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Physical Equivalence of Energy Bands in Solids.

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Abstract. – A concept is introduced for physical equivalence of energy bands in solids: two energy bands are physically equivalent if their branches have identical continuity chords (symmetries) and identical Berry phases. 14 pairs of simple bands exist that are described by equivalent band representations but are nevertheless physically inequivalent because they have different topologies. Examples are given of physically equivalent and physically inequivalent composite energy bands. All simple bands on different Wyckoff positions are physically inequivalent and they correspond therefore to different energy bands.

Since the appearance of the classical paper [1], it has been customary to specify the symmetry of energy bands in solids by the symmetry of their Bloch functions at different points in the Brillouin zone. A striking property of the energy spectrum in solids is the continuity of the energy as a function of the Bloch vector $\boldsymbol{k}$. Here a connected question is the continuity of the Bloch functions in $\boldsymbol{k}$. Although much work has been done on the continuity of energy bands [2], the subject is not so well understood [3-5]. For simple bands (one Bloch function at each $\boldsymbol{k}$), it has been proven that the Bloch function $\psi_k(\boldsymbol{r})$ can be chosen to be analytic in $\boldsymbol{k}$ (their Wannier functions are exponentially decaying) [6]. It was recently shown that simple bands can be assigned a topological label, which is the Berry phase of the Bloch function [7]. Correspondingly, simple bands can be specified both by the symmetry (*e.g.*, continuity chord [8]) and the topology of their Bloch functions. Two simple bands will be called physically equivalent if their Bloch functions have the same continuity chords and the same Berry phases. Bloch functions of physically equivalent bands can be connected by a continuous phase. Examples have been established of simple energy bands that have identical continuity chords (*e.g.*, symmetries) but whose Bloch functions cannot be connected by a continuous phase [9]. These latter bands are physically inequivalent.

In this letter we define the general concept of physical equivalence for energy bands in solids. For this purpose we use quasi-Bloch functions [3, 10], and band representations of

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space groups that are built on them [11]. It is shown that a Wyckoff position [$\boldsymbol{w}$] together with the label of an irreducible representation of the isotropy or little group G_w (a point group which leaves the point $\boldsymbol{w}$ in the Wyckoff position [$\boldsymbol{w}$] unchanged) determine a branch quasi-Bloch function $\phi_k^{(w,l)}(\boldsymbol{r})$, which has a well-defined continuity chord and also a well-defined Berry phase. By definition, two composite energy bands (more than one Bloch function at each point in the Brillouin zone) belonging to equivalent band representations of a given space group [12] are called physically equivalent if their corresponding branches have identical continuity chords and identical Berry phases [7]. This definition applies also to simple bands. In the latter case there is a single branch and the quasi-Bloch function becomes the Bloch function. We show that there are numerous energy bands that belong to equivalent band representations (have identical continuity chords) but they are nevertheless physically inequivalent. Most of them are composite bands. For simple bands an example of the latter kind was already given before [9] and a detailed calculation of the Berry phases for the space group F222 (# 22) was carried out in ref. [7c]. In this letter we list all the physically inequivalent simple bands that correspond to equivalent band representations. There are 14 pairs of them: 8 pairs in the space group F222 (# 22) and 6 pairs in the space group F23 (# 196). We present the Berry phases for these physically inequivalent bands. These examples demonstrate for the first time the topological significance of Berry phases in the classification of energy bands in solids.

