad (6)$$

We see therefore that the operation of the point-group element γ_q around $\vec{q}$ can be achieved by applying the same element around the origin $(\gamma \mid \vec{c})$ and by accompanying it by a translation $\vec{R}_q^{(\gamma \mid \vec{c})}$. Correspondingly, the phase factor $\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma \mid \vec{c})})$ in (5) can be interpreted as following from the choice of the point group center at $\vec{q}$. We come therefore to the conclusion that the rule (5) gives the representations of G_q with respect to the fixed point-group center at $\vec{q}$. This shows that the symmetry center $\vec{q}$ can be used as a label (via the Bravais lattice vectors $\vec{R}_q^{(\gamma \mid \vec{c})}$) in specifying the band representations of the group G_q. As was already mentioned, for the space group T_d we have four symmetry centers $\vec{q}_a$, $\vec{q}_a^{(2)}$, $\vec{q}_b$, and $\vec{q}_b^{(2)}$ and by choosing each of these centers as an origin for the point-group elements we obtain four different irreducible-band representations for each irreducible representation $D^{(l)}(\gamma)$ of the point group T_d. The phases of Eq. (5) for these band representations are listed in Table I. Since T_d is a symmorphic space group[15] all the elements in Table I are pure point-group elements.

Having the band representations of T_d we can by induction[4,15] find the corresponding band representations of the full space group O_h^7. Let us denote by $C_s^{(r,l)}(\vec{k},\vec{q})$, $s=1,\ldots,m$ the basis for a band representation of G_r corresponding to the symmetry center $\vec{q}_r$ and the irreducible representation l of the point group of G_r. Correspondingly we denote

$$C_s^{(r_i,l)}(\vec{k},\vec{q})=(\alpha_i\mid\vec{a}_i)C_s^{(r,l)}(\vec{k},\vec{q}) ,$$

where $(\alpha_i\mid\vec{a}_i)$ is an element in the decomposition (2). With this notation the band representation of G that is induced from the band representation $D^{(r,l)}$ of G_r can be written in the following form[4]:

$$(\alpha\mid\vec{a})C_s^{(r_i,l)}(\vec{k},\vec{q})=\exp\{i\vec{k}\cdot[-\vec{q}_r^{(j)}+(\alpha\mid\vec{a})\vec{q}_r^{(i)}]\}\sum_{s'=1}^{m}D_{s's}^{(l)}(\gamma')C_{s'}^{(r_j,l)}(\vec{k},\vec{q}) , \quad (7)$$

where the following relation

$$(\alpha\mid\vec{a})(\alpha_i\mid\vec{a}_i)=(\alpha_j\mid\vec{a}_j)(\gamma'\mid\vec{c}\,') \quad (8)$$

was assumed. In (7) and (8) $(\alpha\mid\vec{a})$ is a general element of the space group G, $(\alpha_i\mid\vec{a}_i)$ and $(\alpha_j\mid\vec{a}_j)$ are the elements of the cosets [Eq. (2)], and $(\gamma'\mid\vec{c}\,')$ is an element of G_r. It is convenient to look at the matrix $D(\alpha\mid\vec{a})$ which represents the element $(\alpha\mid\vec{a})$ in Eq. (7) as consisting of block matrices of dimension $m\times m$. In this form the only nonvanishing block in column i of the matrix $D(\alpha\mid\vec{a})$ is in the row j. Equation (7) induces band representations of the space group G from the band representations of its subgroup G_r.

For the symmetry centers $\vec{q}_a$ and $\vec{q}_b$ Eq. (7) simplifies because the symmetry group of these centers T_d is an invariant subgroup of the full space group O_h^7. When G_r is an invariant subgroup of G, Eq. (8) for the elements $(\gamma\mid\vec{c})$ of G_r assumes the form

$$(\gamma\mid\vec{c})(\alpha_i\mid\vec{a}_i)=(\alpha_i\mid\vec{a}_i)(\gamma'\mid\vec{c}\,') . \quad (9)$$

Correspondingly, the induced-band representation of Eq. (7) for the elements $(\gamma\mid\vec{c})$ of G_r will become[4]

$$(\gamma\mid\vec{c})C_s^{(r_i,l)}(\vec{k},\vec{q})=\exp(-i\vec{k}\cdot\vec{R}_i^{(\gamma\mid\vec{c})})\times\sum_{s'=1}^{m}D_{s's}^{(l)}(\gamma')C_{s'}^{(r_i,l)}(\vec{k},\vec{q}) , \quad (10)$$

where

$$\vec{R}_i^{(\gamma\mid\vec{c})}=(\gamma\mid\vec{c})\vec{q}^{(i)}-\vec{q}^{(i)} . \quad (11)$$

For elements $(\alpha\mid\vec{a})$ of G that do not belong to G_r, the block matrix $D(\alpha\mid\vec{a})$ has only vanishing block matrices on the diagonal. This follows directly from Eq. (8) when written for an invariant subgroup and the general expression (7) for the induced-band representation.

