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Topologically unavoidable points and lines of crossings in the band structure of solids

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Abstract

Rules are developed for a new kind of topologically unavoidable branch crossing in the band structure of solids. It is proved that there exists a great variety of four-branch energy bands in crystalline solids of the orthorhombic system in which the crossings are necessitated by symmetry and topology. These crossings are different from conventional degeneracies that follow from space group symmetry alone, and they can take place on either points or lines in the Brillouin zone.

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Symmetry labelling of eigenfunctions and energies in the band structure of solids was introduced in a famous paper by Bouckaert, Smoluchowski and Wigner (BSW) [1]. They used symmetry points in k-space and the irreducible representations of their symmetry groups G_k for this labelling. This approach reflects the local symmetry of the extended Bloch functions at the symmetry points and their vicinity in the Brillouin zone. As is well known, Bloch functions can be built from atomic-like functions or Wannier functions [2], which are localized in configuration space and carry the full information of the Bloch functions but are not eigenfunctions of the problem. The symmetry properties of Wannier functions were dealt with by Burneika and Levinson [3], des Cloizeaux [4], Kovalev [5] and later Zak [6] who defined the concept of band representations of space groups. Unlike conventional representations which give locally the symmetry in k-space, band representations carry symmetry labels of the entire energy bands and enable one to have a global look at them. One distinguishes between simple energy bands with a single branch (having one Bloch function at each $\vec{k}$-vector in the Brillouin zone), and composite ones with more than one branch (two, or more than one, Bloch function at each $\vec{k}$). When at a given $\vec{k}$ in the Brillouin zone there are d Bloch functions ($d > 1$) with the same energy, we have a d-fold degeneracy at this $\vec{k}$. BSW [1] have carried out an analysis of degeneracies in energy bands based on irreducible representations of space groups. Following this analysis, Herring [7] has raised the possibility of the appearance of accidental degeneracy which may follow from symmetry and continuity of the energy as a function of $\vec{k}$ in the Brillouin zone. The main feature of accidental degeneracy is that it can be removed by changing the potential of the crystal, while keeping the symmetry unchanged. Based on the notion of band representations, it was recently shown that in some crystals with four-branch composite energy bands a special kind of degeneracy exists which is a consequence of symmetry and continuity, and for which the location in k-space of the degeneracy point can be moved by changing the potential, but it cannot be removed as long as the symmetry of the crystal is kept unchanged [8].

In this paper we establish rules for the existence of topologically unavoidable points and lines of branch crossings in the band structure of solids. A point of a crossing is obtained when two energy branches ϵ_1 and ϵ_2 assume the same energy at some given point in the Brillouin zone. When this happens on a whole line, then we have a line of crossing for two energy surfaces. These rules are established for a great variety of crystals with orthorhombic symmetry. The main tool for establishing these rules is the notion of elementary band representations [9], a classification of which was given in [10]. An additional tool is the compatibility relations [1] when applied on a global scale of entire energy bands or the so-called continuity chords (see item 2 in [6]). At the centre of the Brillouin zone, $\vec{k} = 0$ (the Γ-point) all irreducible representations of orthorhombic space groups are one dimensional (because the point groups for these space groups are Abelian [1, 11]). On the other hand, on the surface of the Brillouin zone there are always symmetry points at which all the irreducible representations (irreps) or co-representations of orthorhombic space groups are of dimensionality two or higher (time-reversal included). With these facts in mind it will be shown that there are numerous orthorhombic space groups for which branch crossings are unavoidable by symmetry and topology.

The idea we are going to use for proving the rules for topologically unavoidable crossings in orthorhombic crystals is as follows: let us start with a short description of background material. An elementary energy band which corresponds to an elementary band representation [9] has a number of branches $b(\vec{w}, \rho)$ given by the formula ($\vec{w}$ is a maximal symmetry Wyckoff position [12], and ρ specifies an irreducible representation $D^{(\vec{w},\rho)}$ of the symmetry group G_w of $\vec{w}$):

$$b(\vec{w}, \rho) = \left[\dim D^{(\vec{w},\rho)}\right] \frac{|P|}{|G_w|} \tag{1}$$