Let us explain the idea of this letter on the well-known example of a one-dimensional crystal along the x-axis [3, 7]. Such a crystal has two inequivalent symmetry (inversion) centres at $x = w_1 = 0$ and $x = w_2 = a/2$, where a is the lattice constant. These are the Wyckoff positions [13]. Around each Wyckoff position one can construct Wannier functions which are even (+) or odd (−) $\psi^{w_s,\pm}(x)$, $s = 1, 2$. There are 4 such Wannier functions, and, correspondingly, 4 Bloch functions $\psi_k^{w_s,\pm}(x)$, where k is the Bloch quasi-momentum. The following one-to-one symmetry correspondence exists [3]: the symmetry of the Wannier function $(w_{s,\pm})$ fully determines the symmetry of the Bloch function $\psi_k(x)$ (even or odd) at the symmetry point $k = 0(\Gamma)$ and $k = (\pi/a)(X)$ in the Brillouin zone, and *vice versa*, given the symmetry of $\psi_k(x)$ at Γ and X (analyticity in k of the Bloch function is assumed), this fully determines the Wyckoff position and the symmetry of the Wannier function. In this letter we show that in 3 dimensions this one-to-one correspondence is, in general, no longer true. There are cases, even for simple bands, when for two Wannier functions $\psi^{(w_1)}(\boldsymbol{r})$, $\psi^{w_2}(\boldsymbol{r})$ at inequivalent symmetry centres $\boldsymbol{w}_1$ and $\boldsymbol{w}_2$ (Wyckoff positions) in the crystal, the corresponding Bloch functions $\psi_k^{(w_1)}(\boldsymbol{r})$, $\psi_k^{w_2}(\boldsymbol{r})$ have identical symmetries at all $\boldsymbol{k}$-points in the Brillouin zone. This means that the symmetry alone does not distinguish between these two Bloch functions, and in this letter we add a topological label—the Berry phase [7]—which does tell the difference between them! The Berry phase is a measurable quantity and one should be able to distinguish in the laboratory between Bloch functions with identical symmetries but with different topological labels.

A band representation $D^{(w,l)}$ of a space group G is the induced representation from the representation γ_l of the isotropy group G_w for the $\boldsymbol{w}$-Wyckoff position [11, 12, 14]. The space group can be decomposed into cosets with respect to $G_w T = \overline{G}_w$, where T is the translational group:

$$G = \overline{G}_w + (a_2 \,|\, \boldsymbol{t}_2)\,\overline{G}_w + \ldots + (a_s \,|\, \boldsymbol{t}_s)\,\overline{G}_w\,, \tag{1}$$

where the representative elements $(a_i \,|\, \boldsymbol{t}_i)$ $(i = 1, 2, ..., s)$ define the s star vectors of $\boldsymbol{w}$

$$\boldsymbol{w}_1 = \boldsymbol{w},\ \ \boldsymbol{w}_2 = (a_2 \,|\, \boldsymbol{t}_2)\,\boldsymbol{w},\ \ \ldots,\ \ \boldsymbol{w}_s = (a_s \,|\, \boldsymbol{t}_s)\,\boldsymbol{w}\,. \tag{2}$$

Let $\psi^{(w,l)}(\boldsymbol{r})$ be the basis function for the representation γ_l (assumed to be one-dimensional) of

G_w. Then by definition we have [12] (when G_w is symmorphic)

$$(\beta|\boldsymbol{w} - \beta\boldsymbol{w})\,\psi^{(w,l)}(\boldsymbol{r}) = \gamma_l(\beta)\,\psi^{(w,l)}(\boldsymbol{r}), \tag{3}$$

where $(\beta|\boldsymbol{w} - \beta\boldsymbol{w})$ is an element of G_w which consists of a point group element β and a primitive translation $\boldsymbol{w} - \beta\boldsymbol{w}$. The latter will be later denoted by $\boldsymbol{R}_\beta^{(w)} = \boldsymbol{w} - \beta\boldsymbol{w}$. All the partners for the basis of the band representation $D^{(w,l)}$ are then [11, 12]

$$\psi_i^{(w,l)}(\boldsymbol{r}) = (\alpha_i|\boldsymbol{t}_i)\,\psi^{(w,l)}(\boldsymbol{r}), \qquad i = 1, \ldots, s, \tag{4}$$

where $\psi_1^{(w,l)}(\boldsymbol{r}) \equiv \psi^{(w,l)}(\boldsymbol{r})$ (see eq. (2)). Correspondingly, one can define the quasi-Bloch functions [3, 5] for the orbitals in eqs. (3) and (4), where ($\boldsymbol{R}_m$ is a Bravais lattice vector)

$$\phi_{ik}^{(w,l)}(\boldsymbol{r}) = \sum_m \exp[i\boldsymbol{k}\cdot\boldsymbol{R}_m]\,\psi_i^{(w,l)}(\boldsymbol{r} - \boldsymbol{R}_m) = (\alpha_i|\boldsymbol{t}_i)\,\phi_{1\alpha_i^{-1}k}^{(w,l)}(\boldsymbol{r}). \tag{5}$$

In what follows, $\phi_{ik}^{(w,l)}(\boldsymbol{r})$ will be called the quasi-Bloch functions for the s branches ($i = 1, \ldots, s$) of the composite energy band.