Having Eq. (10) it becomes a simple matter to find the band representations of O_h^7 that are induced from the band representations of T_d. Since T_d is a symmorphic group, $\vec{c}$ is a Bravais lattice vector. For using Eq. (10) we need the multiplication table of Eq. (9) for the decomposition (3). If γ is an element of T_d (ϵ is the unit element), then $I\gamma$ is an element of the second coset in the decomposition (3), and Eq. (9) assumes the form

$$\gamma\epsilon=\epsilon\gamma,\quad \gamma I=I\gamma ,$$
$$(I\gamma)\epsilon=(I\gamma)\epsilon,\quad (I\gamma)I=\epsilon\gamma . \quad (12)$$

With the aid of Table I we can now construct the band representations of O_h^7 that are induced from the symmetry centers $\vec{q}_a$ and $\vec{q}_b$. As an example let us find explicitly the matrices $D^{(a,l)}(C_3^{xyz})$ and $D^{(b,l)}(C_3^{xyz})$. From Table I we find that for C_3^{xyz} the phase factor $\exp(i\vec{k}\cdot\vec{R}^{\gamma})$ assumes the following values: It is 1 for the centers $\vec{q}_a$ and $\vec{q}_a^{(2)}$; it is $\delta\gamma^*$ for $\vec{q}_b$, and $\delta^*\gamma$ for $\vec{q}_b^{(2)}$. By using Eq. (10) and the multiplication table (12) we find that the only nonzero block matrices are on the diagonal

$$D_{11}^{(a,l)}(C_3^{xyz})=D_{22}^{(a,l)}(C_3^{xyz})=D^{(l)}(C_3^{xyz}) ,$$
$$D_{11}^{(b,l)}(C_3^{xyz})=\delta^*\gamma D^{(l)}(C_3^{xyz}) , \quad (13)$$
$$D_{22}^{(b,l)}(C_3^{xyz})=\delta\gamma^* D^{(l)}(C_3^{xyz}) ,$$

where D_{ij} denote block matrices. Similarly, one can find the matrices for the other elements of O_h^7.

Let us now turn to the symmetry centers $\vec{q}_c$ and $\vec{q}_d$. For these centers the symmetry group G_q (which is D_{3d}) is not an invariant subgroup of the full space group O_h^7. Each of the centers has four vectors in the star and in Table II we list the phases $\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma\mid\vec{c})})$ that correspond to the Bravais lattice vectors $\vec{R}_q^{(\gamma\mid\vec{c})}$. By using Eq. (5) we find the irreducible-band representations of the space groups D_{3d} for the different centers $\vec{q}_c$ and $\vec{q}_d$ and their stars. As was already mentioned before, the symmetry groups for different centers in the same star are different (despite the fact that they are denoted by the same symbol D_{3d}). Thus, for $\vec{q}_c$ the symmetry group is D_{3d}^{xyz} while for $\vec{q}_c^{(2)}$ it is $D_{3d}^{\bar{x}\bar{y}z}$, and so on (see Table II). Correspondingly, each vector in the star defines, according to Eq. (5), the band representations of its symmetry group. Thus $\vec{q}_c$ leads to six-irreducible-band representations of D_{3d}^{xyz} (six is the number of irreducible representations of the point group D_{3d}). They are obtained from Eq. (5) by varying l (l runs from one to six over the six irreducible representations[17] of the point group D_{3d}) for the fixed set of phases $\exp(i\vec{k}\cdot\vec{R}_c^{(\gamma|\vec{c})})$ corresponding to $\vec{q}_c$.

Having the band representations of the symmetry groups of $\vec{q}_c$ and $\vec{q}_d$ (and their stars) we use now the induction equation (7) for constructing the corresponding band representations of O_h^7. For using Eq. (7) we need the multiplication table (8) for the decomposition (4). This information is contained in Table III. In this table we list only the point-group elements without their partial translations. Since the space groups D_{3d} in O_h^7 are nonsymmorphic[15] some of the elements in Table III contain partial translations. In fact D_{3d} can be decomposed into two cosets by

$$D_{3d}=C_{3v}+(I\mid a/4,a/4,a/4)C_{3v}\ . \tag{14}$$

Here C_{3v} is a symmorphic group while all the elements of the second coset contain the partial translation $(a/4,a/4,a/4)$. From the point of view of the whole space group O_h^7 the information about pure point-group elements and mixed ones (containing partial translations) is given in the decomposition (3). As was already mentioned T_d is a symmorphic group while the second coset in (3) contains mixed elements. In Table III explicit multiplication results are given for the elements of D_{3d}^{xyz} and the coset elements C_4^z, C_2^z, and C_4^{3z} [see decomposition (4)]. Clearly with the information in Table III, it is a simple matter to find the multiplication rule for any $(\alpha\mid\vec{a})$ because one can always find an $(\alpha_i\mid\vec{a}_i)$ and an $(\gamma\mid\vec{c})$ such that $(\alpha\mid\vec{a})=(\alpha_i\mid\vec{a}_i)(\gamma\mid\vec{c})$. Here $(\gamma\mid\vec{c})$ is an element of ${D_{3d}}^{xyz}$ and $(\alpha_i\mid\vec{a}_i)$ is one of the rotations around the z axis, C_4^z, C_2^z, C_4^{3z}. Since Table III contains the information for the elements of D_{3d}^{xyz} and $(\alpha_i\mid\vec{a}_i)$, the multiplication rule for any other $(\alpha\mid\vec{a})$ can be easily found from it. With Tables II and III at hand we can use Eq. (7) for finding the band representations of O_h^7 that are induced by the symmetry centers $\vec{q}_c$ and $\vec{q}_d$. As an example let us calculate explicitly the matrix $D^{(c,l)}(C_3^{xyz})$ for the element C_3^{xyz}. This band representation is induced from the symmetry center $\vec{q}_c$. From Table III it follows that the only nonvanishing block matrices are $D_{11}^{(c,l)}$, $D_{42}^{(c,l)}$, $D_{23}^{(c,l)}$, and $D_{34}^{(c,l)}$. By using the induction equation (7) and Tables II and III we find

TABLE III. Multiplication table for the decomposition of O_h^7 with respect to D_{3d}. The table contains the products of an element in the left-hand column with an element in the upper row.

