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Band representations and symmetry types of bands in solids

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Symmetry types of bands in solids are specified by means of band representations of space groups. This is a new kind of representation that corresponds to bands of energies rather than to single energies as in the case of usual representations. It is shown that each band representation defines a symmetry type of a band by specifying the symmetry of localized orbitals with respect to a whole lattice of point group centers. In this symmetry specification the quasicoordinate $\vec{q}$ in the Wigner-Seitz cell plays a similar role to what is played by the quasimomentum $\vec{k}$ in the symmetry specification of Bloch states in the Brillouin zone.

I. INTRODUCTION

The concept of bands was first introduced by Bloch[1] and has since been widely used in solid-state physics. On an intuitive level this concept means an isolated interval of energies in the energy spectrum of a crystal. For a more precise definition one has to also give all the Bloch functions that correspond to this interval of energies. Since there is often more than one Bloch function for a given energy ϵ and $\vec{k}$ vector, these two indices are not sufficient for the specification of the Bloch function. One then ends up using the irreducible representations of space groups for labeling Bloch functions at each point $\vec{k}$ in the Brillouin zone.[2] A precise definition of a band involves, therefore, an energy interval and a specification of the corresponding Bloch functions by means of the space-group symmetry at each $\vec{k}$ vector. This definition is adopted in a series of papers by Des Cloizeaux.[3] It involves both the energy spectrum and the symmetry of the crystal. These two pieces of information are of different nature and while it is usually hard to find the first of them, the second is, as a rule, known. In fact, these two parts of information appearing in the definition of a band are to a great extent independent and it should be possible to separate them. This is very much the same as in atomic physics where one can talk about the symmetry without mentioning the energy of the levels. Thus, in atomic physics it is quite simple to specify the symmetry types of atomic levels by the angular momentum quantum numbers or, equivalently, by the rotational symmetry. One should be able to do the same in solids and answer the question about the symmetry types of bands without getting involved with the energy spectrum. This is a much simpler task than the full definition of an energy band in a solid because it is connected with the space-group symmetry only.

The concept of the symmetry type of a band is not new and it has been applied to different band calculation schemes.[4–7] This concept was introduced in Ref. 3 by first defining a band on the basis of Bloch functions as described above and then by showing how to find symmetry adapted Wannier functions that span the band under consideration. These Wannier functions define the symmetry type of the band.

In this paper it is shown how to define the symmetry type of a band by directly using Wannier functions or more generally localized orbitals. This is done by defining new types of representations for a space group; these are called band representations. Unlike the usual representations of space groups which are based on Bloch functions, the band representations have localized orbitals as their bases. Each band representation is infinite dimensional and is also irreducible in the basis of localized orbitals. This new feature of band representations is achieved by restricting the space of functions to localized orbitals only. Such a restriction excludes finite-dimensional representations because the latter are based on Bloch functions which are of extended nature. Different symmetry types of bands are given by different band representations of the space group for the particular solid. As is well known, Wannier functions, or more generally, localized orbitals reproduce energies belonging to a whole band.[4,8] What this means is that a band representation corresponds to a band of energies rather than to a single energy as in the case of a usual representation of a group. But this is exactly the feature that makes a band representation suitable for the definition of the symmetry of a band as a whole entity.

Until quite recently the concept of a band as a whole entity was not utilized because most of the experiments were involved with electronic states at the

Fermi level in metals or at the top and bottom of the valence and conduction bands correspondingly in semiconductors. In recent years, with the application of powerful sources of radiation[9] it became possible to extract information about states ranging over hundreds of eV and in such experiments the data about a band as a whole should become accessible. The concept of a band representation and the symmetry types of bands as entities should therefore, in principle, be connected with experimentally measurable quantities.

There are a number of new concepts that are connected with band representations in solids. It is shown in this paper that the symmetry of localized orbitals can be fully specified with respect to a lattice of point symmetry centers. This lattice was defined in Ref. 3 and will be called the point symmetry lattice. From the point of view of the symmetry types of bands in solids, a space group can be looked upon as consisting of a finite set of point symmetry lattices. Each such lattice is defined by a symmetry center in the Wigner-Seitz cell.[2,10] The symmetry centers by themselves are specified by the quasicoordinate $\vec{q}$. The latter assumes in the band representations a similar role to the one that the quasimomentum $\vec{k}$ has in the usual representation theory of space groups. Thus, it is shown in this paper that the quasicoordinate $\vec{q}$ specifies the band representations of space groups.

In Secs. II and III of this paper the band representation is defined and it is shown how it can be used for the specification of the symmetry types of bands in solids. These sections deal with the basic concepts connected to band representations and methods are outlined for the construction of the latter. In Sec. IV a detailed example is worked out of finding the irreducible band representations of the space group D_4^1. Tables I–IV contain the information connected with these band representations. It is also shown how the band representations specify the symmetry of Bloch functions at different $\vec{k}$ vectors in the Brillouin zone.

II. SYMMETRY SPECIFICATIONS OF BANDS

The symmetry of Bloch functions $\psi_{nk}(\vec{r})$ in a solid for a given quasimomentum $\vec{k}$ is specified by the irreducible representations of the group G_k of the vector $\vec{k}$. The latter is a subgroup of the space group G of the solid and is defined in the following way: to G_k all those elements $(\beta|\vec{b})$ (β is a point group ele-

TABLE I. Symmetry centers and the corresponding sets of Bravais lattice vectors $\vec{R}^\alpha$. The centers a, b, c, d are with symmetry D_4. $e^{(1)}$, $e^{(2)}$ and $f^{(1)}$, $f^{(2)}$ are centers with symmetry D_2 and they form stars in couples. The symmetry centers $g^{(1)}$ and $g^{(2)}$ have the symmetry C_4^z and belong to the same star. $i^{(1)}$, $i^{(2)}$, $i^{(3)}$, and $i^{(4)}$ belong to the same star and have the symmetry C_2^z. $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are the unit cell vectors of the Bravais lattice. C_2^x, C_2^y,C_2^z are rotations by π around the axes x, y, and z correspondingly; C_4^z and C_4^{3z} are rotations by $\frac{1}{2}\pi$ and $\frac{3}{2}\pi$ around the z axis; U^{xy} and $U^{\bar{x}y}$ are rotations by π around the axes xy and $\bar{x}y$, correspondingly.