Let us now show that each branch quasi-Bloch function $\phi_{ik}^{(w,l)}(\boldsymbol{r})$ has a well-defined symmetry and also a well-defined Berry phase. It is instructive to consider first a simple energy band, in which case there is a single branch with one quasi-Bloch function $\phi_k^{(w,l)}(\boldsymbol{r})$ (in the latter case one can also choose the Bloch function $\psi_k(\boldsymbol{r})$ for the analytical description of the band [6]). Denote by P the point group of the space group G which has to be symmorphic for the existence of single branch bands. It is easy to check that for each β of P we have (see eqs. (3) and (5))

$$\beta\phi_k^{(w,l)}(\boldsymbol{r}) = \gamma_l(\beta)\exp[i\beta\boldsymbol{k}\cdot(\boldsymbol{w} - \beta\boldsymbol{w})]\,\phi_{\beta k}^{(w,l)}(\boldsymbol{r}). \tag{6}$$

This equation determines the symmetry at all points in the Brillouin zone, or the continuity chord, of the quasi-Bloch function [5, 8]. For a fixed Wyckoff position $[\boldsymbol{w}]$ and a different representation γ_l of P, eq. (6) gives different $\gamma_l(\beta)$ and therefore different continuity chords. But it might happen that for two different Wyckoff positions $[\boldsymbol{w}]$ and $[\boldsymbol{w}']$, eq. (6) gives the same continuity chords. Examples of this kind are rare and they actually appear only in the space groups # 22 (F222) and # 196 (F23) [9, 12]. From the point of view of symmetry the bands $\phi_k^{(w,l)}(\boldsymbol{r})$ and $\phi_k^{(w',l)}(\boldsymbol{r})$ belong to equivalent band representations $D^{(w,l)}$ and $D^{(w',l)}$.

In addition to a well-defined symmetry, the branch $(\boldsymbol{w}, l)$ has also a well-defined Berry phase which is defined in the following way [7]:

$$\alpha^{(w)}(\boldsymbol{K}) = \int_{\boldsymbol{K}} \boldsymbol{X}_w(\boldsymbol{k})\cdot\mathrm{d}\boldsymbol{k}, \tag{7}$$

where the integration is on the path of a vector $\boldsymbol{K}$ of the reciprocal lattice and where

$$\boldsymbol{X}_w(\boldsymbol{k}) = i\int_{\text{u.c.}} [u_k^{(w,l)}(\boldsymbol{r})]^* \frac{\partial}{\partial\boldsymbol{k}} u_k^{(w,l)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \tag{8}$$

with the integration on a unit cell in the crystal. In eq. (8), $u_k^{(w,l)}(\boldsymbol{r})$ is the periodic part of $\phi_k^{(w,l)}(\boldsymbol{r})$. It can be shown that Berry's phase $\alpha^{(w)}(\boldsymbol{K})$ does not depend on the representation label l, and that it depends on the Wyckoff position only. By using eq. (6) and the definitions (7) and (8) one can show that the following relation holds between the Wyckoff position $\boldsymbol{w}$ and the Berry phase $\alpha^{(w)}(\boldsymbol{K})$ (ref. [7c]):

$$\alpha^{(w)}(\boldsymbol{K}) - \alpha^{(w)}(\beta^{-1}\boldsymbol{K}) = (\boldsymbol{w} - \beta\boldsymbol{w})\cdot\boldsymbol{K} = \boldsymbol{w}\cdot(\boldsymbol{K} - \beta^{-1}\boldsymbol{K}). \tag{9}$$