	E	C_4^z	C_2^z	C_4^{3z}
E	$E\,E$	$C_4^z\,E$	$C_2^z\,E$	$C_4^{3z}\,E$
C_3^{xyz}	$E\,C_3^{xyz}$	$C_4^{3z}\,C_3^{2xyz}$	$C_4^z\,C_2^{\bar{y}z}$	$C_2^z\,C_2^{\bar{x}z}$
C_3^{2xyz}	$E\,C_3^{2xyz}$	$C_2^z\,C_2^{\bar{y}z}$	$C_4^{3z}\,C_2^{\bar{x}z}$	$C_4^z\,C_3^{xyz}$
$C_2^{\bar{x}y}$	$E\,C_2^{\bar{x}y}$	$C_4^{3z}\,C_2^{\bar{x}y}$	$C_2^z\,C_2^{\bar{x}y}$	$C_4^z\,C_2^{\bar{x}y}$
$C_2^{\bar{y}z}$	$E\,C_2^{\bar{y}z}$	$C_4^z\,C_2^{\bar{x}z}$	$C_4^{3z}\,C_3^{xyz}$	$C_2^z\,C_3^{2xyz}$
$C_2^{\bar{x}z}$	$E\,C_2^{\bar{x}z}$	$C_2^z\,C_3^{xyz}$	$C_4^z\,C_3^{2xyz}$	$C_4^{3z}\,C_2^{\bar{y}z}$
I	$E\,I$	$C_4^z\,I$	$C_2^z\,I$	$C_4^{3z}\,I$
S_6^{xyz}	$E\,S_6^{xyz}$	$C_4^{3z}\,S_6^{5xyz}$	$C_4^z\,\sigma^{\bar{y}z}$	$C_2^z\sigma^{\bar{x}z}$
S_6^{5xyz}	$E\,S_6^{5xyz}$	$C_2^z\,\sigma^{\bar{y}z}$	$C_4^{3z}\,\sigma^{\bar{x}z}$	$C_4^z\,S_6^{xyz}$
$\sigma^{\bar{x}y}$	$E\,\sigma^{\bar{x}y}$	$C_4^{3z}\,\sigma^{\bar{x}y}$	$C_2^z\,\sigma^{\bar{x}y}$	$C_4^z\,\sigma^{\bar{x}y}$
$\sigma^{\bar{y}z}$	$E\,\sigma^{\bar{y}z}$	$C_4^z\,\sigma^{\bar{x}z}$	$C_4^{3z}\,S_6^{xyz}$	$C_2^z\,S_6^{5xyz}$
$\sigma^{\bar{x}z}$	$E\,\sigma^{\bar{x}z}$	$C_2^z\,S_6^{xyz}$	$C_4^z\,S_6^{5xyz}$	$C_4^{3z}\,\sigma^{\bar{y}z}$
C_4^z	$C_4^z\,E$	$C_2^z\,E$	$C_4^{3z}\,E$	$E\,E$
C_2^z	$C_2^z\,E$	$C_4^{3z}\,E$	$E\,E$	$C_4^z\,E$
C_4^{3z}	$C_4^{3z}\,E$	$E\,E$	$C_4^z\,E$	$C_2^z\,E$

$$D_{11}^{(c,l)}(C_3^{xyz})=D^{(l)}(C_3^{xyz}) ,$$
$$D_{42}^{(c,l)}(C_3^{xyz})=D^{(l)}(C_3^{2xyz}) , \qquad (15)$$
$$D_{23}^{(c,l)}(C_3^{xyz})=D^{(l)}(C_2^{\bar{y}z}) ,$$
$$D_{34}^{(c,l)}(C_3^{xyz})=D^{(l)}(C_2^{\bar{x}z}) ,$$

where by $D^{(l)}$ we have denoted the irreducible representations of D_{3d}. In a similar way one can find the matrices $D^{(c,l)}$ and also $D^{(d,l)}$ for all the elements of O_h^7. The induction method will give an irreducible-band representation of O_h^7 for each star, e.g., $\vec{q}_c$ or $\vec{q}_d$ and each irreducible representation of the point group D_{3d}. Since the latter has six irreducible representations[17] Eq. (7) will give 12-irreducible-band representations of O_h^7, six for each symmetry center $\vec{q}_c$ and $\vec{q}_d$.