where $[\dim D^{(\vec{w},\rho)}]$ is the dimension of the irreducible representation $D^{(\vec{w},\rho)}$ of G_w and $|P|$ and $|G_w|$ are the number of elements of the groups P (the point group of the space group of the solid) and G_w. The label $(\vec{w}, \rho)$ specifies the band representation in question, which is an induced representation of the space group G induced from $D^{(\vec{w},\rho)}$ of G_w. Being an induced representation from a finite-order subgroup G_w, the band representation $(\vec{w}, \rho)$ is infinite dimensional and covers the infinite set of functions belonging to the corresponding energy band. By reducing the band representation $(\vec{w}, \rho)$, one can find its content in irreducible representations of the space group G at each point $\vec{k}$ in the Brillouin zone. It is, in particular, easy to find this content at the point Γ in the centre $\vec{k} = 0$ of the Brillouin zone [6]. For this, one just has to find the representations of the point group P which are induced from the representation ρ of the symmetry group G_w. For orthorhombic space groups their point groups P are all Abelian and therefore their irreducible representations will all be one dimensional at the Γ-point. As was mentioned above, for all orthorhombic space groups, on the surface of the Brillouin zone there are always symmetry points at which all irreducible representations (including co-representations) are of dimension two or higher [13]. For checking whether a crossing of two branches appears we are going to follow pairs of

Table 1. Irreducible representations of the point group D_{2h}. The U^x is a rotation by π around the x-axis (respectively, y and z-axes), the σ^x is a reflection in the plane perpendicular to x (respectively, y and z). I is the inversion.

$D_{2h} - mmm$	E	U^x	U^y	U^z	σ^x	σ^y	σ^z	I
1	1	1	1	1	1	1	1	1
2	1	1	−1	−1	1	−1	−1	1
3	1	−1	1	−1	−1	1	−1	1
4	1	−1	−1	1	−1	−1	1	1
5	1	1	1	1	−1	−1	−1	−1
6	1	1	−1	−1	−1	1	1	−1
7	1	−1	1	−1	1	−1	1	−1
8	1	−1	−1	1	1	1	−1	−1

one-dimensional representations for a given elementary energy band that initiate at the Γ-point as two separate one-dimensional representations and end up at symmetry points on the surface of the Brillouin zone that have two-dimensional representations only. In order to see how this is done let us consider as an example the orthorhombic space group 61 $\left(D_{2h}^{15},\ \mathrm{Pbca}\right)$. This group has two maximal symmetry Wyckoff positions [12]:

$$a = (000) \qquad b = \left(00\frac{c}{2}\right). \tag{2}$$

For a and b the symmetry groups G_a and G_b contain the unit element E and the inversion I, and are isomorphic to the point group C_i [13]. There are four (two from each Wyckoff position) four-branch elementary band representations $(\vec{w}, \rho)$ ($\vec{w} = a$ or b and $\rho = 1, 2$) for the space group Pbca according to equation (1), since $|P| = 8$, $|G_w| = |C_i| = 2$ and each of the two irreducible representations of C_i are one dimensional ($\dim D^{(\vec{w},\rho)} = 1$). The elementary band representation $(a,\ 1)$ induced from the trivial representation of C_i contains the four even representations of the point group D_{2h} (see table 1, irreps 1–4) at the symmetry centre Γ in the Brillouin zone. On the surface of the Brillouin zone there are usually a number of symmetry points which have two-dimensional representations only. In table 2 we list those points for the orthorhombic space groups that are continuously connected by symmetry points inside the Brillouin zone (column 2 in table 2) with non-trivial symmetry elements (column 3 in table 2). It is important to point out that this possibility to follow continuously some symmetry elements along lines from the centre Γ of the Brillouin zone to the surface will be used below as the main tool in establishing the rules of branch crossings. For the example under consideration (group D_{2h}^{15}), we give in table 3 the characters of the two-dimensional representations at the symmetry points on the surface of the Brillouin zone $X, Y, Z\ A, D$ and H at which there are only two-dimensional irreps (the characters are taken from [13], pp 101, 102). In the upper row of table 3 the point group elements of Pbca are given (in general, they appear with partial translations [12, 13]). In the first column of table 3 we list the symmetry points on the surface of the Brillouin zone (see table 2 for their coordinates), which have two-dimensional irreps only for the space group D_{2h}^{15}. The subscripts 1 and 2 number the different irreducible representations. In the last column of table 3 we list the symmetry points in the Brillouin zone which continuously connect the centre Γ with the corresponding symmetry points on the surface of the Brillouin zone in the first column. The underlined characters in table 3 identify the symmetry elements of the symmetry points in the last column (see also table 2). We are now ready to discuss crossings of the branches of the elementary energy band that correspond to the elementary band representation $(a,\ 1)$ of the orthorhombic group Pbca. As was pointed out above, the band representation $(a,\ 1)$ contains the irreps 1–4 of D_{2h} at the Γ-point

Table 2. Symmetry points and symmetry elements on the surface and inside the Brillouin zone for the orthorhombic space groups. For the latter their symmetry elements are given in column 3. For notations see caption for table 1.