Symmetry center	$\vec{R}^\alpha=\vec{q}-\alpha\vec{q}$							
	E	C_2^x	C_2^y	C_2^z	C_4^z	C_4^{3z}	U^{xy}	$U^{\bar{x}y}$
$a(0,0,0)$	0	0	0	0	0	0	0	0
$b(0,0,\frac{1}{2}c)$	0	$\vec{a}_3$	$\vec{a}_3$	0	0	0	$\vec{a}_3$	$\vec{a}_3$
$c(\frac{1}{2}a,\frac{1}{2}a,0)$	0	$\vec{a}_2$	$\vec{a}_1$	$\vec{a}_1+\vec{a}_2$	$\vec{a}_1$	$\vec{a}_2$	0	$\vec{a}_1+\vec{a}_2$
$d(\frac{1}{2}a,\frac{1}{2}a,\frac{1}{2}c)$	0	$\vec{a}_2+\vec{a}_3$	$\vec{a}_1+\vec{a}_3$	$\vec{a}_1+\vec{a}_2$	$\vec{a}_1$	$\vec{a}_2$	$\vec{a}_3$	$\vec{a}_1+\vec{a}_2+\vec{a}_3$
$e^{(1)}(\frac{1}{2}a,0,0)$	0	0	$\vec{a}_1$	$\vec{a}_1$				
$e^{(2)}(0,\frac{1}{2}a,0)$	0	$\vec{a}_2$	0	$\vec{a}_2$				
$f^{(1)}(\frac{1}{2}a,0,\frac{1}{2}c)$	0	$\vec{a}_3$	$\vec{a}_1+\vec{a}_3$	$\vec{a}_1$				
$f^{(2)}(0,\frac{1}{2}a,\frac{1}{2}c)$	0	$\vec{a}_2+\vec{a}_3$	$\vec{a}_3$	$\vec{a}_2$				
$g^{(1)}(0,0,z)$	0			0	0	0		
$g^{(2)}(0,0,\bar{z})$	0			0	0	0		
$i^{(1)}(0,\frac{1}{2}a,z)$	0			$\vec{a}_2$				
$i^{(2)}(0,\frac{1}{2}a,\bar{z})$	0			$\vec{a}_2$				
$i^{(3)}(\frac{1}{2}a,0,z)$	0			$\vec{a}_1$				
$i^{(4)}(\frac{1}{2}a,0,\bar{z})$	0			$\vec{a}_1$				

TABLE II. Characters of irreducible representations of the point group D_4 and the phases for the band representations corresponding to the symmetry centers a, b, c, and d. $\xi=\exp(-ik_x a)$, $\eta=\exp(-ik_y a)$, $\zeta=\exp(-ik_z c)$.

D_4	E	C_2^x	C_2^y	C_2^z	C_4^z	C_4^{3z}	U^{xy}	$U^{\bar{x}y}$
$D^{(1)}$	1	1	1	1	1	1	1	1
$D^{(2)}$	1	−1	−1	1	1	1	−1	−1
$D^{(3)}$	1	1	+1	1	−1	−1	−1	−1
$D^{(4)}$	1	−1	−1	1	−1	−1	+1	1
$D^{(5)}$	2	0	0	−2	0	0	0	0
q_a	1	1	1	1	1	1	1	1
q_b	1	ζ	ζ	1	1	1	ζ	ζ
q_c	1	η	ξ	$\xi\eta$	ξ	η	1	$\xi\eta$
q_d	1	$\eta\zeta$	$\xi\zeta$	$\xi\eta$	ξ	η	ζ	$\xi\eta\zeta$

ment and $\vec{b}$ is a translation) of G belong that have the property

$$\beta\vec{k}=\vec{k}+\vec{K}_i \ , \tag{1}$$

where $\vec{K}_i$ is a vector of the reciprocal lattice. The symmetry of $\psi_{nk}(\vec{r})$ is defined by means of the irreducible representations $D(\beta|\vec{b})$ of G_k

$$(\beta|\vec{b})\psi_{nk}^{(l)}(\vec{r})=\sum_{n'} D_{n'n}^{(k,l)}(\beta|\vec{b})\psi_{n'k}^{(l)}(\vec{r}) \ . \tag{2}$$

The index l labels different representations of G_k. In this approach one can assign a definite representation to each $\vec{k}$ and each energy level. By defining in such a way the representations for all the $\vec{k}$ vectors in a Brillouin zone and for all the energies belonging to a band, one specifies the symmetry of the given band.[2,3,10] Such a symmetry specification has the disadvantage that is uses many different representations which do not seem to have anything in common for defining a band as one entity. Thus, it does not seem to reflect any characteristic symmetry features of the band as a whole. In what follows it is shown that such characteristic features exist and that

TABLE III. Characters of irreducible representations of the point group D_2 and the phases for the band representations corresponding to the symmetry centers $e^{(1)}$, $e^{(2)}$, $f^{(1)}$, $f^{(2)}$. $\xi=\exp(-ik_x a)$, $\eta=\exp(-ik_y a)$, $\zeta=\exp(-ik_z c)$.

D_2	E	C_2^x	C_2^y	C_2^z
$D^{(1)}$	1	1	1	1
$D^{(2)}$	1	1	−1	−1
$D^{(3)}$	1	−1	−1	1
$D^{(4)}$	1	−1	1	−1
$e^{(1)}$	1	1	ξ	ξ
$e^{(2)}$	1	η	1	η
$f^{(1)}$	1	ζ	$\xi\zeta$	ξ
$f^{(2)}$	1	$\eta\zeta$	ζ	η

TABLE IV. Matrix elements $D_{ij}^{(l,r)}$ of the band representations of D_4^1 induced from the band representations of D_2 for the stars $e^{(1)}$, $e^{(2)}$ and $f^{(1)}$, $f^{(2)}$. The matrices are given for the elements of D_2 only. l denotes different irreducible representations of the point group D_2; the index r denotes different symmetry centers.

	E	C_2^x	C_2^y	C_z^z
$D_{11}^{(1,e)}$	1	1	ξ	ξ
$D_{22}^{(1,e)}$	1	η	1	η
$D_{11}^{(2,e)}$	1	1	$-\xi$	$-\xi$
$D_{22}^{(2,e)}$	1	$-\eta$	1	$-\eta$
$D_{11}^{(3,e)}$	1	−1	$-\xi$	ξ
$D_{22}^{(3,e)}$	1	$-\eta$	−1	η
$D_{11}^{(4,e)}$	1	−1	ξ	$-\xi$
$D_{22}^{(4,e)}$	1	η	−1	$-\eta$
$D_{11}^{(1,f)}$	1	ζ	$\xi\zeta$	ξ
$D_{22}^{(1,f)}$	1	$\eta\zeta$	ζ	η
$D_{11}^{(2,f)}$	1	ζ	$-\xi\zeta$	$-\xi$
$D_{22}^{(2,f)}$	1	$-\eta\zeta$	ζ	$-\eta$
$D_{11}^{(3,f)}$	1	$-\zeta$	$-\xi\zeta$	ξ
$D_{22}^{(3,f)}$	1	$-\eta\zeta$	$-\zeta$	η
$D_{11}^{(4,f)}$	1	$-\zeta$	$\xi\zeta$	$-\xi$
$D_{22}^{(4,f)}$	1	$\eta\zeta$	$-\zeta$	$-\eta$

a definition of a band in a solid can be given based entirely on a single representation of its space group.

Let us compare the symmetry of a crystal with that of an atom. The atomic levels are specified by the rotational symmetry around one fixed center. In a crystal there is, as a rule, more than one center of point group symmetry. Consider, for example, a crystal with the symmetry D_4^1. This is a crystal of the tetragonal system. In Fig. 1 two kinds of symmetry centers are given in the plane perpendicular to the C_4 axis.[11] The squares denote centers with D_4-point symmetry and the ovals with D_2 symmetry correspondingly. Crystals have, in general, a number of point group centers of different symmetry. What is characteristic to the crystalline point symmetry is that each center of a given kind appears not as a single center but as an infinite lattice of symmetry centers. Such a lattice is obtained by choosing one center of given point symmetry and by applying to it all the elements of the space group.[3] This lattice differs, in general, from the Bravais lattice of the crystal. Only for centers with the full point symmetry of the crystal (e.g., points a and c in Fig. 1) will this lattice coincide with the Bravais lattice. In the general case, the unit cell of the lattice will have a structure assigned to it. Thus, in Fig. 1, the points $e^{(1)}$ and $e^{(2)}$ form the structure of the unit cell. For a full description of the lattice of the symmetry centers we have to also give its position with respect to the origin of the crystal. Thus, the points a and c in Fig. 1 lead to identical lattices in the space group D_4^1. However, they are located in different positions with respect to the origin of the crystal. A lattice of symmetry centers is therefore specified by the point symmetry of one of its centers, by the structure of the unit cell, and by its location with respect to the origin. This lattice of symmetry centers in a crystal replaces the single center in an atom. Because of its important role in the symmetry specification of bands it will be called the point symmetry lattice. One can visualize a space group symmetry as consisting of a finite number of point symmetry lattices. As is shown below, the specification of the symmetry of states with respect to a point symmetry lattice leads one to the symmetry notion of a band as a whole in much the same way as an array of localized orbitals on a lattice leads to an energy band.

