Connectivity of energy bands in crystals

L. Michel* and J. Zak
Department of Physics, Technion, Israel Institute of Technology, 32000 Haifa, Israel
(Received 30 September 1998)

It is shown that in crystals with nonsymmorphic space groups all energy bands corresponding to elementary band representations are composite and connected; i.e., these bands have several branches, and there are enough contact points among them so that one can travel continuously through all of them. The concept of elementary band representations is explained. The proof is essentially based on the property of monodromy occurring for families of representations of nonsymmorphic space groups. [S0163-1829(99)03909-0]

One of the most striking features of the quantum theory of solids is the band structure of their energy spectrum. A central role in this theory is played by the Bloch functions $\psi_k(\mathbf{r})$ and the quasimomentum $\mathbf{k}$, which specifies the translational symmetry of the crystal.[1] Qualitatively, the existence of bands and gaps in the energy spectrum is the basis for the classification of solids into metals, semiconductors, and insulators.[2] An energy band is called ''simple'' if one Bloch function only corresponds to each $\mathbf{k}$ vector in the Brillouin zone. It is called composite if $b>1$ Bloch functions correspond to a given $\mathbf{k}$ vector. In addition, an energy band is called ''connected'' if there are enough contact points between its branches so one can travel continuously through all its branches. A connected energy band, be it simple or composite, covers a continuous interval on the energy axis.

The continuity of energy band branches was proven in Ref. 3, and the study of contacts between them began in 1936 in Refs. 3 and 4. But at that time, the concept of energy bands as whole entities had no symmetry-based definition. In 1980, after interesting preliminary works,[5–7] Zak introduced[8] the concept of band representations: they are characterized by the label $(\mathbf{w},\rho)$, with $\mathbf{w}$ a point of the Wigner-Seitz cell with a given symmetry (the different cases are listed for each space group as ''Wyckoff positions'' in the ITC = International Tables for Crystallography[9]), and ρ labels an irreducible representation $D_w^{(\rho)}$ of G_w, the little group (=stabilizer) of $\mathbf{w}$; indeed, they are the representations of the space group G induced from the irreducible representations of the different stabilizers G_w. These representations are infinite dimensional since the G_w's are finite groups isomorphic to subgroups of the point group $P=G/\mathcal{T}$, with $\mathcal{T}$ denoting the invariant subgroup of translations of G. The band label is a purely group-theoretical one; it does not reflect the specific form of the periodic potential in the Schrödinger equation. One can compare it with the labeling of spherical harmonics in atoms; in the latter case, the radial functions are determined by the explicit form of the atomic potential. The label $(\mathbf{w},\rho)$ in solids describes the global symmetry properties of the energy band, while the detailed structure of the band is determined by the potential. It turns out that the Wyckoff position $\mathbf{w}$ is closely related to a geometrical phase of the energy band.[10] Like $\mathbf{w}$, this geometrical phase describes global properties of energy bands and it has recently acquired much interest in electric polarization in solids.[11] On the other hand, the Bloch momentum $\mathbf{k}$ is a local label in the Brillouin zone for an energy band which specifies the eigenvalues of the translations. So, as shown in Refs. 3 and 4, at the point $\mathbf{k}$ of the Brillouin zone, the symmetry group of an energy band is the little space group $G_{\mathbf{k}}$.

Of central interest are the band representations which cannot be decomposed as direct sums of band representations. They were first introduced in Ref. 8 where Zak called them irreducible-band representations (here, as in Ref. 12, we call them *elementary*), and he showed that it is necessary for the $\mathbf{w}$ of their label to have a maximal symmetry (equivalently, G_w has to be a maximal finite subgroup of the space group G). In Ref. 12 it was shown that this condition might not be sufficient and the full list of the 40 exceptions was given; the longer list of equivalent elementary band representations with distinct labels was also established. The energy bands whose band representations are elementary are simply called *elementary energy bands*. The number of branches of an elementary band representation labeled by $(\mathbf{w},\rho)$ is given by Eq. (21) of Ref. 12:

$$b_{(w,\rho)}=(\dim D_{G_w}^{(\rho)})|P|/|G_w|, \tag{1}$$

where $|P|$ and $|G_w|$ are, respectively, the number of elements of the groups P and G_w.