So far we have considered the symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$ in the Wigner-Seitz cell and have pointed out how to find the irreducible-band representations of O_h^7 that are induced from these centers. Many other symmetry centers exist for the diamond space group.[14] However, as can be checked, symmetry groups G_q of these additional centers are subgroups of one of the above considered groups T_d or D_{3d}. One can also show that the set of the Bravais lattice vectors [Eq. (1)] for the subgroups G_q of any additional centers coincides on this subgroup with the corresponding set for a center of T_d or D_{3d}. As was proven in Ref. 4 such symmetry centers will not lead to new irreducible-band representations of O_h^7. An example of such a symmetry center is $q_e=(xxx)$ which has C_{3v} as its symmetry group.[14] The latter is a subgroup of both T_d and D_{3d}. One can also check that, for example, the Bravais lattice vectors corresponding to the symmetry centers $\vec{q}_a$ and $\vec{q}_e$ coincide, $R_e^{(\gamma|\vec{c})}=R_a^{(\gamma|\vec{c})}$ for $(\gamma|\vec{c})$ belonging to C_{3v}. The results of Ref. 4 show that the irreducible-band representations of O_h^7 that are induced from the symmetry center $\vec{q}_e$ are all contained among those induced from the center $\vec{q}_a$. If one is interested in irreducible-band representations only then the symmetry center $\vec{q}_e$ can be left out as long as $\vec{q}_a$ was considered. We come, therefore, to a conclusion that for the construction of all different irreducible-band representations of O_h^7 it is sufficient to consider the symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$. The latter by using Eq. (5) and the induction equation (7) lead to all the irreducible-band representations of O_h^7.

III. CONTINUITY CHORDS OF BANDS

Having the irreducible-band representations of a space group one can answer the question about 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_l, and so on, of irreducible representations for symmetry groups G_k at different points $\vec{k}$ in the Brillouin zone. By definition[15] all those elements $(\beta|\vec{b})$ of the space group G belong to G_k for which

$$\beta\vec{k}=\vec{k}+\vec{K} , \qquad (16)$$

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 $D^{(\vec{q},l)}[(\alpha|\vec{t}),\vec{k}]$ be a band representation of G. Then by definition[4] the matrix corresponding to $(\alpha_2|\vec{t}_2)(\alpha_1|\vec{t}_1)$ is

$$D^{(\vec{q},l)}[(\alpha_2|\vec{t}_2)(\alpha_1|\vec{t}_1),\vec{k}]=D^{(\vec{q},l)}[(\alpha_2|\vec{t}_2),\vec{k}]D^{(\vec{q},l)}[(\alpha_1|\vec{t}_1),\alpha_2^{-1}\vec{k}] , \qquad (17)$$

where in the last matrix $\alpha_2^{-1}\vec{k}$ appears, showing that $\vec{k}$ is a variable. For the elements of G_k Eq. (17) will assume the usual form of a multiplication rule for a representation. This follows from Eq. (16) for the elements of G_k and the fact that the band-representation matrices $D[(\alpha|\vec{t}),\vec{k}]$ 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 [Eq. (7)] and for each $\vec{k}$ we find the representation $D^{(k)}$ of G_k that is given by the same equation (7). 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 what we call the continuity chord of the band $(\vec{q},l)$.

As an example we consider the group O_h^7. We start with the symmetry centers $\vec{q}_a$ and $\vec{q}_b$. Their symmetry group is T_d. The point group T_d has five irreducible representations which we denote by $l=1, 2, \ldots, 5$, as in Ref. 17. Correspondingly we have ten-irreducible-band representations $(\vec{q}_a,l)$ and $(\vec{q}_b,l)$. Let us consider in detail the symmetry point $\vec{k}=(0,2\pi/a,0)$ (point X) in the Brillouin zone. Its symmetry group is $G_x=D_{4h}^{y}$. In Table IV we list the characters of the representations of G_x that are obtained from the band representations $(\vec{q}_a,l)$ and $(\vec{q}_b,l)$ at $\vec{k}=(0,2\pi/a,0)$ (point X). These characters are denoted by $\chi^{(a,l)}$ and $\chi^{(b,l)}$, correspondingly. They are obtained from Eq. (10) by using Table I and the multiplication table given in Eq. (12). In particular, from Eq. (12) it follows that the characters $\chi^{(a,l)}$ and $\chi^{(b,l)}$ vanish for the elements of D_{4h} that do not belong to T_d. By reducing the representations given in Table IV we find the irreducible representation of G_x that they contain. In Table IV we also list the irreducible representations of G_x, X_1, X_2, X_3, X_4 (see Ref. 17). The reduction leads to the following results:

$$\begin{aligned}
\chi^{(a,1)}&=\chi^{(b,1)}=X_1\,,\\
\chi^{(a,2)}&=\chi^{(b,2)}=X_2\,,\\
\chi^{(a,3)}&=\chi^{(b,3)}=X_1+X_2\,,\\
\chi^{(a,4)}&=\chi^{(b,4)}=X_1+X_3+X_4\,,\\
\chi^{(a,5)}&=\chi^{(b,5)}=X_2+X_3+X_4\,.
\end{aligned} \tag{18}$$

By carrying out the same process for all the symmetry points in the Brillouin zone[17] we find the continuity chords of the bands $(\vec{q}_a,l)$ and $(\vec{q}_b,l)$. The results are given in Table V. As is seen from this table the centers $\vec{q}_a$ and $\vec{q}_b$ lead to the same representations at all the symmetry points in the Brillouin zone with the only exception of the point W. At this point the representation $l=3$ of the point group T_d leads to the same representations (W_1+W_2) for both centers $\vec{q}_a$ and $\vec{q}_b$. For all the other representations of T_d $(l=1, 2, 4, 5)$ the centers $\vec{q}_a$ and $\vec{q}_b$ give different representations at the symmetry point W. All the symbols in Table V are according to Ref. 17.

