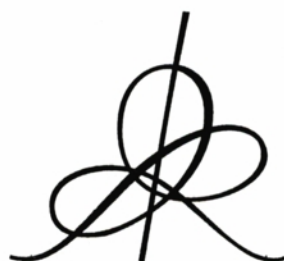


SYMMETRY AND TOPOLOGY OF ENERGY BANDS IN CRYSTALS

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§0. Introduction.

These lectures contain work carried out with Josuah Zak, at the Technion Physics department; they are the direct continuation of the previous ones given two years ago [MIC97]. They ended by the presentation of a conjecture made with J. Zak:

The graph of an elementary band is connected

and showed on an example the idea of the proof for non-symmorphic space groups; it was essentially based on the monodromy on the Brillouin zone of the unitary irreducible representations of the non-symmorphic space groups. We also explained that this idea did not work for the 73 symmorphic groups. This year we will present the basic ideas we need to complete the proof of our conjecture and show them at work on a characteristic example.

§1. Study of the symmetry of a crystal.

We will explain again the concepts appearing in this very short introduction; sometimes we will be somewhat sketchy and will refer for more details to the quoted reference of the 1996 Zajęczkovo school and even the [MIC95] 1994 Zajęczkovo lectures. Let us begin by recalling the group theory topics we shall need. We are interested by 3-dimensional or 2-dimensional crystals; however when the dimension does not need to be specified¹, we denote it by n . By definition, a basis $\{\vec{b}_j\}$, $j = 1, 2, \dots, n$, of a n -dimensional real vector space E_n generates, by addition and subtraction of vectors, a *lattice* L ; it is a group isomorphic to $Z^n \sim L$.

The group of symmetry of a crystal is called *space group* and we denote it here by G . It contains a lattice of translations which is an invariant subgroup: $L \triangleleft G$. The corresponding quotient $P = G/L$ is the point group; it is a finite group which must have a faithful representation by matrices with integral elements, i.e. it can be identified to a finite subgroup of $GL_n(Z)$. A conjugation of P in $GL_n(Z)$ corresponds simply to a change of basis of L ; so a symmetry classification is made by the different conjugacy classes of finite subgroups of $GL_n(Z)$. The crystallographers (e.g. [ITC] p. 719) call them *arithmetic classes*. There are 13, 73 of them in dimension 2,3 while these different point groups form only 10, 32 *geometric classes*², i.e. conjugacy classes in the general linear group $GL_n(R)$ or, equivalently, conjugacy classes in the orthogonal group O_n . Here, we will consider only the arithmetic classes of point groups; the standard notation for them is that of [ITC]. Each arithmetic class defines a distinct point group action on the lattice of translations; it defines also a space group: the semi-direct product $G = L \rtimes P$. The tables [ITC] use the same notation for the arithmetic classes and the corresponding 13, 73 space-groups $L \rtimes P$; they call them *symmorphic* space groups. The other 4, 157 space groups are called *non-symmorphic*; they exist in 3, 61 arithmetic classes. By definition, given an arithmetic class defined by the point group P , the space groups (in dimension 3) which satisfy:

$$P \text{ finite} < GL_3(Z); \quad L \sim Z^3 \triangleleft G; \quad G \xrightarrow{\theta} G/L = P. \quad 1(1)$$

¹ Part of crystallography in dimension 4,5,6 is useful for the study of modulated and of “quasi” crystals.

² The classification of crystals into geometric classes is sufficient for studying most macroscopic physical properties of crystals but not for their microscopic properties.

are called extensions of P by L and they belong to the same “arithmetic class of space groups”.