Among the 230 space groups, the 73 of them which have stabilizers G_w isomorphic to P are called symmorphic. The 157 space groups all of whose stabilizers G_w are isomorphic to strict subgroups of P are called nonsymmorphic. Equation (1) shows that their elementary bands are composite. In this paper we show that in crystals with nonsymmorphic space group symmetry all elementary bands are connected.

As shown in Ref. 3, contacts between band branches may occur at the points $\mathbf{k}$ of the Brillouin zone where the little space group $G_{\mathbf{k}}$ has an irreducible representation of dimension $d>1$. Indeed, the corresponding d distinct states belong to d different branches and have the same energy. In his thesis (summarized in Ref. 4) Herring made a thorough study of the points $\mathbf{k}$ and the irreducible representations of $G_{\mathbf{k}}$ which are transformed by the addition of time reversal into a corepresentation of double dimension. These two types of contact are not sufficient for proving the connectivity of elementary bands existing in nonsymmorphic groups, e.g., those with only Abelian $G_{\mathbf{k}}$'s. To prove the connectivity of the branches of elementary bands for such groups, we will have to use another property of the irreducible representations of nonsymmorphic groups: it was found in 1942 by Herring[13] in a paper constructing all unitary irreducible representations of two nonsymmorphic space groups: $Fm\overline{3}d$ (diamond structure) and $P6_3/mmc$ (hexagonal close packing). We shall establish this property when we need it.

In a space group G, if no element of the translation coset $\mathcal{T}r = r\mathcal{T}$ leaves fixed a point of space, the coset elements are called nonsymmorphic (e.g., Ref. 4). In three dimensions these elements are glide reflections or screw rotations, i.e., that the reflection (its order is $n=2$) or the rotation by $2\pi/n$, $n=2,3,4,6$, is followed (or preceded) by a translation in the reflection plane or along the rotation axis; so the square of a glide reflection or the nth power of the screw rotation is a pure translation. In the coset of nonsymmorphic elements we choose, and denote by r, an element such that the translation $r^n \in \mathcal{T}$ is as small as possible:

$$r^n = p\mathbf{t}_r, \quad 0<p<n, \tag{2}$$

with $\mathbf{t}_r$ a lattice translation such that there are no shorter lattice vectors colinear to it. For a glide reflection, the glide vector is $(1/2)\mathbf{t}_r$ and $(p/n)\mathbf{t}$ for the screw rotation. If a space group has a nonsymmorphic element, it is nonsymmorphic. The converse is not always true: the two exceptions are the space groups $I2_12_12_1$ and $I2_13$ (for the notations, see Ref. 9).

We begin our proof with the study of the simplest case of space groups generated by the translations $\mathcal{T}$ and one nonsymmorphic element satisfying Eq. (2) with $p=1$. There are nine such space groups which are denoted in ITC=[9] by

$$Pc, Cc; \quad P2_1, \; P3_1 \sim P3_2, \quad P4_1 \sim P4_3, \quad P6_1 \sim P6_5. \tag{3}$$

The first two contain a glide reflection, the others a screw rotation. The symbol $\sim$ between three pairs of space groups indicates their isomorphism: ITC=[9] distinguishes between them because they correspond to opposite helicity (the groups of these *enantiomorphic pairs* are transformed into each other by reflections through a plane containing the rotation axis). For each of the nine groups of Eq. (3), the stabilizers of all points of space are trivial: $G_w=1$; i.e., there is only one Wyckoff position, the whole space. So all elementary band representations are equivalent to the unique induced representation from the trivial subgroup 1; it is called the regular representation of G. From Eq. (1) we see that the number of branches is $b=|P|=n$, the smallest power of r, which is a pure translation, as defined in Eq. (2). Let us consider first the four isomorphic classes of groups in Eq. (3) with screw rotations. We take as basis of the $\mathcal{T}$ lattice $\mathbf{e}_3=\mathbf{t}_r$ [defined in Eq. (2)] and, as $\mathbf{e}_1, \mathbf{e}_2$, two lattice vectors orthogonal to $\mathbf{e}_3$. Then the reciprocal lattice is generated by the vectors $2\pi\mathbf{e}_i^*$ which satisfy