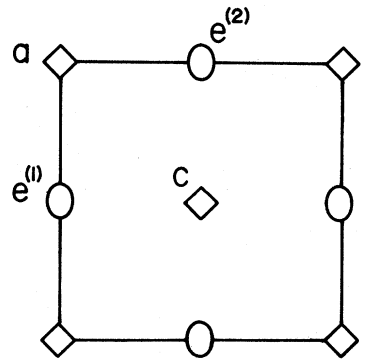

FIG. 1. Space group D_4^1: the squares denote centers with point symmetry D_4, the ovals with point symmetry D_2.

In defining the symmetry notion of a band in a crystal it should be more suitable to use Wannier functions (or more generally, localized functions) than Bloch functions. The reason for this is that while a Bloch function defines a single energy in the band, a Wannier function reproduces energies belonging to a whole band.[4,8] In fact, there is no need to restrict oneself to Wannier functions and the same can be said about a more general localized function.[12] What this means is that in solids one can find localized functions that correspond to a band of energies. By specifying the symmetry of such localized functions we shall clearly specify the symmetry of a band as a whole entity.

We shall define a band in a solid as consisting of a set of localized orbitals which are invariant under all the operations of the space group. Such a set of orbitals will form an infinite-dimensional representation of the space group. The reason for this is that the translation operators do not have eigenfunctions in the space of localized functions and since there is an infinite number of translations the invariant set will necessarily contain an infinite number of functions. This can best be seen when the functions are expressed in kq representation.[13] A function $C(\vec{k},\vec{q})$ in the kq representation is connected with the corresponding function $\psi(\vec{r})$ in the r representation by the following formula

$$C(\vec{k},\vec{q})=\Omega^{-1}\sum_m \exp(i\vec{k}\cdot\vec{R}_m)\psi(\vec{q}-\vec{R}_m) \ , \qquad (3)$$

where Ω is the volume of a unit cell in the reciprocal lattice and $\vec{R}_m$ are vectors of the Bravais lattice. When a translation by $\vec{R}_l$ is applied to $C(\vec{k},\vec{q})$ one obtains the shifted function

$$\exp(-i\vec{k}\cdot\vec{R}_l)C(\vec{k},\vec{q}) \ . \qquad (4)$$

This means that when all the translations of a space group are applied to a function $C(\vec{k},\vec{q})$ we get in Eq. (4) an infinite set of independent functions. We come to the conclusion that if we insist on considering only localized functions, all the representations of space groups will be infinite dimensional. We shall call them band representations. Since the only thing that pure translations do in the kq representation is to shift a function according to Eq. (4), it is clear that the bases of band representations contain a limited number of functions

$$C_1(\vec{k},\vec{q}),C_2(\vec{k},\vec{q}),\ldots,C_m(\vec{k},\vec{q}) \ , \qquad (5)$$

and the same functions shifted by the phases as in Eq. (4). When the space group elements $(\alpha|\vec{t})$ (α a point group element and $\vec{t}$ a translation[2]) are applied to these functions we get

$$(\alpha|\vec{t})C_s(\vec{k},\vec{q}) = \sum_{s'=1}^{m} D_{s's}[(\alpha|\vec{t}),\vec{k}]C_{s'}(\vec{k},\vec{q}) \ , \tag{6}$$

where $D[(\alpha|\vec{t}),\vec{k}]$ is, in general, a $\vec{k}$-dependent matrix. The knowledge of these matrices for all the elements $(\alpha|\vec{t})$ defines the symmetry properties of the functions $C_s(\vec{k},\vec{q})$. From Eq. (3) it follows that the operation of $(\alpha|\vec{t})$ on a function $C(\vec{k},\vec{q})$ in the kq representation is

$$(\alpha|\vec{t})C(\vec{k},\vec{q}) = C(\alpha^{-1}\vec{k},\alpha^{-1}\vec{q}-\vec{t}) \ . \tag{7}$$

Equation (6) defines a correspondence between the elements $(\alpha|\vec{t})$ of the space group and finite-dimensional $\vec{k}$-dependent matrices $D[(\alpha|\vec{t}),\vec{k}]$

$$(\alpha|\vec{t}) : D[(\alpha|\vec{t}),\vec{k}] \ . \tag{8}$$

This correspondence gives what we call a band representation of the space group. It is only by working in the kq representation that we get a correspondence of the form Eq. (8). Thus, in the r representation Eq. (6) would become

$$(\alpha|\vec{t})\psi_s(\vec{r}-\vec{R}_l) = \sum_{s'R_l'} D_{s's}[(\alpha|\vec{t}),\vec{R}_l-\vec{R}_{l'}]\psi_{s'}(\vec{r}-\vec{R}_{l'}) \ , \tag{9}$$

where by translational symmetry D depends on the difference $\vec{R}_l-\vec{R}_{l'}$ only. Equation (9) defines an infinite-dimensional representation of the space group. The matrix in Eq. (9) is nothing else but the Fourier transform of the matrix in Eq. (8). We see therefore that in the kq representation we get finite-dimensional matrices representing the elements $(\alpha|\vec{t})$ of the space group on the basis of localized orbitals. The form of the band representations in the kq representation [Eqs. (6) or (8)] is also important from another point of view. The kq functions $C(\vec{k},\vec{q})$ satisfy the same boundary conditions as the Bloch functions do[13]

$$C(\vec{k}+\vec{K}_n,\vec{q}) = C(\vec{k},\vec{q}) \ , \tag{10}$$

$$C(\vec{k},\vec{q}-\vec{R}_m) = \exp(-i\vec{k}\cdot\vec{R}_m)C(\vec{k},\vec{q}) \ . \tag{11}$$

The function $C(\vec{k},\vec{q})$ can therefore be given a double meaning. When $\vec{k}$ and $\vec{q}$ are the variables of the kq representation, the function $C(\vec{k},\vec{q})$ is a localized orbital. However, the same function for a fixed quasimomentum is a Bloch-like function in the r representation. This is seen from Eq. (3) which is the same as the relation connecting a Bloch function and a Wannier function in the r representation.[4] This dual meaning of the functions in the kq representation allows one to define the symmetry of the Bloch functions at each point of the Brillouin zone from the knowledge of the band representation. Thus, assume that the band representation in Eq. (6) is given. Let us choose a definite $\vec{k}$ vector and the corresponding G_k with the elements $(\beta|\vec{b})$ as defined in Eq. (1). By using Eq. (7) for the elements of G_k we can assume that β does not operate on $\vec{k}$ [see Eqs. (1) and (10)]. The elements of G_k therefore transform a function $C(\vec{k},\vec{q})$ for the fixed $\vec{k}$ (that was chosen for G_k) to a function with the same $\vec{k}$. It follows that by looking at $C(\vec{k},\vec{q})$ as at Bloch-like functions in the r representation, Eq. (6) will define a representation of G_k for each $\vec{k}$ in the Brillouin zone. But this is exactly what is needed for specifying the symmetry of a band in the framework of the commonly used definition.[2,3] From the symmetry specification of a band given by a band representation in Eq. (6) we arrive at the usual representations of the groups of $\vec{k}$ specifying the Bloch functions at each point in the Brillouin zone. It follows therefore that a single-band representation of the space group fully specifies the symmetry of a band in a solid and it replaces the commonly used definition which is based on many different representations of the groups G_k.