For the centers $\vec{q}_c$ and $\vec{q}_d$ the symmetry group is D_{3d}. This point group has six irreducible representations which we denote by $l=1, 2, \ldots, 6$ as in Ref. 17. Having this in mind we expect 12-irreducible-band representations which are labeled by $(\vec{q}_c,l)$ and $(\vec{q}_d,l)$. As an example, let us consider the symmetry point $\vec{k}=(\pi/a,\pi/a,\pi/a)$ (point L) in the Brillouin zone.[17] Its symmetry $G_L=D_{3d}^{(xyz)}$. In Table VI we list the characters of the representations of G_L that are obtained from the band representations $(\vec{q}_c,l)$ and $(\vec{q}_d,l)$ at $\vec{k}=(\pi/a,\pi/a,\pi/a)$ (point L). They are denoted by $\chi^{(c,l)}$ and $\chi^{(d,l)}$, correspondingly. In obtaining these characters we use Eq. (7), Table II, and the multiplication table, Table III. In order to find the continuity chords for each band we reduce the representations $\chi^{(c,l)}$ and $\chi^{(d,l)}$ into the irreducible constituents of the group G_L. The latter are also listed in Table VI under $L_1, L_2, \ldots, L_6$. The reduction of $\chi^{(c,l)}$ and $\chi^{(d,l)}$ at the point L leads to the following results:

TABLE IV. Character table for the group D_{4h} of the symmetry point X. The symbols in the upper line have the same meaning as in Table I. The upper part of the table are the characters of the representations that are obtained from the band representations (a,l) and (b,l). The lower part are the characters of the irreducible representations for the symmetry point X (see Ref. 17).

$G_x=D_{4h}^{y}$	E	C_2^{y}	σ^{xz}	$\sigma^{\bar{x}z}$	$C_2^{\bar{x}z}$	C_2^{xz}	Other elements
$\chi^{(a,1)}=\chi^{(b,1)}$	2	2	2	2	0	0	
$\chi^{(a,2)}=\chi^{(b,2)}$	2	2	−2	−2	0	0	
$\chi^{(a,3)}=\chi^{(b,3)}$	4	4	0	0	0	0	0
$\chi^{(a,4)}=\chi^{(b,4)}$	6	−2	2	2	0	0	
$\chi^{(a,5)}=\chi^{(b,5)}$	6	−2	−2	−2	0	0	
X_1	2	2	2	2	0	0	
X_2	2	2	−2	−2	0	0	
X_3	2	−2	0	0	2	−2	0
X_4	2	−2	0	0	−2	2	

TABLE V. Continuity chords for the bands (a,l) and (b,l). a and b denote the symmetry centers $\vec{q}_a$ and $\vec{q}_b$. l denotes the irreducible representations of the point group T_d, $l=1, 2, 3, 4, 5$. The notations for the symmetry points in the Brillouin zone follow Ref. 17.

$\vec{k}$ \ $(\vec{q},l)$	$(a,1)$		$(b,1)$	$(a,2)$		$(b,2)$	$(a,3)(b,3)$	$(a,4)$		$(b,4)$	$(a,5)$		$(b,5)$
Γ		$\Gamma_1\Gamma_7$			$\Gamma_2\Gamma_6$		$\Gamma_3\Gamma_8$		$\Gamma_4\Gamma_{10}$			$\Gamma_5\Gamma_9$	
Δ		$\Delta_1\Delta_4$			$\Delta_2\Delta_3$		$\Delta_1\Delta_2\Delta_3\Delta_4$		$\Delta_1\Delta_4(2\Delta_5)$			$\Delta_2\Delta_3(2\Delta_5)$	
Σ		$\Sigma_1\Sigma_4$			$\Sigma_2\Sigma_3$		$\Sigma_1\Sigma_2\Sigma_3\Sigma_4$		$2(\Sigma_1\Sigma_4)\Sigma_2\Sigma_3$			$\Sigma_1\Sigma_4 2(\Sigma_2\Sigma_3)$	
Λ		$2\Lambda_1$			$2\Lambda_2$		$2\Lambda_3$		$2(\Lambda_1\Lambda_3)$			$2(\Lambda_2\Lambda_3)$	
Ξ		$\Xi_1\Xi_2$			$\Xi_1\Xi_2$		$2(\Xi_1\Xi_2)$		$3(\Xi_1\Xi_2)$			$3(\Xi_1\Xi_2)$	
Θ		$2\Theta_1$			$2\Theta_2$		$2(\Theta_1\Theta_2)$		$4\Theta_1 2\Theta_2$			$2\Theta_1 4\Theta_2$	
X		X_1			X_2		X_1X_2		$X_1X_3X_4$			$X_2X_3X_4$	
W	W_1		W_2	W_2		W_1	W_1W_2	W_1		$(2W_1)W_2$	$(2W_1)W_2$		$W_1(2W_2)$
K		K_1K_3			K_2K_4		$K_1K_2K_3K_4$		$2(K_1K_3)K_2K_4$			$K_1K_3 2(K_2K_4)$	
L		L_1L_4			L_2L_5		L_3L_6		$L_1L_3L_4L_6$			$L_2L_3L_5L_6$	
U		U_1U_2			U_3U_4		$U_1U_2U_3U_4$		$2(U_1U_2)U_3U_4$			$U_1U_2 2(U_3U_4)$	
Z		Z_1			Z_1		$2Z_1$		$3Z_1$			$3Z_1$	
Q		Q_1Q_2			Q_1Q_2		$2(Q_1Q_2)$		$3(Q_1Q_2)$			$3(Q_1Q_2)$	
S		S_1S_2			S_3S_4		$S_1S_2S_3S_4$		$2(S_1S_2)S_3S_4$			$S_1S_2 2(S_3S_4)$	
A		A_1A_2			A_1A_2		$2(A_1A_2)$		$3(A_1A_2)$			$3(A_1A_2)$	
B		B_1B_2			B_1B_2		$2(B_1B_2)$		$3(B_1B_2)$			$3(B_1B_2)$	
M		$2M_1$			$2M_2$		$2(M_1M_2)$		$(4M_1)(2M_2)$			$(2M_1)(4M_2)$	
N		N_1N_2			N_1N_2		$2(N_1N_2)$		$3(N_1N_2)$			$3(N_1N_2)$	