$$\mathbf{e}_i^* \cdot \mathbf{e}_j = \delta_{ij}. \tag{4}$$

So the components k_i of a $\mathbf{k}=\Sigma_i k_i \mathbf{e}_i^*$ of the Brillouin zone are defined modulo 2π. The groups $G_{\mathbf{k}_3}$ with $\mathbf{k}_3 = k_3\mathbf{e}_3^*$ are all equal to the space group G, and their irreducible representations are one dimensional. Indeed, any lattice translation vector $\mathbf{t}=\Sigma_j n_j \mathbf{e}_j$, n_j integers, is represented by $D_{\mathbf{k}_3}(\mathbf{t}) = \exp i\mathbf{k}\cdot\mathbf{t} = \exp(n_3k_3)$. In particular, $D_{\mathbf{k}_3}(\mathbf{t}_r)=\exp(ik_3)$; so the screw rotation r has n inequivalent one-dimensional representations corresponding to the different nth roots of $D_{\mathbf{e}_3}(\mathbf{e}_3)$:

$$\mathbf{k}_3 = k_3\mathbf{e}_3^*, \quad \rho \equiv 0,1,2,\ldots,n-1, \mathrm{mod}\, n,$$
$$D_{\mathbf{k}_3}^{(\rho)}(r) = e^{i(2\pi\rho+k_3)/n}. \tag{5}$$

We remark that the values of the powers of r generate the full image of a representation ρ. When k_3 varies on a full period, it is transformed into $k_3+2\pi$; this transformation has the same effect in Eq. (5) as the change of ρ into $\rho+1$:

$$\text{in Eq. (5)} \quad k_3 \mapsto k_3 + 2\pi \Leftrightarrow \rho \mapsto \rho+1. \tag{6}$$

In plain words, when we change the value of the coordinate k_3 we move on a circle of the Brillouin zone that we denote by Γ_3; making one turn on this circle makes a circular permutation of the n representations $D_{\mathbf{k}_3}^{(\rho)}$ of $G_{\mathbf{k}_3} \sim G$. This phenomenon, discussed by Herring in Ref. 13, is called *monodromy* in mathematics. The circular permutation defined by Eq. (6) is denoted by the cycle $\gamma = (12\ldots n)$, and it must be emphasized that the n-element cyclic group generated by γ acts transitively on the n representations (equivalently, these n representations form one orbit of the monodromy group). Each of these n representations corresponds to a distinct branch of the elementary band. So proof of the connection of the n branches is straightforward: follow the continuous energy function along the branch labeled by the representation ρ; this function is not necessarily periodic since after a complete turn on the circle Γ_3 we are over the starting point, but on the branch corresponding to the representation labeled by $\rho+1$, etc. After n turns on the circle Γ_3, we will have followed the continuous energy value through all the branches; that means that they form a connected graph. The proof is similar (with $n=2$) for the groups Pc, Cc generated by a glide reflection (choose again $\mathbf{e}_3=\mathbf{t}_c$), but since the elementary bands have only two branches, time reversal is sufficient for proving connectivity.

TABLE I. Contacts imposed by time reversal between branches whose band representations are labeled by $\rho, 0 \leqslant \rho < n$ in Eq. (5) for the nine space groups listed in Eq. (3). For the space groups $P2_1$, $P4_1 \sim P4_3$, $P6_1 \sim P6_5$, since they contain $P2_1$ as subgroup, Ref. 4 shows that the contacts listed in the last line of this table extend to the whole face (k_1, k_2, π) of the Brillouin zone.