Points on the surface of the BZ	Points inside the BZ	Symmetry for points inside the BZ
$Z(00\frac{\pi}{c})$	$(00k_z)$	$U^z\sigma^x\sigma^y$
$X(\frac{\pi}{a}00)$	(k_x00)	$U^x\sigma^y\sigma^z$
$Y(0\frac{\pi}{b}0)$	$(0k_y0)$	$U^y\sigma^x\sigma^z$
$U(\frac{\pi}{a}0\frac{\pi}{c})$	(k_x0k_z)	σ^y
$T(0\frac{\pi}{b}\frac{\pi}{c})$	$(0k_yk_z)$	σ^x
$S(\frac{\pi}{a}\frac{\pi}{b}0)$	(k_xk_y0)	σ^z
$A(k_x0\frac{\pi}{c})$	(k_x0k_z)	σ^y
$C(k_x\frac{\pi}{b}0)$	(k_xk_y0)	σ^z
$B(0k_y\frac{\pi}{c})$	$(0k_yk_z)$	σ^x
$D(\frac{\pi}{a}k_y0)$	(k_xk_y0)	σ^z
$G(\frac{\pi}{a}0k_z)$	(k_x0k_z)	σ^y
$H(0\frac{\pi}{b}k_z)$	$(0k_yk_z)$	σ^x

Table 3. Symmetry points on the surface of the Brillouin zone (BZ) and the characters of the corresponding irreps of the space group Pbca (taken from [13]). The underlined characters correspond to symmetry elements of the points inside the BZ.

Points on the surface of the BZ	Symmetry elements and characters								Points inside the BZ
	E	U^x	U^y	U^z	I	σ^x	σ^y	σ^z	
$X_{1,2}$	$\underline{2}$	$\underline{0}$	0	0	0	0	$\underline{\pm 2}$	$\underline{0}$	(k_x00)
$Y_{1,2}$	$\underline{2}$	0	$\underline{0}$	0	0	$\underline{0}$	0	$\underline{\pm 2}$	$(0k_y0)$
$Z_{1,2}$	$\underline{2}$	0	0	$\underline{0}$	0	$\underline{\pm 2}$	$\underline{0}$	0	$(00k_z)$
A	$\underline{2}$	0					$\underline{0}$	0	(k_x0k_z)
D	$\underline{2}$		0			0		$\underline{0}$	(k_xk_y0)
H	$\underline{2}$			0		$\underline{0}$	0		$(0k_yk_z)$

(see table 1). In which order these representations arrange according to energy cannot be determined from symmetry considerations alone and this order depends on the specific form of the periodic potential of the crystal. However, no matter which order is chosen for these four irreps, it is shown in what follows that the branches in the $(a, 1)$ energy band have to cross. This is seen from the fact (see table 3) that in the Γ–X direction (including X) the character $\chi(\sigma^y) = \pm 2$, while in the Γ–A direction including A, $\chi(\sigma^y) = 0$. This leads to unavoidable crossing in either the X- or A-direction. Indeed, by pairing the irreps 1–4 as in figure 1 (1 & 3 and 2 & 4) in order to avoid crossing in the X-direction for $\chi(\sigma^y) = \pm 2$, we necessarily have crossing in the A-direction for $\chi(\sigma^y) = 0$ (in this direction there are two choices of pairings with each of them leading to crossing (see figures 2(a) and (b)). This leads us to the first rule of crossings:

*Rule 1***.** If there exists a symmetry element which has different characters in two different directions of the Brillouin zone, then in one of these two directions there is necessarily a crossing. Rule 1 needs no proof because it is clear that different characters for the same element requires a different pairing of the irreps which has to lead to a crossing in one of these directions.

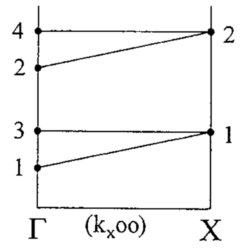

Figure 1. Schematic energy graphs for the band representation (a, 1) of the space group 61 in the direction X in the BZ. The numbers on the left are for the irreps of D_{2h}, and on the right for the irreps of G_X, the symmetry group of the symmetry point X.