This equation can be written for three independent $\boldsymbol{K}$-vectors, *e.g.*, the basis vectors $\boldsymbol{K}_1$, $\boldsymbol{K}_2$

and $\boldsymbol{K}_3$ of a unit cell for the reciprocal lattice. One can then find $\alpha^{(w)}(\boldsymbol{K}_i)$, $i = 1, 2, 3$. In particular, if $\beta^{-1}\boldsymbol{K} = -\boldsymbol{K}$, it follows from eq. (9) that $\alpha^{(w)}(\boldsymbol{K}) = \boldsymbol{w}\cdot\boldsymbol{K}$. On the other hand, if $\beta^{-1}\boldsymbol{K} = \boldsymbol{K}$, then $\alpha^{(w)}(\boldsymbol{K})$ is undetermined in the corresponding $\boldsymbol{K}$-direction. This is always the case for polar point groups which consist of a single rotation axis and (or) a reflection plane containing this axis [12]. But in the latter case, also the Wyckoff position does not have a fixed value.

Consider now two equivalent band representations $D^{(w,l)}$ and $D^{(w',l)}$ for one-branch energy bands (simple energy bands) at different Wyckoff positions $[\boldsymbol{w}]$ and $[\boldsymbol{w}']$. As was pointed out above, they can belong to the space groups # 22 or # 196 only. There are 8 pairs of such band representations in # 22 (4 representations for the pair a and b Wyckoff positions, and 4 for the pair c and d) and 6 pairs in # 196 (3 representations for the pair a and b, and 3 for the pair c and d) [12]. There are altogether 14 pairs of such equivalent band representations on different Wyckoff positions. We now use eqs. (7) and (9) in order to find the Berry phases for each pair of these band representations. It is clear that a Berry phase $\alpha^{(w)}$ is defined modulo 2π. It is interesting to point out that despite the fact that for a given Wyckoff position $[w]$ the Berry phase $\alpha^{(w)}$ will depend on the choice of the origin, $\alpha^{(w)} - \alpha^{(w')}$ for two different Wyckoff positions $[\boldsymbol{w}]$ and $[\boldsymbol{w}']$ is origin independent. Thus, for the space groups F222 and F23 we have [13] $\boldsymbol{w}_b - \boldsymbol{w}_a + \boldsymbol{w}_d - \boldsymbol{w}_c = 0$ and therefore $\alpha^{(b)} - \alpha^{(a)} + \alpha^{(d)} - \alpha^{(c)} = 0$, independent of the choice of origin. The results for the Berry phases for the groups # 22 and # 196 are summarized in table I (for the group # 22, the Berry phases were already computed in ref. [7c]). We see from this table that for each pair of these equivalent band representations $D^{(a,l)}$ and $D^{(b,l)}$

TABLE I. – *Berry phases for branch quasi-Bloch functions* $\phi_k^{(w,l)}(\boldsymbol{r})$ *in the space groups* F222, F23. *The Wyckoff positions are given in column* 2. *The superscript in the quasi-Bloch function gives the Wyckoff position* $[\boldsymbol{w}]$ *and the label* l *of the irreducible representation of the isotropy group* G_w. *The Berry phases* $\alpha(\boldsymbol{K})$ (*column* 4) *are listed for the basis vectors* $\boldsymbol{K}_j$ ($j = 1, 2, 3$) *of the reciprocal lattice* (*column* 5).