$\mathbf{k}_3 = k_3\mathbf{e}_3^*$	$Pc, Cc, P2_1$	$P3_1 \sim P3_2$	$P4_1 \sim P4_3$	$P6_1 \sim P6_5$
$k_3=0$		$E_1=E_2$	$E_1=E_3$	$E_1=E_5$, $E_2=E_4$
$k_3=\pi$	$E_0'=E_1'$	$E_0'=E_2'$	$E_0'=E_3'$, $E_1'=E_2'$	$E_0'=E_5'$, $E_1'=E_4'$, $E_2'=E_3'$

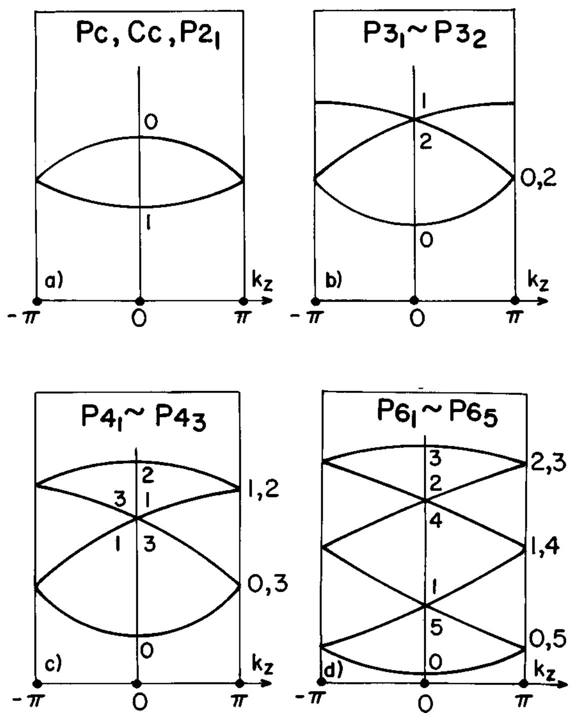

FIG. 1. Schematic plots of the energy function $E(k_3)$ for the space groups listed in Eq. (3). With the chosen ordering of the energy levels at $k=0,\pi$, no accidental degeneracy occurs.

The given proof of the connectivity of the elementary bands for the nine space groups listed in Eq. (3) does not tell where the contacts between the branches are. Their position is given by time reversal symmetry. At the Brillouin zone point $\mathbf{k}_3$ with $k_3=0$ and π, the screw rotation r is represented by the phases $\exp(i2\pi\rho/n)$ and $\exp[i\pi(2\rho+1)/n]$, respectively. We know from Ref. 4 that the branches corresponding to complex conjugate representations meet at these points. Let us denote by E_ρ and E'_ρ the energy of the branch ρ at these two points. Table I gives the energy degeneracy for the different groups.

In Fig. 1 we have drawn the connected graph of the energy over Γ_3 for the different groups. We have chosen the order of the energy levels E_ρ and E'_ρ such that there is no other crossing over Γ_3 than those imposed by time reversal. In Fig. 2, by changing the order of the levels at $k_3=0$ for the group $P4_1$ two more contacts must appear. They correspond

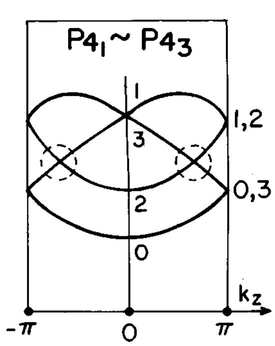

FIG. 2. Alternative ordering of the energy levels at $k=0$ for the space groups $P4_1$ and $P4_3$ imposes two accidental degeneracies indicated by the dashed-line circles.