Many experiments on crystals (e.g. those involving the scattering of a beam of photons, electrons,...) yields Fourier transforms of functions on the space of the crystals; they are defined on the *reciprocal space* whose vectors are called quasi-momenta and are usually denoted by \vec{k} . As for the Fourier transform on our space, \vec{k} defines a unirrep (unitary irreducible linear representation) $\vec{x} \xrightarrow{\vec{k}} \exp(i\vec{k}.\vec{x})$ of the group of space translations. However the crystal symmetry contains only a lattice of translations, so there is a discrete infinity of vectors \vec{K} in the reciprocal space which define the trivial representation of L ; indeed they must satisfy the conditions:

$$\forall \ell \in L, \quad e^{i\vec{K}.\vec{\ell}} = 1 \Leftrightarrow \vec{K}.\vec{\ell} = 2\pi\nu, \quad \nu \in \mathbb{Z}. \quad 1(2)$$

The vectors \vec{K} which satisfy these conditions form the *reciprocal lattice*, i.e. the lattice $2\pi L^*$, where L^* (called dual lattice) is the lattice generated by the dual basis $\{\vec{b}_i^*\}$ of $\{\vec{b}_j\}$ defined by:

$$\vec{b}_i^*.\vec{b}_j = \delta_{ij}. \quad 1(3)$$

To summarize: the set of unirreps of the translation lattice L is the set of \vec{k} 's (reciprocal vectors modulo the reciprocal lattice); they form a group isomorphic to U_1^n and whose topology is that of a n -dimensional torus. This group is called *Brillouin zone*³ (denoted here BZ) by the solid state physicists and it is called *dual group* by the mathematicians, with the usual notation \hat{L} . We recall a natural coordinate system for L and \hat{L} :

$$L \ni \vec{t} = \sum_j n_j \vec{b}_j, \quad \hat{L} \ni \vec{k} = \sum_j k_j \vec{b}_j^*, \quad n_j \text{ integers, } k_j \bmod 2\pi, \quad \vec{k}.\vec{\ell} = \sum_j k_j n_j. \quad 1(4)$$

For any unirrep of a group it is useful to know its kernel and its image; for the unirrep \vec{k} of L we have:

$$\text{Ker } \vec{k} = \{\vec{t} \in L, \vec{k}.\vec{t} = 0\} \triangleleft L; \quad \text{Im } \vec{k} = \{e^{i\vec{k}.\vec{t}}, \vec{t} \in L\} = L / \text{Ker } \vec{k}. \quad 1(5)$$

The invariant subgroup of translations of G acts trivially on BZ , so the natural action of G on the BZ defines an effective action of the point group P ; this action depends only on the arithmetic class. We denote by $P_{\vec{k}}$ the stabilizer⁴ of \vec{k} . We will have also to consider the stabilizers $G_{\vec{k}}$ of \vec{k} by the actions of the space groups of an arithmetic class. The stabilizers $G_{\vec{k}}$ contain all translations of $L \triangleleft G$, so they are space groups which, for a given $P_{\vec{k}}$, are different subgroups of the different G 's of the arithmetic class we study.

³ There is an interesting representation of this group by the Voronoï cell of the reciprocal lattice with the opposite faces identified; we call it Brillouin cell. We shall not need it here.

⁴ Physicists often use instead the expression “little group”. We prefer stabilizer because this word indicates the definition of the concept.

Let us recall the definition of the group $P(\vec{k})$ introduced by Herring [HER42]. It is easy to show that $\text{Ker } \vec{k} \triangleleft G_k$; the Herring group is simply the quotient $P(\vec{k}) = G_k / \text{Ker } \vec{k}$. One shows easily that $P(\vec{k})$ is a central extension of P_k by $\text{Im } \vec{k}$:

$$P(\vec{k}) = G_k / \text{Ker } \vec{k} \Rightarrow \text{Im } \vec{k} \leq C(P(\vec{k})) \text{ and } P(\vec{k}) / \text{Im } \vec{k} = P_k. \quad 1(6)$$

In the particular case of a symmorphic space group G :

$$G_k = L \rtimes P_k, \text{ then } P(\vec{k}) = \text{Im } \vec{k} \times P_k. \quad 1(7)$$

Beware that the Herring group may also be of this form for non-symmorphic G or G_k .