Space group	Wyckoff position	Branch quasi-Bloch functions	Berry phases $\alpha(\boldsymbol{K}_1)$	$\alpha(\boldsymbol{K}_2)$	$\alpha(\boldsymbol{K}_3)$	Vectors of the reciprocal lattice
		$l = 1, 2, 3, 4$				
F222 (# 221)	$a(0\,0\,0)$	$\phi_k^{(a,l)}(\boldsymbol{r})$	0	0	0	$\boldsymbol{K}_1 = \left(\frac{2\pi}{a}, \frac{2\pi}{b}, -\frac{2\pi}{c}\right)$
	$b\left(0\,0\,\frac{c}{2}\right)$	$\phi_k^{(b,l)}(\boldsymbol{r})$	π	π	π	$\boldsymbol{K}_2 = \left(\frac{2\pi}{a}, \frac{2\pi}{b}, -\frac{2\pi}{c}\right)$
	$c\left(\frac{a}{4}\,\frac{a}{4}\,\frac{c}{4}\right)$	$\phi_k^{(c,l)}(\boldsymbol{r})$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\boldsymbol{K}_3 = \left(-\frac{2\pi}{a}, \frac{2\pi}{b}, \frac{2\pi}{c}\right)$
	$d\left(\frac{a}{4}\,\frac{a}{4}\,\frac{3c}{4}\right)$	$\phi_k^{(d,l)}(\boldsymbol{r})$	$-\frac{\pi}{2}$	$-\frac{\pi}{2}$	$-\frac{\pi}{2}$	
		$l = 1, 2, 3$				
F23 (# 196)	$a(0\,0\,0)$	$\phi_k^{(a,l)}(\boldsymbol{r})$	0	0	0	$\boldsymbol{K}_1 = \left(\frac{2\pi}{a}, \frac{2\pi}{a}, -\frac{2\pi}{a}\right)$
	$b\left(\frac{a}{2}\,\frac{a}{2}\,\frac{a}{2}\right)$	$\phi_k^{(b,l)}(\boldsymbol{r})$	π	π	π	$\boldsymbol{K}_2 = \left(-\frac{2\pi}{a}, \frac{2\pi}{a}, \frac{2\pi}{a}\right)$
	$c\left(\frac{a}{4}\,\frac{a}{4}\,\frac{a}{4}\right)$	$\phi_k^{(c,l)}(\boldsymbol{r})$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\boldsymbol{K}_3 = \left(\frac{2\pi}{a}, -\frac{2\pi}{a}, \frac{2\pi}{a}\right)$
	$d\left(\frac{3a}{4}\,\frac{3a}{4}\,\frac{3a}{4}\right)$	$\phi_k^{(d,l)}(\boldsymbol{r})$	$-\frac{\pi}{2}$	$-\frac{\pi}{2}$	$-\frac{\pi}{2}$	

(or $D^{(c,l)}$ and $D^{(d,l)}$) the Berry phases are different. This shows that in all the 14 cases the one-branch bands are physically inequivalent, despite their being equivalent according to their band symmetry. From the point of view of continuity of these bands the inequality of their Berry phases means that there is no continuous phase that connects their Bloch functions $\psi_k^{(a,l)}(\boldsymbol{r})$ with $\psi_k^{(b,l)}(\boldsymbol{r})$ (or $\psi_k^{(c,l)}(\boldsymbol{r})$ with $\psi_k^{(d,l)}(\boldsymbol{r})$). It follows therefore that there are no physically equivalent one-branch bands in solids that correspond to different Wyckoff positions!

Let us now explain our results on an example of a tight-binding approximation. In the latter case the localized $\psi^{(w,l)}(\boldsymbol{r})$ can be represented by an atomic function $A^{(w,l)}(\boldsymbol{r})$. In particular, let us consider the a and b Wyckoff positions in the F222 space groups [13]: $a = (0, 0, 0)$, $b = (0, 0, c/2)$, where c is the lattice constant in the z-direction. And for simplicity let us consider the trivial representation of the D_2-point group [15], $l = 1$. The connection between the atomic functions $A(\boldsymbol{r})$ and the corresponding Bloch functions is as follows:

$$\psi_k^{(w,1)}(\boldsymbol{r}) = \sum_{\boldsymbol{R}} \exp[i\boldsymbol{k}\cdot\boldsymbol{R}]\, A^{(w,1)}(\boldsymbol{r}-\boldsymbol{R}), \tag{10}$$

where w can be a or b, and the summation is over the Bravais lattice. By definition of the band representation, we have for $A^{(w,1)}(\boldsymbol{r})$

$$g_a A^{(a,1)}(\boldsymbol{r}) = A^{(a,1)}(\boldsymbol{r}); \qquad g_b A^{(b,1)}(\boldsymbol{r}) = A^{(b,1)}(\boldsymbol{r}); \tag{11}$$