The possibility of specifying the symmetry of a band by a single-band representation is consistent both with usual representation theory of space groups and the very notion of a band in a solid. From the point of view of usual representations a band representation is infinite dimensional and it can contain therefore all the necessary representations for the symmetry specification of Bloch functions at different points in the Brillouin zone. As to the notion of a band we find that while a usual representation corresponds to a single energy value, a band representation, by definition, is based on localized orbitals and it corresponds therefore to a band of energies.

We have come to the conclusion that each band representation specifies a possible symmetry type of a band. Clearly, each space group should have different band representations and we will therefore have different symmetry types of bands for a given solid. As will be shown in the next section the symmetry of the localized orbitals belonging to a given band is specified with respect to the point symmetry lattices that were defined above. Since the number of point symmetry lattices in a crystal is finite and since the point symmetry itself is of finite order, each crystal will have a limited number of bands with different symmetry types. This is unlike in atoms where an infinite number of different symmetry types exists for atomic orbitals.

For distinguishing between different band representations one can use the concepts of equivalency and reducibility as for usual representa-

tions. Band representations can be reducible or irreducible depending on whether or not the basis in Eq. (5) can be split into invariant sub-bases with respect to the full space group of the solid. By definition of a band representation, the splitting is allowed in the framework of localized functions only. Thus, a linear combination of the function in Eq. (4) that leads to a Bloch function $C_{k'}(\vec{k},\vec{q})$ for the quasimomentum $\vec{k}'$

$$C_{k'}(\vec{k},\vec{q})=\sum_l \exp(i\vec{k}'\cdot\vec{R}_l-i\vec{k}\cdot\vec{R}_l)C(\vec{k},\vec{q})$$
$$=\Omega\Delta(\vec{k}'-\vec{k})C(\vec{k},\vec{q}) \quad (12)$$

should be excluded. The Δ function in Eq. (12) is an infinite sum of Dirac δ functions

$$\Delta(\vec{k})=\sum_n \delta(\vec{k}-\vec{K}_n) \ . \quad (13)$$

The function in Eq. (12) is excluded because it is not square integrable. The irreducible band representations play the same role in the framework of band representations as usual irreducible representations play in the general representation theory. Thus, the irreducible band representations serve as elementary building bricks in the symmetry specification of bands in solids.

III. BAND REPRESENTATIONS OF SPACE GROUPS

A band representation was defined in the previous section as an infinite-dimensional representation of the space group with a basis of localized orbitals. Alternatively, Eq. (6) defines a finite-dimensional band representation but with matrices $D[(\alpha|\vec{t}),\vec{k}]$ that are $\vec{k}$ dependent. Since $\vec{k}$ is a variable of the wave function, this means that strictly speaking Eq. (6) does not define a representation of the space group because the matrix elements in Eq. (6) are not constants. It is nevertheless meaningful to talk about a m-dimensional band representation (a band representation means also that in a finite-dimensional space the matrices of the representation are $\vec{k}$ dependent) with m having the meaning of the number of independent orbitals that form the band. By applying to Eq. (6) another space group element $(\beta|\vec{u})$ we find that the matrix corresponding to the product $(\beta|\vec{u})(\alpha|\vec{t})$ will be

$$D[(\beta|\vec{u}),\vec{k}]D[(\alpha|\vec{t}),\beta^{-1}\vec{k}] \ . \quad (14)$$

This multiplication rule shows clearly that band representations do not behave as usual representations but have some similarity with the corepresentation theory for time reversal.[14] This can also be seen on the concept of equivalent band representations. Thus, if $\bar{C}_s(\vec{k},\vec{q})$ is a new basis given by the matrix $T(\vec{k})$

$$\bar{C}_s(\vec{k},\vec{q})=\sum_{s'=1}^{m} T_{s's}(\vec{k})C_{s'}(\vec{k},\vec{q}) \ , \quad (15)$$

then the equivalent band representation will be given by the matrices

$$T^{-1}(\vec{k})D[(\alpha|\vec{t}),\vec{k}]T(\alpha^{-1}\vec{k}) \ . \quad (16)$$

In the matrix on the right the vector $\vec{k}$ is replaced by $\alpha^{-1}\vec{k}$. With the aid of Eq. (16) one can define the concepts of reducible and irreducible band representations. The band representation $D[(\alpha|\vec{t}),\vec{k}]$ is reducible if a matrix $T(\vec{k})$ exists for which all the matrices in Eq. (16) assume a quasidiagonal form. This is equivalent to saying that the basis in Eq. (5) can be split into invariant sub-bases by the transformation Eq. (15). If such a matrix T does not exist then $D[(\alpha|\vec{t}),\vec{k}]$ is called an irreducible band representation. Like in usual group representations, the irreducible band representations play a central role in specifying bands on the basis of space group symmetries.

In general, the matrices of the band representations are nonunitary. However, if the basis in Eq. (5) is chosen to be orthonormal [in this case, we shall denote the functions by $a_s(\vec{k},\vec{q})$]

$$\Omega\int a_s^*(\vec{k},\vec{q})a_{s'}(\vec{k},\vec{q})\,d\vec{q}=\delta_{ss'} \ , \quad (17)$$

then as can be checked the band representation is unitary

$$D^+[(\alpha|\vec{t}),\vec{k}]D[(\alpha|\vec{t}),\vec{k}]=E \ . \quad (18)$$

In Eq. (18), E is a unit matrix. The basis functions $a_s(k,q)$ satisfying Eq. (17) are the Wannier functions of the problem.[15] In general, there is, however, no need to work with orthogonal functions and often this is not even desirable because orthogonality and localization are mutually exclusive properties.[12]

It is easy to construct band representations of symmorphic space groups. A space group is symmorphic if together with $(\alpha|\vec{t})$ also $(\alpha|0)$ and $(\epsilon|\vec{t})$ are elements of the group.[2] This also means that the point group elements appear with pure translations $\vec{R}_m$ only. Thus, one can check that the correspondence

$$(\alpha|\vec{R}_m):\exp(-i\vec{k}\cdot\vec{R}_m)D(\alpha) \quad (19)$$

gives a band representation of G if $D(\alpha)$ is a representation of the point group of G. Also, if $D(\alpha)$ is an irreducible representation of the point group of G then Eq. (19) gives an irreducible band representation of G. In order to construct additional band representations of G let us define the groups G_q of the symmetry points $\vec{q}$ in the Wigner-Seitz cell.[2,10] To G_q belong all those elements $(\gamma|\vec{c})$ of the space

group for which

$$(\gamma|\vec{c}) = \gamma\vec{q} + \vec{c} = \vec{q} - \vec{R}_m \ , \tag{20}$$

where $\vec{R}_m$ is a Bravais lattice vector. G_q always contains all the pure translations. Relation (20) is similar to the definition Eq. (1) for G_k with the difference, however, that in Eq. (20) the translation $\vec{c}$ also operates on $\vec{q}$. G_q can be chosen to be a symmorphic space group. This is achieved by choosing $\vec{q}$ itself as the origin for the point group elements.[11] $(\gamma|\vec{c})$ in Eq. (20) is written with respect to the origin of the crystal. Let γ_q be the point group element γ when written with respect to $\vec{q}$ as the center. Then, by definition

$$\gamma_q = (\epsilon|\vec{q})\gamma(\epsilon|-\vec{q}) = (\epsilon|\vec{q} - \gamma\vec{q} - \vec{c})(\gamma|\vec{c}) \ . \tag{21}$$