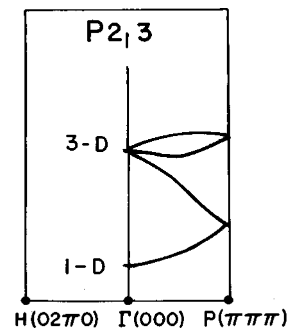

FIG. 3. For the band $(a,1)$ of the space group $I2_13$, at the point $\mathbf{k}_\Gamma$ we have a one-dimensional and a three-dimensional irreducible representation. At the point $\mathbf{k}_P$ there are 2 inequivalent irreducible two-dimensional representations. Connectivity of all the four branches is unavoidable. At the point $\mathbf{k}_H$, like at $\mathbf{k}_\Gamma$, there is a one-dimensional and a three-dimensional representation, with the order determined by the potential.

to the accidental degeneracies studied in Ref. 4. They can be moved over Γ_3 by changing the potential and they can be removed as Fig. 1(c) shows.

The five other space groups generated by the translations and one nonsymmorphic element are $P4_2$, $I4_1$, $P6_2 \sim P6_4$, $P6_3$: their value of p in Eq. (2) is >1; it is 2,2,2,2,3, respectively. These groups have several band representations, and an application of the same method proves their connectivity. The $14=9+5$ groups studied contain all nonsymmorphic symmetry operations defined by Eq. (2) and all nonsymmorphic elements existing in the nonsymmorphic three-dimensional space groups belong to one of these 14 types. So we can apply the same method to all other nonsymmorphic groups except two of them that we have to study directly: they are the two nonsymmorphic groups which do not contain nonsymmorphic elements. The space group $I2_12_12_1$ has three Wyckoff positions with maximal symmetry (they are labeled *a,b,c* in Ref. 9). Each one yields 2 two-branch elementary band representations. To prove their connectivity, it is sufficient to read tables of irreducible representations (see, e.g., Ref. 14) of space groups and notice that all those of $G_{\mathbf{k}_R}$ ($\mathbf{k}_R$ represents the vertices of the Brillouin cell) are two dimensional.

The space group $I2_13$ has two Wyckoff positions a and b with maximal symmetry whose stabilizers are the cyclic groups C_3 and C_2; we label their irreducible representations by $1,\omega=\exp(2i\pi/3)$, $\overline{\omega}$ and by $+$, $-$, respectively. So the labels of their five elementary band representations are $(a,1)$, (a,ω), $(a,\overline{\omega})$, $(b,+)$, $(b,-)$. The 12-element (tetrahedral) point group $T=23$ leaves fixed four isolated points of the Brillouin zone:[14] $\mathbf{k}_\Gamma=0=4\mathbf{k}_P$, $\mathbf{k}_P$, $\mathbf{k}_H=2\mathbf{k}_P$, $\mathbf{k}_{P'}=3\mathbf{k}_P$ (H and P,P' represent, respectively, the 6 four-edge vertices and the 8 three-edge vertices on the surface of the Brillouin zone with 12 rhombic faces). We denote by 1, ω, $\overline{\omega}$, and v the four irreducible representations of T (the first three are one-dimensional representations and v is its three-dimensional vector one). From Ref. 14 we read that $G_{\mathbf{k}_P} \sim G_{\mathbf{k}_{P'}}$ have only two-dimensional irreducible representations. For the four-branch band $(a,1)$, a straightforward computation yields for the representations of the $G_{\mathbf{k}}$, $1\oplus v$ at $\mathbf{k}_\Gamma$, $\mathbf{k}_H$ and the direct sum of 2 two-dimensional irreducible representations at $\mathbf{k}_P$, $\mathbf{k}_{P'}$. This is obviously sufficient for proving the connectivity of the energy band by using the same simple argument given in Ref. 15 for the diamondlike structure: see Fig. 3. By replacing 1 by ω and $\overline{\omega}$, in the sets of representations at $\mathbf{k}_\Gamma$ and $\mathbf{k}_H$, the same argument applies to the elementary bands (a,ω) and $(a,\overline{\omega})$. We remark that time reversal combines the two corresponding complex conjugate elementary band representations into 1 eight-branch elementary band *corepresentation*, which is globally connected because the representations $\omega,\overline{\omega}$ of $G_{\mathbf{k}_\Gamma},G_{\mathbf{k}_H}$, are combined into an irreducible two-dimensional corepresentation.