where g_a is an element of G_a (the isotropy group of the Wyckoff position a), and, similarly, g_b is an element of G_b [9]. Let us concentrate on the rotation by π around the x-axis, U^x. In G_a this is a pure rotation, while in G_b it is $(U^x|00c)$, *e.g.*, it contains a translation by c in the z-direction. A simple calculation shows that for the Bloch functions one gets the following result (use is made of eqs. (10) and (11)):

$$U^x \psi_k^{(a,1)}(\boldsymbol{r}) = \psi_{U^x k}^{(a,1)}(\boldsymbol{r}), \qquad U^x \psi_k^{(b,1)}(\boldsymbol{r}) = \exp[-ik_z c]\, \psi_{U^x k}^{(b,1)}(\boldsymbol{r}), \tag{12}$$

where $U^x k = (k_x, -k_y, -k_z)$. Similar results can be obtained for U^y and U^z (rotations about y and z by π). One can now check that at all symmetry points in the Brillouin zone [15] the Bloch functions $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$ have identical symmetries. This means that under all the elements of the point group D_2 these two Bloch functions behave in the same way at all symmetry points in the Brillouin zone. For example, at point $Z(0, 0, 2\pi/c)$ [15], the phase factor in eq. (12) for the b-function is 1. In a similar way one can check the disappearance of this phase factor at all points in the Brillouin zone. The conclusion is that from the point of view of symmetry, the two Bloch functions $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$ are identical. However, the atomic functions $A^{(a,1)}(\boldsymbol{r})$ and $A^{(b,1)}(\boldsymbol{r})$ out of which these two Bloch functions were built (eq. (10)) have different symmetries (eq. (11)), because their symmetries are determined with respect to inequivalent Wyckoff positions a and b. The question is then whether one can distinguish between the Bloch functions $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$. As we have just shown, from the point of view of symmetry, they are identical. What we show in this letter is that the Bloch functions $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$ are distinguishable by their topologies! Namely, as follows from table I, their Berry phases are different. We come therefore to a very striking result, that there are cases of simple bands with identical symmetries of their Bloch functions, but with different topologies for them. In other words, the Bloch functions $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$ cannot be connected by a continuous k-dependent phase factor (otherwise they would have identical Berry phases):

$$\psi_k^{(b,1)}(\boldsymbol{r}) \neq \exp[i\alpha(\boldsymbol{k})]\, \psi_k^{(a,1)}(\boldsymbol{r}). \tag{13}$$

In particular, it follows from eq. (13) that $\psi_k^{(a,1)}(\boldsymbol{r})$ and $\psi_k^{(b,1)}(\boldsymbol{r})$ cannot belong to the same energy band (otherwise one would be able to connect them by a phase).

For composite energy bands we find a very rich variety of band representations that have identical symmetries for their Bloch functions, but with different Barry phases. A detailed account for composite bands will be published elsewhere.

In conclusion, topology of quasi-Bloch functions was used, in addition to their symmetry, for the introduction of the notion of physical equivalence of energy bands in solids. In a recent publication [12] a complete symmetry classification of energy bands in solids was carried out based on their band representations. By adding topology, the symmetry classification can be subdivided into physically equivalent and inequivalent energy bands. Simple bands on different Wyckoff positions are never physically equivalent. On the other hand, composite bands on different Wyckoff positions can be physically equivalent. For simple bands the following remark can be made: for them one can choose the actual Bloch functions $\psi_k^{(w,l)}(\boldsymbol{r})$ and $\psi_k^{(w',l)}(\boldsymbol{r})$ to be analytic, where $[\boldsymbol{w}]$ and $[\boldsymbol{w}']$ are different Wyckoff positions for one of the space groups F222 or F23. For a fixed l, these Bloch functions have identical symmetries; they cannot, however, describe energy bands with coinciding energies because their Berry phases $\alpha^{(w)}$ and $\alpha^{(w')}$ are different and they therefore cannot be connected by a continuous phase.

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