In solid state physics one calls allowed representations of G_k those unirreps of G_k whose kernel contains $\text{Ker } \vec{k}$; so the images of the allowed representations of G_k are unirreps of the Herring group. From [SEI35] it is known that all inequivalent unirreps of the space groups are obtained by inducing the allowed unirreps of G_k ; we denote the latter by $\chi_{G_k}^{(\alpha)}$ and the corresponding unirrep of G by $\chi_G^{(k,\alpha)}$:

$$\chi_G^{(k,\alpha)} = \text{Ind}_{G_k}^G \chi_{G_k}^{(\alpha)}; \quad \dim \chi_G^{(k,\alpha)} = |G : G_k| \cdot \dim \chi_{G_k}^{(\alpha)}, \quad 1(8)$$

where $|G : G_k| = |P : P_k|$ is the index (= the number of cosets) of G_k in G and P_k in P . When there is no confusion we use the same symbols for the representations and their characters.

§2. Already known energy degeneracy in bands.

Electron bound states play a great role in physical properties of crystals. Their energy spectrum is a union of continuous segments separated by gaps. A better knowledge is obtained by the “band structure” i.e. the functions (labelled sequentially by the integer m) $E_m(\vec{k})$ of the energy over the Brillouin zone. These functions are continuous; this property is already proven in the one-electron Schrödinger problem with a potential which has the symmetry of the space group G e.g. [BOU36]. Note that the derivative may have discontinuities (a general study was made in [VHO53]) for the mathematically similar problem of the vibration spectra). The set of these energy curves must be invariant by the space group G of the crystal; beware that each curve separately need not to have this symmetry.

When we consider a given point \vec{k} of the Brillouin zone, the one electron Schrödinger problem has symmetry G_k ; its study is similar to that of a molecule. The Hamiltonian commutes with G_k and the space of its eigenfunctions carries a unitary representation χ_{G_k} whose decomposition into unirreps give quantum numbers for the electron states. To an unirrep $\chi_{G_k}^{(\alpha)}$ of dimension d corresponds a degeneracy of d states with the same energy. What is different in crystals is the continuity of the energy on BZ and the topology of BZ itself. There exists in a neighbourhood $\mathcal{V}(\vec{k}_{(0)}) \subset BZ$ of a given $\vec{k}_{(0)}$ such that the groups G_k ’s are, up to a conjugation, subgroups of $G_{k_{(0)}}$ (that we also denote by $\leq G_{k_{(0)}}$) and [BOU36] established the “compatibility conditions”:

$$\vec{k} \in \mathcal{V}(\vec{k}_{(0)}) \subset BZ \Rightarrow \chi_{G_k} \subseteq \text{Res}_{G_k}^{G_{k_{(0)}}} \chi_{G_{k_{(0)}}}, \quad 2(1)$$

where Res means “restriction of the group representation to the subgroup” and \subseteq indicates a direct sum of components appearing in the decomposition into unirreps of the representation to which it applies.

The electron bound states of an energy band are invariant under time reversal \mathcal{T} . This symmetry changes \vec{k} into $-\vec{k}$. The \mathcal{T} invariant points of BZ are not only the C-element of this group, but all elements which satisfy:

$$\vec{k} \equiv -\vec{k} \bmod 2\pi L^* \Leftrightarrow 2\vec{k} \equiv 0 \bmod 2\pi L^* \Leftrightarrow 2k_j \equiv 0 \bmod 2\pi \Leftrightarrow k_j = 0 \text{ or } \pi \bmod 2\pi \quad 2(2)$$

in any coordinate system of type 1(4); so there are, including 0, eight such points of the BZ . For them the *co-stabilizer* $\tilde{G}_k = \langle G_k, \mathcal{T} \rangle$ is generated by G_k and \mathcal{T} . The physical representation of \tilde{G}_k uses an antiunitary operator for \mathcal{T} and it is called a *corepresentation*. If the d -dimensional unirrep $\chi_{G_k}^{(\alpha)}$ is not equivalent to a real representation, the irreducible corepresentation, $\chi_{G_k}^{(\alpha)} \oplus \bar{\chi}_{G_k}^{(\alpha)}$, has double dimension, so time reversal introduces a new type of degeneracy. Herring, in [HER37]a, studied the more general case in which \tilde{G}_k is generated by G_k and a product $r\mathcal{T}$, $r \in G_k$ and obtained a nearly complete set⁵ of the degeneracies occurring for specified \vec{k} . In the second part of his thesis, [HER37]b, Herring studied the accidental degeneracies⁶. He showed that they can be moved by modifying the potential in the Schrödinger equation; physically that can be obtained by varying the pressure, temperature, etc... (or moving in a column of the Mendeleev table). That explains the reversible transition from metal (with accidental degeneracy between two bands) to insulator (in which the degeneracy is removed).