TABLE VI. Character table for the group D_{3d} of the symmetry point L. The symbols in the upper line have the same meaning as in Tables I and II. The upper part of the table is the characters of the representations that are obtained from the band representations (c,l) and (d,l). The lower part is the characters of the irreducible representation for the symmetry point L (see Ref. 17).

$G_L=D_{3d}^{(xyz)}$	E	$C_3^{xyz}C^{2xyz}$	I	$S_6^{xyz}S_6^{5xyz}$	$\sigma^{\bar{x}z}\sigma^{\bar{y}z}\sigma^{\bar{x}y}$	$C_2^{\bar{x}z}C_2^{\bar{x}y}C_2^{\bar{x}y}$
$\chi^{(c,1)}=\chi^{(d,4)}$	4	1	−2	1	2	0
$\chi^{(c,2)}=\chi^{(d,5)}$	4	1	−2	1	−2	0
$\chi^{(c,3)}=\chi^{(d,6)}$	8	−1	−4	−1	0	0
$\chi^{(c,4)}=\chi^{(d,1)}$	4	1	2	−1	2	0
$\chi^{(c,5)}=\chi^{(d,2)}$	4	1	2	−1	−2	0
$\chi^{(c,6)}=\chi^{(d,3)}$	8	−1	4	1	0	0
L_1	1	1	1	1	1	1
L_2	1	1	1	1	−1	−1
L_3	2	−1	2	−1	0	0
L_4	1	1	−1	−1	1	−1
L_5	1	1	−1	−1	−1	1
L_6	2	−1	−2	1	0	0

$$
\begin{aligned}
&\chi^{(c,1)}=\chi^{(d,4)}=L_1+L_4+L_6\,,\\
&\chi^{(c,2)}=\chi^{(d,5)}=L_2+L_5+L_6\\
&\chi^{(c,3)}=\chi^{(d,6)}=L_1+L_4+L_5+2L_6\,,\\
&\chi^{(c,4)}=\chi^{(d,1)}=L_1+L_3+L_4\\
&\chi^{(c,5)}=\chi^{(d,2)}=L_2+L_3+L_5\,,\\
&\chi^{(c,6)}=\chi^{(d,3)}=L_1+L_2+2L_3+L_6\,.
\end{aligned}
\tag{19}
$$

This process can be carried out for all the symmetry points in the Brillouin zone. The results are summed up in Table VII. The symmetry centers $\vec{q}_c$ and $\vec{q}_d$ lead to the same representations at all the points in the Brillouin zone with the only exception at point L at which they are different. In Table VII this is shown by listing the representations for $\vec{q}_c$ in the upper line and for $\vec{q}_d$ in the lower line. For all the other symmetry points in the Brillouin zone they are identical.

In summing up this section let us point out that Tables V and VII contain the continuity chords for all the irreducible-band representations of the space group O_h^7 that are induced from the symmetry centers $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$. There is no need to consider other symmetry centers of O_h^7 in the Wigner-Seitz cell because, as was already mentioned in the preceding section, they don't lead to additional irreducible-band representations of O_h^7. Tables V abd VII give, therefore, all the continuity chords for all the possible symmetry types of bands for the diamond structure O_h^7.

IV. DISCUSSION

We introduced the concept of a continuity chord for defining all those Bloch states at different symmetry points in a Brillouin zone that can possibly belong to a band with a given symmetry type. In finding continuity chords we used band representations which are fully defined by the symmetry group of the solid. It might therefore appear that continuity chords can be established from symmetry arguments only. This is, however, not so because band representations are given by $\vec{k}$-dependent matrices $D[(\gamma|\vec{c}),\vec{k}]$ [see Eq. (5)] containing the phases $\exp(i\vec{k}\cdot\vec{R}_q^{(\gamma|\vec{c})})$. The latter are continuous and periodic in $\vec{k}$. Band representations have, therefore, a built-in continuity in $\vec{k}$ by their definition. This continuity also appears in the concepts of equivalency and reducibility of band representations.[4] Since continuity chords are found by using band representations they depend both on their symmetry and their continuity. In this sense the continuity chords are closely related to the compatibility[2] or connectivity[3] relations of bands which are also defined by symmetry and continuity arguments. However, in establishing compatibility relations the only symmetry tool at hand is the reduction of representations at neighboring points in the Brillouin zone. In simple situations this

TABLE VII. Continuity chords for the bands (c,l) and (d,l). c and d denote the symmetry centers $\vec{q}_c$ and $\vec{q}_d$. l denotes the irreducible representations of the point group D_{3d}, $l=1, 2, 3, 4, 5, 6$. The notations for the symmetry point in the Brillouin zone follow Ref. 17.