From Eq. (20) it follows that $\vec{q} - \gamma\vec{q} - \vec{c}$ is a Bravais lattice vector $\vec{R}_m$ and Eq. (21) can be rewritten in the following form

$$(\gamma|\vec{c}) = (\epsilon|c + \gamma\vec{q} - \vec{q})\gamma_q \ . \tag{22}$$

It therefore follows that each γ_q appears with a pure translation, which means that G_q with respect to $\vec{q}$ as a center is a symmorphic space group. This simplifies considerably the construction of band representations for G_q. According to Eq. (19), if $D(\gamma_q)$ is an irreducible representation of the point group of G_q then the correspondence

$$(\gamma_q|\vec{R}_m) : \exp(-i\vec{k}\cdot\vec{R}_m)D(\gamma_q) \tag{23}$$

defines an irreducible band representation of G_q. In this way, each irreducible representation of the point group of G_q will define an irreducible band representation of the space group G_q.

For symmorphic space groups there are usually a number of symmetry centers $\vec{q}_r$ with the full space group symmetry G. Thus, in the space group D_4^1 these are the symmetry centers a, b, c, and d (see Table I). For these centers Eq. (22) becomes

$$\alpha = (\alpha_r|\alpha\vec{q}_r - \vec{q}_r) \ . \tag{24}$$

We denote by α_r the point group element α with respect to the center $\vec{q}_r$. There is no $\vec{c}$ in Eq. (24) because we assumed that the space group is symmorphic. By using Eqs. (23) and (24) we can now build additional band representations [in addition to the one given by Eq. (19)] of the symmorphic space group. They are given by the correspondence

$$(\alpha|\vec{R}_m) : \exp[i\vec{k}\cdot(\vec{R}_r^{\alpha} - \vec{R}_m)]D(\alpha_r) \ , \tag{25}$$

where by $\vec{R}_r^{\alpha}$ we denoted the Bravais lattice vector

$$\vec{R}_r^{\alpha} = \vec{q}_r - \alpha\vec{q}_r \ . \tag{26}$$

Equation (26) defines a set of Bravias lattice vectors (they vary with α) for each symmetry center $\vec{q}_r$. Two sets $\vec{R}_r^{\alpha}$ and $\vec{R}_{r'}^{\alpha}$ for the centers $\vec{q}$ and $\vec{q}_{r'}$ are called different if there is an α for which $\vec{R}_r^{\alpha} \neq \vec{R}_{r'}^{\alpha}$. Correspondingly, two symmetry centers $\vec{q}$ and $\vec{q}_{r'}$ are called inequivalent if their Bravais lattice sets $\vec{R}_r^{\alpha}$ and $\vec{R}_{r'}^{\alpha}$ are different; otherwise they are equivalent. Here the following remark is in order: $\vec{q}_r$ and $\vec{q}_{r'}$ are also equivalent if they differ by a Bravais lattice vector

$$\vec{q}_{r'} = \vec{q}_r + \vec{R} \ . \tag{27}$$

What is meant by the equivalency of the centers $\vec{q}_r$ and $\vec{q}_{r'}$ is that they lead to equivalent band representations in the formula (25). This is easy to check. Denote by $D^{(r)}[(\alpha|R_m), \vec{k}]$ the band representation that corresponds to $\vec{q}_r$ as given by Eq. (25). The one corresponding to $\vec{q}_{r'}$ will then be

$$D^{(r')}[(\alpha|\vec{R}_m), \vec{k}] = \exp[i\vec{k}\cdot(\vec{R} - \alpha\vec{R})] \times D^{(r)}[(\alpha|\vec{R}_m), \vec{k}] \ , \tag{28}$$

where $\vec{R}$ is defined in Eq. (27). Equation (28) shows that $D^{(r')}$ and $D^{(r)}$ are equivalent band representations [see Eq. (16)] with the matrix $T(\vec{k}) = \exp(-i\vec{k}\cdot\vec{R})$. It is clear that if for two symmetry centers $\vec{q}_r$ and $\vec{q}_{r'}$ their Bravais lattice sets as given in Eq. (26) are identical then the corresponding band representations are the same. We come to an interesting conclusion that assigns to the quasicoordinate $\vec{q}$ a role similar to the one played by the quasimomentum $\vec{k}$. As is well known only the $\vec{k}$ vectors in the Brillouin zone lead to different representations of the space group. From what we have shown a similar result holds for $\vec{q}$: only those symmetry centers lying in the Wigner-Seitz cell[2,10] lead to different band representations of the space group. This explains why in constructing band representations it is sufficient to consider the groups G_q for the symmetry centers in the Wigner-Seitz cell.

Given the inequivalent symmetry centers $\vec{q}_r$ with the whole group symmetry G and the irreducible representations $D(\alpha)$ of the point group of G, Eq. (25) defines a number of different irreducible band representations of the space group G. For some groups of low symmetry this actually gives all the irreducible band representations. There is a number of such groups and one of them (C_i^1) is considered in detail in Zak.[16]

In a general case, irreducible band representations of a space group G can be found by using the simple induction method that is widely used in the usual representation theory of space groups.[2] The space group G is decomposed into cosets with respect to the subgroup G_q

$$G = G_q + (\alpha_2|\vec{a}_2)G_q + \cdots + (\alpha_f|\vec{a}_f)G_q \ , \tag{29}$$

where

$$(\alpha_2|\vec{a}_2), \ldots, (\alpha_f|\vec{a}_f)$$

are different elements that do not belong to G_q [by definition $(\alpha_1|\vec{a}_1)$ is the unit element $(\epsilon|0)$ of the space group]. Given the decomposition Eq. (29) one can assign a star to each vector $\vec{q}$ which together with $\vec{q}$ contains the vectors

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

Thus, the stars of the q vectors labeled by squares in Fig. 1 contain only $\vec{q}$ itself, while those labeled by ovals contain two vectors, $e^{(1)}$ and $e^{(2)} = C_4^z e^{(1)}$. C_4^z is a rotation by $\frac{1}{2}\pi$ around the axis z. A list of different symmetry centers with their stars for D_4^1 are given in Table I. Now let

$$C_1(\vec{k}, \vec{q}), C_2(\vec{k}, \vec{q}), \ldots, C_m(\vec{k}, \vec{q}) \tag{30}$$

be a basis for an irreducible band representation of G_q. Then it can be checked that the set of functions

$$C_s(\vec{k}, \vec{q}), (\alpha_2|\vec{a}_2)C_s(\vec{k}, \vec{q}), \ldots, (\alpha_f|\vec{a}_f)C_s(\vec{k}, \vec{q}) \ , \tag{31}$$

with $s = 1, \ldots, m$ form a basis for a band representation of the space group G. This shows that each band representation of a subgroup G_q leads to a band representation of the space group G itself. In such a way one can arrive at band representations of G from the band representations of its subgroups G_q. The latter as we saw are given by the simple formula (23).