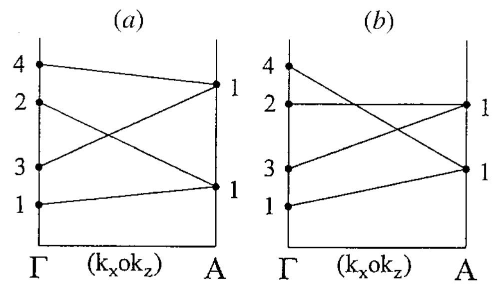

Figure 2. (a) and (b) are schematic energy graphs as in figure 1, but for the A-direction. (a) and (b) give different allowed pairings or irreps.

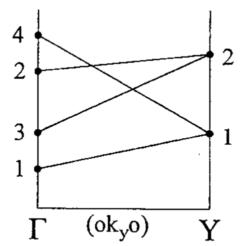

Figure 3. Schematic energy graphs as in figure 1 but for the Y-direction.

Before discussing rule 1, we turn to the derivation of an additional crossing rule. In the above analysed example for the Pbca space group we had $\chi(\sigma^y) = \pm 2$ for the X-direction. Table 3 shows that in the Y-direction the character of σ^z is $\chi(\sigma^z) = \pm 2$. Such a character requires the pairing of 1 & 4 and 2 & 3. Comparing this with figure 1 for the X-direction, the conclusion is that there is unavoidable crossing in one of the directions X and Y. Having chosen the order of the irreps as in figure 1 to have $\chi(\sigma^y) = \pm 2$ in the X-direction, we shall necessarily get a crossing in the Y-direction (figure 3).

Consider now the directions A, D and H in table 3 and notice that in the A-direction, $\chi(\sigma^y) = 0$, in the D-direction $\chi(\sigma^z) = 0$ and in the H-direction $\chi(\sigma^x) = 0$. From table 1 it is seen that no pairing of the irreps 1–4 exists that would lead to the vanishing of the characters for all the three elements $\sigma^x, \sigma^y, \sigma^z$. This means that crossing is unavoidable in one of the directions A, D and H.[1] A possible crossing situation is shown in figure 4, where we have

[1] An example of such a crossing was already encountered in the space group $P2_12_12_1$ [8].

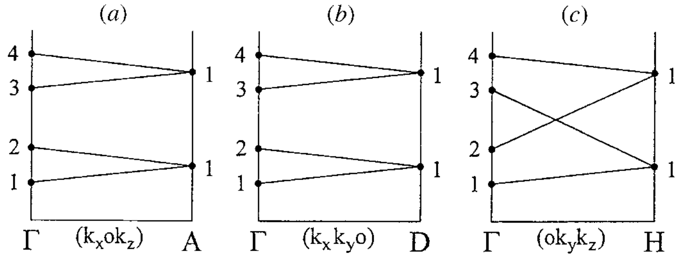

Figure 4. (*a*), (*b*) and (*c*) are schematic energy graphs as in figure 1, but for the directions A, D and H, respectively. The order of the irreps of D_{2h} was chosen in such a way that there is no crossing in A- and D-directions, but then there is a necessary crossing in the H-direction.

chosen the ordering of the irreps 1–4 of D_{2h} at Γ in such a way as to avoid crossing in the A- and D-directions, but then there is necessarily a crossing in the H-direction (if we had chosen the ordering of the irreps as in figure 1, then there would be no crossing in the D- and H-directions, and the crossing would necessarily appear in the A-direction). We can now formulate rule 2 for branch crossing.

*Rule 2***.** It consists of two parts 2a and 2b. (2a) If there exist two symmetry elements which have characters ± 2 in two different directions in the Brillouin zone, then in one of these directions there is necessarily a crossing. (2b) If there exist three symmetry elements which have characters zero in two or three different directions in the Brillouin zone, then in one of these directions there is necessarily a crossing. The proof of rule 2 is as follows. The induction of four-branch band representations for orthorhombic space groups is determined by four elements of the following point groups (in view of the fact that the possible symmetry groups G_w for such four-branch bands are C_1, C_i, C_2 and C_s) [12, 13]:

$$D_2, \quad C_{2v} \quad \text{and} \quad C_{2h}. \tag{3}$$

These are Abelian point groups having only one-dimensional irreps at the Γ-point . It is easy to check that any pairing of their irreps gives a character ± 2 for one of the non-trivial elements (non-unit elements) and 0 for the other two. This means that for a fixed pairing we can have no two elements with character ± 2 and no three elements with 0-character. This proves rule 2.