$\vec{k}$ \ $(\vec{q},l)$	$(c,1)$ $(d,1)$	$(c,2)$ $(d,2)$	$(c,3)$ $(d,3)$	$(c,4)$ $(d,4)$	$(c,5)$ $(d,5)$	$(c,6)$ $(d,6)$
Γ	$\Gamma_1\Gamma_4$	$\Gamma_2\Gamma_5$	$\Gamma_3\Gamma_4\Gamma_5$	$\Gamma_7\Gamma_{10}$	$\Gamma_6\Gamma_9$	$\Gamma_8\Gamma_9\Gamma_{10}$
Δ	$\Delta_1\Delta_4\Delta_5$	$\Delta_2\Delta_3\Delta_5$	$\Delta_1\Delta_2\Delta_3\Delta_4\Delta_5$	$\Delta_1\Delta_4\Delta_5$	$\Delta_2\Delta_3\Delta_5$	$\Delta_1\Delta_2\Delta_3\Delta_4 2\Delta_5$
Σ	$(2\Sigma_1)\Sigma_3\Sigma_4$	$(2\Sigma_2)\Sigma_3\Sigma_4$	$2(\Sigma_1\Sigma_2\Sigma_3\Sigma_4)$	$\Sigma_1\Sigma_2(2\Sigma_4)$	$\Sigma_1\Sigma_2(2\Sigma_3)$	$2(\Sigma_1\Sigma_2\Sigma_3\Sigma_4)$
Λ	$(2\Lambda_1)\Lambda_3$	$(2\Lambda_2)\Lambda_3$	$\Lambda_1\Lambda_2(3\Lambda_3)$	$(2\Lambda_1)\Lambda_3$	$(2\Lambda_2)\Lambda_3$	$\Lambda_2\Lambda_2(3\Lambda_3)$
Ξ	$2(\Xi_1\Xi_2)$	$2(\Xi_1\Xi_2)$	$4(\Xi_1\Xi_2)$	$2(\Xi_1\Xi_2)$	$2(\Xi_1\Xi_2)$	$4(\Xi_2\Xi_2)$
Θ	$(3\Theta_1)\Theta_2$	$\Theta_1(3\Theta_2)$	$4(\Theta_1\Theta_2)$	$(3\Theta_1)\Theta_2$	$\Theta_1(3\Theta_2)$	$4(\Theta_1\Theta_2)$
X	X_1X_3	X_2X_4	$X_1X_2X_3X_4$	X_1X_4	X_2X_3	$X_2X_2X_3X_4$
W	W_1W_2	W_1W_2	$2(W_1W_2)$	W_1W_2	W_1W_2	$2(W_1W_2)$
K	$(2K_1)K_3K_4$	$(2K_2)K_3K_4$	$2(K_1K_2K_3K_4)$	$K_1K_2(2K_3)$	$K_1K_2(2K_4)$	$2(K_1K_2K_3K_4)$
$L(c)$	$L_1L_4L_6$	$L_2L_5L_6$	$L_3L_4L_5(2L_6)$	$L_1L_3L_4$	$L_2L_3L_5$	$L_1L_2(2L_3)L_6$
$L(d)$	$L_1L_3L_4$	$L_2L_3L_5$	$L_1L_2(2L_3)L_6$	$L_1L_4L_6$	$L_2L_5L_6$	$L_3L_4L_5(2L_6)$
U	$U_1(2U_2)U_3$	$U_1U_3(2U_4)$	$2(U_1U_2U_3U_4)$	$(2U_1)U_2U_4$	$U_2(2U_3)U_4$	$2(U_1U_2U_3U_4)$
Z	$2Z_1$	$2Z_1$	$4Z_1$	$2Z_1$	$2Z_1$	$4Z_1$
Q	$2(Q_1Q_2)$	$2(Q_1Q_2)$	$4(Q_1Q_2)$	$2(Q_1Q_2)$	$2(Q_1Q_2)$	$4(Q_1Q_2)$
S	$S_1(2S_2)S_3$	$S_1S_3(2S_4)$	$2(S_1S_2S_3S_4)$	$(2S_1)S_2S_4$	$S_2(2S_3)S_4$	$2(S_1S_2S_3S_4)$
A	$2(A_1A_2)$	$2(A_1A_2)$	$4(A_1A_2)$	$2(A_1A_2)$	$2(A_1A_2)$	$4(A_1A_2)$
B	$2(B_1B_2)$	$2(B_1B_2)$	$4(B_1B_2)$	$2(B_1B_2)$	$2(B_1B_2)$	$4(B_1B_2)$
M	$(3M_1)M_2$	$M_1(3M_2)$	$4(M_1M_2)$	$(3M_1)M_2$	$M_1(3M_2)$	$4(M_1M_2)$
N	$2(N_1N_2)$	$2(N_1N_2)$	$4(N_1N_2)$	$2(N_1N_2)$	$2(N_1N_2)$	$4(N_1N_2)$

gives a connection between Bloch states at different symmetry points but, in general, there is no way to connect all the symmetry points by compatibility arguments. Band representations specify bands as whole entities and this is the reason that they enable one to establish continuity chords for bands in solids.