It turns out, however, that in order to find different irreducible band representations of a space group G there is no need to consider all the subgroups G_q. This can be seen in the following way. Let G be a space group and consider all the symmetry centers $\vec{q}_a$ that have as their symmetry G itself. For the case of a symmorphic group this was already discussed and formula (25) gives the irreducible band representations of G that are connected with the corresponding inequivalent centers. For a nonsymmorphic space group G, by definition, no symmetry centers exist with the full symmetry G. For the latter there are therefore no band representations that correspond to symmetry centers with G itself as their symmetry group. Next, let us consider a subgroup G_1 or G. For definiteness, let G_1 be the highest symmetry subgroup. In may happen that there is more than one such subgroup and then we shall consider all of them. As with G we look for the symmetry centers $\vec{q}_b$ with the symmetry G_1. Let γ_b be the point group elements of G_1 with respect to the center $\vec{q}_b$. By using Eqs. (22) and (23) we find the band representations of G_1 that correspond to the symmetry centers $\vec{q}_b$.

$$(\gamma|\vec{c}+\vec{R}_m) : \exp[i\vec{k}\cdot(\vec{R}_b^{(\gamma|\vec{c})} - \vec{R}_m)]D(\gamma_b) \ , \tag{32}$$

where like in Eq. (26) $\vec{R}_b^{(\gamma|\vec{c})}$ are Bravais lattice vectors

$$\vec{R}_b^{(\gamma|\vec{c})} = \vec{q}_b - (\gamma|\vec{c})\vec{q}_b \tag{33}$$

corresponding to the symmetry center q_b. $D(\gamma_b)$ in Eqs. (32) denotes irreducible representations of the point group of G_1. Again, two sets $\vec{R}_b^{(\gamma|\vec{c})}$ and $\vec{R}_{b'}^{(\gamma|\vec{c})}$ of Bravais lattice vectors are considered different if there exists an element $(\gamma|\vec{c})$ for which $\vec{R}_b^{(\gamma|\vec{c})} \neq \vec{R}_{b'}^{(\gamma|\vec{c})}$. Correspondingly, the symmetry centers $\vec{q}_b$ and $\vec{q}_{b'}$ for different sets of Bravais lattice vectors are inequivalent. When $\vec{R}_b^{(\gamma|\vec{c})} = \vec{R}_{b'}^{(\gamma|\vec{c})}$ for all $(\gamma|\vec{c})$, then $\vec{q}_b$ and $\vec{q}_{b'}$ are equivalent. As in Eq. (25), Eq. (32) defines for inequivalent centers different irreducible band representations of the space group G_1. Having the irreducible band representations of G_1 we can construct band representations of the full space group G by the induction procedure which was outlined in the Eqs. (30) and (31). The question is, however, whether this will lead to new irreducible band representations of G. For the particular case we are considering here the answer is affirmative for a nonsymmorphic space group G because for the latter we have not as yet constructed any band representations. For a symmorphic group G we already have the band representations that are given in Eq. (25) and the question is whether by induction we can obtain new band representations of G from those of its subgroup G_1. This question is answered by the following general rule. Let G_1 be any space group (it can be the space group G itself) and G_2 its subgroup. Denote by $(\gamma|\vec{c})$ the elements of G_1 and by $(\delta|\vec{d})$ the elements of G_2. Since G_2 is a subgroup of G_1 the elements $(\delta|\vec{d})$ belong also to G_1. Let $\vec{q}_f$ by a symmetry center of G_2. We can write for it the Eq. (33)

$$\vec{R}_f^{(\delta|\vec{d})} = \vec{q}_f - (\delta|\vec{d})\vec{q}_f \ . \tag{34}$$

This relation according to Eq. (32) will lead to different band representations of G_2. From them, by induction we can find band representations of G_1. However, if the symmetry centers $\vec{q}_b$ [Eq. (33)] and $\vec{q}_f$ [Eq. (34)] are equivalent on the elements of the subgroup G_2, then the band representation of G_1 that is induced from $\vec{q}_f$ of G_2 will coincide with the band representation of G_1 corresponding to $\vec{q}_b$. This follows from the fact that band representations of G_1 for its own centers $\vec{q}_b$ can also be obtained by induction from G_2 but then the set of the corresponding Bravais lattice vectors will be

$$\vec{R}_b^{(\delta|\vec{d})} = \vec{q}_b - (\delta|\vec{d})\vec{q}_b \ . \tag{35}$$

It is therefore clear that when the Bravais lattice vectors in Eq. (33) coincide with those in Eq. (34) (or when $\vec{q}_b$ and $\vec{q}_f$ are equivalent on G_2) then the band representations of G_2 corresponding to $\vec{q}_f$ will not lead to new band representations of G_1. This is an

important rule and we can summarize it in the following way. Given G_1 with a symmetry center $\vec{q}_b$ and its subgroup G_2 with a center $\vec{q}_f$, then the band representations of G_1 for $\vec{q}_b$ coincide with the ones induced from G_2 for the center $\vec{q}_f$ if $\vec{q}_b$ and $\vec{q}_f$ are equivalent on G_2. It should be pointed out that for being equivalent $\vec{q}_b$ and $\vec{q}_f$ do not have to be equal. The above established rule is of much importance because it reduces considerably the number of G_q that have to be considered in the construction of the irreducible band representations of a given space group. It will be called the equivalency rule.

Given a space group G it is simple to find the inequivalent centers $\vec{q}$ for it and its subgroups G_q. We start with the symmetry centers q of the highest symmetry. For symmorphic space groups these are the centers with the symmetry of the space group G itself. Thus, for the space group D_4^1 these symmetry centers are[11] a, b, c, and d (see Fig. 1 and Table I). Next we go down one step with the symmetry. In the space group D_4^1 we come to the D_2-symmetry centers denoted by e and f on page 179 of Ref. 11. These points with their stars are listed in Table I. In general, we go to symmetry centers with lower symmetry until we reach symmetry centers that are equivalent to the ones already considered above. Thus, for the group D_4^1 we list in Table I as examples the symmetry centers g and i with the symmetry C_4 and C_2 correspondingly. As is seen from this table, $g^{(1)}$ and $g^{(2)}$ are equivalent with the higher-symmetry centers a and b, $i^{(1)}$ and $i^{(2)}$ are equivalent with $e^{(2)}$ and $f^{(2)}$, while $i^{(3)}$ and $i^{(4)}$ with $e^{(1)}$ and $f^{(1)}$. The group D_4^1 also has other symmetry centers in the Wigner-Seitz cell (see Ref. 11, page 179). However, as can be easily checked, their G_q are subgroups of the groups that were already considered with equivalent symmetry centers. This means that the other symmetry points of D_4^1 will not lead to new irreducible band representations. Thus, in constructing the irreducible band representations of D_4^1 it is sufficient to consider the symmetry centers a to f only.