The following remark should be made concerning the above rules 1 and 2. When dealing with induced representations the induction process imposes connections between characters of different elements. The most often encountered of such connections in the application of rules 1 and 2 is for the induction from the symmetry group C_i, where the character of a rotation U by π is closely connected to that of a reflection σ through a plane perpendicular to the rotation axes. This is so because $\sigma = IU$ where I is the inversion. See another remark about these connections later.

In table 4 we give a list of orthorhombic space groups whose four-branch energy bands have topologically unavoidable branch crossings in one or more directions. The information in this table in the first 4 columns is taken from [12]. Column 5 shows the rule number according to which the branch crossing materializes, and in the last column we give the possible directions of the crossings. For rules 1 and 2a they take place in one of two such directions, while for rule 2b in one of two or three directions. For each direction the symmetry element is given which persists for the whole line from the centre Γ to the surface of the Brillouin zone. With the information in table 4, the character table 1 for D_{2h}, and the characters for the irreps of the corresponding orthorhombic space groups [13], it is easy to draw branch crossing graphs similar to those given in figures 1–4 for group 61.

Table 4. Topologically unavoidable crossing directions for four-branch energy bands of the orthorhombic system. The first four columns are taken from [12]. The information in the last column is explained in the text.

Space group	Space group symbol	WYCKOFF position	Isotropy group	Rule	Symmetry elements and directions in Brillouin zone
19	P$2_1 2_1 2_1$ D_2^4	$a(xyz)$	E	2b	$U^x(X), U^y(Y), U^z(Z)$
29	Pca2_1 C_{2v}^5	$a(xyz)$	E	1	$\sigma^y(Z), \sigma^y(X)$
				2b	$U^z(Z), \sigma^x(Z), \sigma^y(X)$
33	Pna2_1, C_{2v}^9	$a(xyz)$	E	1	$\sigma^y(Z), \sigma^y(X)$
				2b	$U^z(Z), \sigma^x(Z), \sigma^y(X)$
48	Pnnn D_{2h}^2	$e(\frac{a}{2}\frac{b}{2}\frac{c}{2})$, $f(000)$	C_i	2a	$U^x(X), U^y(Y)$
				2b	$\sigma^y(A), \sigma^x(B), \sigma^z(C)$
50	Pban D_{2h}^4	$e(000)$, $f(00\frac{c}{2})$	C_i	2a	$U^x(X), U^y(Y)$
				2b	$\sigma^x(U), \sigma^y(T), \sigma^z(C)$
52	Pnna D_{2h}^6	$a(000)$, $b(00\frac{c}{2})$	C_i	1	$\sigma^z(Y), \sigma^z(D)$
				2a	$U^x(X), U^z(Z)$
				2b	$\sigma^x(Z), \sigma^y(Z), \sigma^z(X)$
		$c(\frac{a}{4}0z)$	C_2^z	1	$\sigma^z(Y), \sigma^z(D)$
		$d(x\frac{b}{4}\frac{c}{4})$	C_2^x	1	$\sigma^z(Y), \sigma^z(D)$
53	Pmna D_{2h}^7	$g(\frac{a}{4}y\frac{c}{4})$	C_2^y	2a	$U^x(X), \sigma^x(Z)$
54	Pcca D_{2h}^8	$a(000)$, $b(0\frac{b}{2}0)$	C_i	1	$\sigma^y(X), \sigma^y(A)$
				2a	$U^z(Z), \sigma^y(X)$
				2b	$\sigma^z(X), \sigma^y(Z), \sigma^x(B)$
		$c(0y\frac{c}{4})$	C_2^y	1	$\sigma^y(X), \sigma^y(A)$
				2a	$U^z(Z), \sigma^y(X)$
		$d(\frac{a}{4}0z)$, $e(\frac{a}{4}\frac{b}{2}z)$	C_2^z	1	$\sigma^y(X), \sigma^y(A)$
56	Pccn D_{2h}^{10}	$a(000)$, $b(00\frac{c}{2})$	C_i	1	$\sigma^y(X), \sigma^y(A)$
				2a	$\sigma^x(Y), \sigma^y(X)$
				2b	$\sigma^x(B), \sigma^y(A), \sigma^z(C)$
		$c(\frac{a}{4}\frac{b}{4}z)$, $d(\frac{a}{y}\frac{3b}{4}z)$	C_2^z	1	$\sigma^y(X), \sigma^y(A)$
57	Pbcm D_{2h}^{11}	$a(000)$, $b(\frac{a}{2}00)$	C_i	1	$\sigma^x(Z), \sigma^x(H)$
				2a	$\sigma^z(Y), \sigma^x(Z)$
		$c(x\frac{b}{4}0)$	C_2^x	1	$\sigma^x(Z), \sigma^x(H)$
				2a	$\sigma^z(Y), \sigma^x(Z)$
		$d(xy\frac{c}{4})$	C_s^z	1	$\sigma^x(Z), \sigma^x(H)$
59	Pmmn D_{2h}^{13}	$c(\frac{a}{4}\frac{b}{4}0)$, $d(\frac{a}{4}\frac{b}{4}\frac{c}{2})$	C_i	2a	$\sigma^y(U), \sigma^x(T)$
60	Pbcn D_{2h}^{14}	$a(000)$, $b(0\frac{b}{2}0)$	C_i	1	$\sigma^y(X), \sigma^y(A)$
				2a	$U^y(Y), \sigma^x(Z)$
				2b	$\sigma^z(D), \sigma^x(H), \sigma^y(A)$
		$c(0y\frac{c}{4})$	C_2^y	1	$\sigma^y(X), \sigma^y(A)$
				2a	$\sigma^y(X), \sigma^x(Z)$
61	Pbca D_{2h}^{15}	$a(000)$, $(00\frac{c}{2})$	C_i	1	$\sigma^x(Z), \sigma^x(H)$
				2a	$\sigma^x(Z), \sigma^z(Y)$
				2b	$\sigma^x(H), \sigma^z(D), \sigma^y(A)$
62	Phma D_{2h}^{16}	$a(000)$, $b(00\frac{c}{2})$	C_i	1	$\sigma^z(Y), \sigma^z(X)$
				2a	$\sigma^y(X), \sigma^z(Y)$
				2b	$U^x(X), U^y(Y), U^z(Z)$
		$c(x\frac{b}{4}z)$	C_s^y	1	$\sigma^x(Y), \sigma^z(X)$
				2b	$U^x(X), U^y(Y), U^z(Z)$
64	Cmca D_{2h}^{18}	$e(\frac{a}{4}y\frac{c}{4})$	C_2^y	1	$\sigma^x(Z), \sigma^z(S) = \sigma^x(S)$
68	Ccca D_{2h}^{22}	$c(\frac{a}{4}0\frac{c}{4})$, $d(0\frac{b}{4}\frac{c}{4})$	C_i	1	$U^z(Z), \sigma^z(S) = U^z(S)$
				2b	$\sigma^y(A), \sigma^x(B), \sigma^z(S)$
70	Fddd D_{2h}^{24}	$c(000)$, $d(\frac{a}{2}\frac{b}{2}\frac{c}{2})$	C_i	2a	$U^x(X), U^y(Y)$
				2b	$\sigma^x(X), \sigma^z(X), \sigma^x(B)$
73	Ibca D_{2h}^{27}	$a(000)$, $b(\frac{a}{4}\frac{b}{4}\frac{c}{4})$	C_i	2b	$\sigma^x(T), \sigma^y(U), \sigma^z(S)$