Tables V and VII contain the continuity chords for all the irreducible-band representations of the diamond space group O_h^7. Thus, in the first column of Table V the continuity chords are listed for the band representations $(a,1)$ and $(b,1)$. These are two-dimensional band representations that are built on an s orbital of the group T_d corresponding to the symmetry centers $\vec{q}_a=(0,0,0)$ $\vec{q}_b=(a/2,0,0)$ in the Wigner-Seitz cell. The continuity chords for the symmetry types $(a,1)$ and $(b,1)$ differ only at the point W in the Brillouin zone. At all other points they coincide. As another example, consider the fourth column of Table V. Here the continuity chords are listed for a p orbital of T_d, again, around the symmetry centers $\vec{q}_a$ and $\vec{q}_b$. They correspond to six-dimensional band representations. These chords also differ only at the point W in the Brillouin zone. If columns one and four of Table V are combined one obtains continuity chords that belong to reducible-band representations. Thus, one can combine $(a,1)$ and $(a,4)$ to obtain an eight-dimensional band representation that is built on s and p orbitals for T_d around $\vec{q}_a$. This band representation is clearly reducible. Similarly, one can build three other eight-dimensional reducible-band representations by combining columns one and four of Table V. All of them will be built on s and p orbitals of T_d. Such s and p orbitals are often assumed to be possible candidates for band-structure calculations in diamondlike crystals.[8,12,18,19] In such calculations one starts with bases built on s-p localized orbitals and it is expected that they will lead to a separation of the valence and conduction bands each containing four branches. It is of interest to discuss this approach from the point of view of band representations and the continuity chords of Table V. From this table it follows that the s-p orbitals (columns 1 and 4) lead together to an eight-dimensional band representation. As was already mentioned this is a reducible band representation. It reduces, as one can show, into the following irreducible band representations: either a two- and a six-dimensional one for the center a, or two four-dimensional ones for the center c. The latter possibility corresponds to the valence and conduction bands in the diamond-type crystals, and as it follows from Ref. 19 the s-p orbitals lead to a satisfactory band-structure calculation. In fact, it follows from Table V that the only way to build irreducible four-dimensional band representations out of the symmetry centers $\vec{q}_a$ and $\vec{q}_b$ is using the orbitals $(a,3)$ or $(b,3)$ of T_d (column 3 of Table V).

An alternative way of building irreducible four-dimensional band representations is by using the centers $\vec{q}_c$ and $\vec{q}_d$ of Table VII. They are obtained by using orbitals that correspond to the irreducible representations with $l=1$, 2, 4, 5 of the point groups D_{3d} (columns 1, 2, 4, and 5 in Table VII). In particular $(c,1)$ or $(d,1)$ correspond to the full symmetric representation of D_{3d} around the centers $\vec{q}_c$ and $\vec{q}_d$, respectively. Similarly $(c,4)$ or $(d,4)$ give the antisymmetric (in which the inversion element is represented by -1) representation of D_{3d}. The possibility of using such orbitals in calculations of the diamond-type band structures was first considered by Hall.[6] From Table VII it follows that these orbitals will lead to four-branch conduction for valence bands. This only means that from the point of view of symmetry the band representations $(c,1)$, $(d,1)$, $(c,4)$, and $(d,4)$ are suitable candidates for band-structure calculations of the diamond-type crystals. This possibility was criticized in Ref. 18, however, as was pointed out in Ref. 12 it should not be excluded on general grounds.

An interesting general conclusion that follows from Tables V and VII about the clustering of different Bloch states at a given symmetry point in the Brillouin zone. As is seen from these tables, the smallest number of states that form a band is two. These are the band representations $(a,1)$, $(b,1)$, $(a,2)$, and $(b,2)$. At the Γ point only two possible clusterings with two branches in a band are allowed: $\Gamma_1\Gamma_7$ and $\Gamma_2\Gamma_6$. For example, Γ_1 and Γ_2 or Γ_1 and Γ_6, and so on, never come together in an irreducible set of states. Similar clusterings appear at other points. Of particular interest is the point X in the Brillouin zone. Here, as is well known from representation theory of space groups,[1] there is sticking together of bands, and all the representations at this point are two-dimensional (see Table IV). However, as is seen from Tables V and VII only the states X_1 and X_2 can appear in a separate band. Neither X_3 nor X_4 can appear in an irreducible band of dimension two. The smallest dimensionality bands in which X_3 or X_4 can appear are of dimension four. It is of interest to point out that the band-representation arguments lead to very-well defined clusters of Bloch states of the symmetry point X. Thus, for the p orbitals around $\vec{q}_a$ or $\vec{q}_b$, column four of Table V shows that the only possible clustering is $X_1X_3X_4$. This is in agreement with the results quoted in Ref. 8.

The author has enjoyed discussions on the subject with Professor H. Bacry, Professor J. L. Birman, Professor G. Dresselhaus, Professor J. Genossar, Professor M. Lax, and Professor A. Peres.

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