The connectivity of the 2 six-branch elementary bands $(b\pm)$ is obtained for both bands from the fact that the representations of G_{k_P} and $G_{k_{P'}}$ are the direct sum of their 3 inequivalent two-dimensional irreducible representations and, for some other $G_{\mathbf{k}}$, the direct sum of 2 three-dimensional irreducible representations. Indeed, the $G_{\mathbf{k}}$ representations reduce to $v\oplus v$ both at $\mathbf{k}_\Gamma$ for the $(b,+)$ band representation and at $\mathbf{k}_H$ for the $(b,-)$ one.

In Ref. 15 the connectivity of the branches of the frequency bands in the vibration spectrum of solids has also been proven for some other crystals (e.g., close hexagonal packing) by using the supplementary property that the three acoustic branches meet at zero frequency. Presently, we are also studying the connectivity of elementary bands for the symmorphic groups. To prove it for some of them, we have to use a new property (not explained here) of the elementary band representations. We will present it in another publication.

In conclusion, we have shown in this paper the powerfulness of the symmetry band label $(\mathbf{w},\rho)$ of an elementary band representation. Namely, the energy band, corresponding to such a band representation in crystals with nonsymmorphic space groups, has all its branches necessarily connected by some remarkable combination of symmetry, continuity, and periodicity.

L.M. is grateful to the Physics Department of the Technion for its warm hospitality. J.Z. acknowledges the Erica and Sheila Samson Chair in Physics for its support. The authors acknowledge with thanks helpful discussions with Professor Jan Genossar.

---

*Permanent address: IHES, 91440 Bures-sur-Yvette, France.

[1] F. Bloch, Z. Phys. **52**, 555 (1928).
[2] F. Seitz, *The Modern Theory of Solids* (McGraw-Hill, New York, 1940).
[3] L. P. Bouckaert, R. Schmoluchovski, and E. P. Wigner, Phys. Rev. **50**, 58 (1936).
[4] C. Herring, Phys. Rev. **52**, 361 (1937); **52**, 365 (1937).
[5] I. P. Burneika and I. B. Levinson, Tr. Akad. Nauk Lit. SSR, Ser. B **4**, 21 (1961).
[6] J. des Cloizeaux, Phys. Rev. **129**, 219 (1963); Phys. Rev. **135**, A685 (1964); **135**, A698 (1964).
[7] O. V. Kovalev, Fiz. Tver. Tela (Leningrad) **17**, 1700 (1975) [Sov. Phys. Solid State **17**, 1106 (1975)].
[8] J. Zak, Phys. Rev. Lett. **45**, 1025 (1980); Phys. Rev. B **25**, 1344 (1982); **26**, 3010 (1982).
[9] ITC=*International Tables for Crystallography*, edited by T. Hahn (Reidel, Boston, 1983), Vol. A.
[10] J. Zak, Phys. Rev. Lett. **62**, 2747 (1989); Europhys. Lett. **9**, 615 (1989); L. Michel and J. Zak, *ibid.* **18**, 239 (1992).
[11] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993); R. Resta, Rev. Mod. Phys. **66**, 899 (1994); R. Resta and S. Sorella, Phys. Rev. Lett. **74**, 4738 (1995).
[12] H. Bacry, L. Michel, and J. Zak, *Lectures Notes in Physics* (Springer, New York, 1988), Vol. 313, p. 291.
[13] C. Herring, J. Franklin Inst. **233**, 525 (1942).
[14] A. Casher, M. Glück, and Y. Gur, in *The Irreducible Representations of Space Groups*, edited by J. Zak (Benjamin, New York, 1969).
[15] L. Michel, M. B. Walker, and J. Zak, Phys. Rev. Lett. **74**, 4871 (1995).