In establishing the equivalency of different symmetry centers the following result is useful. Let $\vec{q}_a^{(1)}$ and $\vec{q}_a^{(2)}$ be two symmetry centers belonging to the same star

$$\vec{q}_a^{(2)} = (\alpha_2|\vec{q}_2)\,\vec{q}_a^{(1)} \ , \tag{36}$$

and assume that both centers have the same symmetry group G_1 with the same set of Bravais lattice vectors

$$(\gamma|\vec{c})\,\vec{q}_a^{(1)} = \vec{q}_a^{(1)} - \vec{R}^{(\gamma|\vec{c})} \ , \tag{37}$$

$$(\gamma|\vec{c})\,\vec{q}_a^{(2)} = \vec{q}_a^{(2)} - \vec{R}^{(\gamma|\vec{c})} \ . \tag{38}$$

Then it is simple to check that the symmetry center $\vec{q}_0$ given by

$$\vec{q}_0 = \tfrac{1}{2}(\vec{q}_a^{(1)} + \vec{q}_a^{(2)}) \tag{39}$$

has at least the symmetry G_1 with the same set of $R^{(\gamma|\vec{c})}$. What this means is that by the equivalency rule it is sufficient to consider the symmetry center $\vec{q}_0$ only.

Let us now show how one can actually construct the irreducible band representations of a space group. We have already pointed out that any group G_r when written with respect to $\vec{q}_r$ as the origin is a purely symmorphic space group. Let γ_r be one of its point group elements and let $(\gamma|\vec{c})$ be the same element when written with respect to the common origin of the crystal. Then from Eqs. (22) and (23) and by using the basis in Eq. (30) we can write the representations of G_r with respect to the origin of the crystal.

$$\begin{aligned}(\gamma|\vec{c})\,C_s^{(l,r)}(\vec{k},\vec{q}) &= \exp\{i\vec{k}\cdot[\vec{q}_r - (\gamma|\vec{c})\,\vec{q}_r]\} \\ &\quad\times \sum_{s'=1}^{m} D_{s's}^{(l)}(\gamma_r)\,C_{s'}^{(l,r)}(\vec{k},\vec{q}) \\ &= \sum_{s'=1}^{m} D_{s's}^{(l,r)}[(\gamma|\vec{c}),\vec{k}] \\ &\quad\times C_{s'}^{(l,r)}(\vec{k},\vec{q}) \ , \end{aligned} \tag{40}$$

where the latter form is as in Eq. (6). The index l denotes different irreducible representations of the point group of G_r and r shows that the symmetry specification of the localized functions is being carried out with respect to the point symmetry lattice centered at $\vec{q}_r$. Having the explicit form of the band representations in Eq. (40) we can now construct the band representations of the whole space group G that are induced by the basis in Eq. (31). This is done in very much the same way as in the case of finding usual representations of space groups by using the well-known relation[2]

$$(\alpha|\vec{a})(\alpha_i|\vec{a}_i) = (\alpha_j|\vec{a}_j)(\gamma'|\vec{c}') \ ; \tag{41}$$

$(\alpha|\vec{a})$ is an arbitrary element of the space group G, $(\alpha_i|\vec{a}_i)$ are the elements in the decomposition Eq. (29), and $(\gamma'|\vec{c}')$ belongs to G_r. From Eq. (41) we can find the matrix that corresponds to $(\alpha|\vec{a})$ for the basis in Eq. (31). By also using Eq. (32) we have

$$\begin{aligned}&(\alpha|\vec{a})[(\alpha_i|\vec{a}_i)\,C_s^{(l,r)}(\vec{k},\vec{q})] \\ &\quad= \sum_{s'=1}^{m} D_{s's}^{(l,r)}[(\gamma'|\vec{c}'),\alpha_j^{-1}\vec{k}] \\ &\qquad\times[(\alpha_j|\vec{a}_j)\,C_{s'}^{(l,r)}(\vec{k},\vec{q})] \ . \end{aligned} \tag{42}$$

This relation fully defines the matrix $D(\alpha|\vec{a})$ corresponding to the element $(\alpha|\vec{a})$. It is convenient to look at $D(\alpha|\vec{a})$ as consisting of block matrices of dimension $m \times m$. From Eq. (42) it then follows that the only nonvanishing block in the column i of the matrix $D(\alpha|\vec{a})$ is in row j and this block matrix is fully defined by the band representations of the space group G_r. Formula (42) therefore gives the band representations of the space group G for any symmetry center. In general, these are reducible band representations and their consideration will be left for a separate publication.

The construction of band representations of a space group G are simplified when G_r is an invariant subgroup of G. In this case, Eq. (41) for the elements of G_r assumes the form

$$(\gamma|\vec{c})(\alpha_i|\vec{a}_i) = (\alpha_i|\vec{a}_i)(\gamma'|\vec{c}') \ , \tag{43}$$

where $(\gamma|c)$ and $(\gamma'|\vec{c}')$ are elements of G_r. It is easy to see from Eq. (43) that G_r is also the symmetry group for any vector of the star of $\vec{q}_r$. Thus, if

$$\vec{q}_r^{(i)} = (\alpha_i|\vec{a}_i)\vec{q}_r \tag{44}$$

is a general vector of the star of $\vec{q}_r$, then the symmetry elements for the group of $\vec{q}_r^{(i)}$ are

$$(\alpha_i|\vec{a}_i)(\gamma|\vec{c})(\alpha_i|\vec{a}_i)^{-1} \ . \tag{45}$$

According to Eq. (44) all the elements given by Eq. (45) belong to G_r. The latter is therefore the symmetry group for all the vectors of the star. Having this in mind one can look at Eq. (40) as defining different irreducible band representations of the group G_r for different vectors $\vec{q}_r^{(i)}$ in the star. If all $\vec{q}_r^{(i)}$ are inequivalent then they will define different irreducible band representations of G_r.

From Eq. (43) it also follows that the matrices $D(\alpha|\vec{c})$ of the band representation given by Eq. (42) for the elements of G_r have a quasidiagonal form. They can be written in the following way

$$(\gamma|\vec{c})C_s^{(l,r)}(\vec{k},\vec{q}) = \exp\{i\vec{k}\cdot[\vec{q}_r^{(i)} - (\gamma|\vec{c})\vec{q}_r^{(i)}]\} \times \sum_{s'=1}^{m} D_{s's}^{(l)}(\gamma')C_{s'}^{(l,r_i)}(\vec{k},\vec{q}) \ . \tag{46}$$

This result shows that the band representation in Eq. (42) contains all the different irreducible band representations of the group G_r corresponding to all the vectors in the star of $\vec{q}_r$. It therefore proves that the band representation of the space group G in Eq. (42) is irreducible. We come to the following irreducibility theorem: If the symmetry group of $\vec{q}_r$, G_r is an invariant subgroup of G and if all the vectors $\vec{q}_r^{(i)}$ in the star of $\vec{q}_r$ are inequivalent, then each irreducible band representation of G_r induces an irreducible band representation of the whole space group G.

In general, the groups $G_r^{(i)}$ corresponding to different vectors $\vec{q}_r^{(i)}$ in the star are different and then G_r is not an invariant subgroup of G. However, an important case is when the different groups $G_r^{(i)}$ have a common subgroup H_r. This latter will clearly be an invariant subgroup of the full space group. Let us denote its elements by $(\delta|\vec{d})$. If all the vectors $\vec{q}_r^{(i)}$ of the star are inequivalent on the subgroup H_r then Eq. (46) when written for $(\delta|\vec{d})$ defines different band representations of H_r for all the $\vec{q}_r^{(i)}$. These band representations of H_r will all appear in the band representation of G [see formula (42)] and the latter will therefore be irreducible. This leads us to the following extended formulation of the above irreducibility theorem. Given a symmetry center $\vec{q}_r$, its star vectors $\vec{q}_r^{(i)}$, and their symmetry groups $G_r^{(i)}$ the following can be proven: If the groups $G_r^{(i)}$ have a common subgroup H_r and the centers $\vec{q}_r^{(i)}$ are inequivalent on H_r then the band representation of G induced from G_r according to the formula (42) is irreducible. It turns out that in this form the irreducibility theorem covers a great variety of symmetry centers and it becomes a simple matter to construct irreducible band representations of space groups. In the next section this theorem is applied to the construction of the irreducible band representations of the space group D_4^1.