We would like to make a number of remarks about table 4 which contains the main results of this paper. First, it contains only a part of the crossing directions for each given group and that a full listing will be given elsewhere. For example, for group 48, one can check, by using the tables on p 81 of [13], that for rule 2a there will also be crossings in one of the two directions $U^x(X)$ or $U^z(Z)$ and $U^y(Y)$ or $U^z(Z)$. Second, we would like to point out that there are very many materials that crystallize with orthorhombic symmetry and that, according to [14], there are about 2000 different crystals belonging to the 18 space groups in table 4, which makes the results of branch crossings of much practical interest. Third, as was mentioned above, because of the induction process, there are connections between some characters of different elements (see space group 64 and line 1 for group 68). And finally, one should keep in mind that some of the branch crossings, as mentioned in the introduction, can take place on lines in the Brillouin zone. Consider, for example, figure 4 for group 61. According to figure 4(*c*) there is a crossing in the Γ–H direction between branches 2 and 3, which means that $\epsilon_2(k_y k_z) = \epsilon_3(k_y k_z)$. From here a line of crossing follows in the $k_y k_z$-plane.

In conclusion, we have established rules of branch crossings in four-branch bands in crystals with orthorhombic symmetry and have applied these rules for discovering a great variety of materials in which branch crossing is a topologically unavoidable feature.

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