IV. EXAMPLE

As an example of constructing irreducible band representations let us consider in detail the group D_4^1 that was already mentioned on different occasions in this paper. The inequivalent symmetry points $\vec{q}$ for this group are listed in Table I.

For the symmetry centers with the symmetry $G_q = D_4^1$ (denoted by squares in Fig. 1 and by the letters a, b, c, d in Table I), there is only one vector in the star. In this case the point symmetry lattice coincides with the Bravais lattice of the crystal. The quasicoordinates $\vec{q}_a$, $\vec{q}_b$, $\vec{q}_c$, and $\vec{q}_d$ define four different origins for the point symmetry lattices. The symmetry specification of the localized orbitals is carried out with respect to these four point symmetry lattices. The space group D_4^1 is symmorphic and its band representations for the symmetry centers a, b, c, and d are given by formula (25). The sets of the Bravais lattice vectors [see Eq. (26)] for these symmetry centers are given in Table I, while the phases corresponding to these vectors [see the phases in formula (25)] are given in Table II. The latter also contains the characters of all the irreducible representations of the point group D_4. With the help of Table II, formula (25) gives 20 different band representations of the group D_4^1, four different band representations for each irreducible representation of the point group of D_4.

Next we consider the symmetry centers with D_2 symmetry. These centers are denoted by ovals in Fig. 1 and by e and f in Table I. They have two vectors in each star, $e^{(1)}$, $e^{(2)}$ and $f^{(1)}$, $f^{(2)}$ correspondingly. Each such star defines the structure of the unit cell for the point symmetry lattice. In this case the latter differs from the Bravais lattice. In Table I we list the sets of the Bravais lattice vectors corresponding to these symmetry centers. Table III gives the irreducible representations of the point group D_2 and the phases of the band representations of the space group D_2 for the centers e and f. Each such center, as we see from Table III, gives a different band representation of the space group D_2. The latter is an invariant subgroup of D_4^1. If follows from the irreducibility theorem that the band representations of the space group D_2 corresponding to a given star induce an irreducible band representation of D_4^1. Table IV gives the matrices of these band representations for the elements of D_2 [see formula (46)]. The matrices for the other elements of D_4^1 can be found from the formula (42) and the multiplication table [Eq. (41)] which is given in Table V. This table is written for the decomposition

$$D_4^1 = D_2 + C_4^z D_2 \ . \tag{47}$$

Since the point group D_2 has four irreducible representations, the induction method will give us eight irreducible band representations of D_4^1, 4 for each star (see Table IV).

One can check that the other symmetry centers of the space group D_4^1 do not lead to any new irreducible band representations. This follows from the equivalency rule that was proven in the previous section. The symmetry groups of all the other symmetry centers are subgroups of either D_4^1 or D_2 with coinciding sets of Bravais lattice vectors. Therefore there are altogether 28 different irreducible band representations of D_4^1. Of them 16 are one dimensional and 12 two-dimensional ones. They define 28 different symmetry types of bands for solids with the space-group symmetry D_4^1.

Having the band representations of the space group D_4^1 we can find the symmetry behavior of the corresponding Bloch functions at different points in the Brillouin zone. As was already pointed out, Table II gives 20 different symmetry types of bands. Let us show how to find the symmetries of the corresponding Bloch functions from this table. This is very simple and the only thing we have to do is to replace ξ, η, and ζ appearing in the table by the values they assume for the particular $\vec{k}$ vectors of the Bloch functions. Thus, for $k=0$ we have to assume $\xi=\eta=\zeta=1$. Table II shows that for the Bloch function $\psi_0(\vec{r})$ all the phases [see Eq. (25)] following from $\vec{R}_r^{\alpha}$ are zero. This means that for all the different centers $\psi_0(\vec{r})$ behave according to the representations of the point group of D_4^1. Now take the point $k=(\pi/a, \pi/a, \pi/c)$ in the Brillouin zone. For this point we get four different symmetry types of the Bloch function $\psi_{\pi/a,\pi/a,\pi/c}(\vec{r})$ corresponding to the centers $\vec{q}_a$ to $\vec{q}_d$. This is obtained by putting $\xi=\eta=\zeta=-1$ in Table II. Similarly, Table II gives the symmetry behavior for the Bloch function at all other k vectors in the Brillouin zone. We see therefore that the knowledge of the band representations fully defines the symmetry of the Bloch functions at different points in the Brillouin zone.

TABLE V. Multiplication table for the decomposition of the space group D_4^1 with respect to D_2. The table contains the products of an element in the left-hand column with an element in the upper row.

	E	C_4^z
E	$E\,E$	$C_4^z E$
C_2^x	$E\,C_2^x$	$C_4^z C_2^y$
C_2^y	$E\,C_2^y$	$C_4^z C_2^x$
C_2^z	$E\,C_2^z$	$C_4^z C_2^z$
C_4^z	$C_4^z E$	$E\,C_2^z$
C_4^{3z}	$C_4^z C_2^z$	$E\,E$
U^{xy}	$C_4^z C_2^x$	$E\,C_2^x$
$U^{\bar{x}y}$	$C_4^z C_2^y$	$E\,C_2^y$

V. CONCLUSIONS

It is shown in this paper how a new kind of a representation, called the band representation, can be used for defining symmetry types of bands in solids. In the r representation this is an infinite-dimensional representation of the space group but it assumes a finite dimension when written in the kq representation. In the latter case the matrices of the band representation are k dependent. The infinite-dimensional representation based on localized orbitals was already discussed in Ref. 3. In this reference the symmetry of a band is defined on the basis of Bloch functions and it is shown how the latter can be expressed in symmetry-adapted Wannier functions. In the present paper the order is inverted and symmetry types of bands are directly specified by means of band representations.

In addition to solving the symmetry specification problem of bands in solids, band representations assign a new meaning to the quasicoordinate $\vec{q}$ in the theory of solids. As is well known, the quasimomentum $\vec{k}$ and the quasicoordinate $\vec{q}$ form the symmetric coordinates of translationally invariant systems.[13] The quasimomentum $\vec{k}$ is a conserved quantity in

periodic systems and it serves as a label for specifying representations of space groups. With the introduction of band representations the quasicoordinate $\vec{q}$ acquires the role of labeling them in much the same way as $\vec{k}$ labels the usual representations. Thus, only those $\vec{q}$ limited to two Wigner-Seitz cells lead to different band representations. In addition, the quasicoordinate $\vec{q}$ specifies the point symmetry lattice which is an invariant structure for each given crystal. As follows from the results of this paper there is a close connection between the point symmetry lattice and the symmetry type of a band as a whole. Having the information about a band it should, in principle, be possible to measure the corresponding point symmetry lattice. The latter is, in general, different from the Bravais lattice of the solid.[3] A good idea about these point symmetry lattices can be obtained from the drawings in the international tables[11] that accompany the information about the space group symmetries in crystals.

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