In [MIC97], fig. 2 we showed an example of removable accidental degeneracy. In this paper we shall show that symmorphic group symmetry may require a new type of accidental degeneracies: they can be moved but not removed!

§3. Elementary energy bands of a crystal.

Obviously, the first step for studying the complicated “band structures” obtained in experiments is to try to decompose them into simpler systems by “removing” the accidental degeneracies until one obtains “indecomposable elements” which are so simple that one can classify them. It is a long story partly told in [MIC97]; here we just recall very few steps. There has been a feeling that the quantum numbers of band representations (i.e. the G representation acting on the Hilbert space spanned by the wave functions of the infinite set of bound states belonging to a band) were related to the quantum numbers of the electronic states of the atoms but it became clear on examples that this was not always true. For the similar case of vibration spectra, a straightforward generalisation of the problem for molecules [BUR61] showed that band representations of G are induced

⁵ For instance when r is a screw rotation 2_1 (of angle π) around an axis defined by $\vec{k} \neq 0$, $2\vec{k} \equiv 0$, then \vec{k} is the center of a face of the Brillouin cell and the degeneracy extends to the whole face.

⁶ In general these degeneracies occur on a two dimensional subspace of BZ . Indeed the energy function over BZ of a branch is represented by a 3-dimensional hypersurface in a 4 dimensional space; so the intersection of two function graphs is most often of dimension 2 when it occurs.

from a the vector representation of the stabilizers G_q of the atom positions⁷. For the electron energy bands, their band representations could be induced from any representation $\chi_{G_q}^{(\rho)}$ of the stabilizer G_q of any point of space. For example, this was consider by de Cloizeaux [CLO63]; moreover in p. 561 of this paper he gave the obvious definition for the indecomposable multi-branch bands: *their energy graph should always be connected*. In 1980, as “building bricks in the symmetry definition of bands in solids”, Zak proposed in [ZAK80], *the band representations which cannot be decomposed into a direct sum of band representations*. We call them the *elementary band representations* and we simply say that they give the symmetry of *elementary bands*. Moreover Zak established the natural necessary conditions that elementary band representations must satisfy: they are induced from *irreducible representations of a stabiliser $G_q < G$ maximal among those of the points of space*⁸. These necessary conditions are not sufficient. In [BAC88] we established the complete classification of elementary band representations. All band representations satisfying the necessary conditions are elementary except 40 of them belonging to 25 space groups: they all occur for the two dimensional representations of 7 stabilisers G_q (out of 73)

$$P422, P\bar{4}m2, P\bar{4}2m, R32, P321, P312, P622. \quad 3(1)$$

Among the elementary band representations there are 152 equivalent pairs: 57 at the same q and 95 at different q 's. Among the last ones, 63 occur for all G_q unirreps of 17 pairs of Wyckoff positions in 14 space groups. For this last class of equivalent representations a (Berry phase like) topological invariant seems⁹ to distinguish them [MIC92].

Those results have been obtained with the assumption that Frobenius reciprocity is still valid for the band representations although they are infinite dimensional induced representations¹⁰. In that case we have only to study the restriction $\text{Res}_{G_q}^G \chi_G^{(k,\alpha)}$; its components on the different unirreps of G_q are

$$\text{Res}_{G_q}^G \chi_G^{(k,\alpha)} = \oplus_{\rho} m_{q,\rho}^{k,\alpha} \chi_{G_q}^{(\rho)}; \quad m_{q,\rho}^{k,\alpha} = \langle \text{Res}_{G_q}^G \chi_G^{(k,\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q}, \text{ integer } \geq 0. \quad 3(2)$$

The unirreps of G and of G_q are finite dimensional and well known to physicists; so we can compute easily the coefficient $m_{q,\rho}^{k,\alpha}$. We have shown that G_k is the symmetry group of the problem at each point $\vec{k} \in BZ$. It is very interesting to introduce the local symmetry group on BZ G_k in the expression giving $m_{q,\rho}^{k,\alpha}$; we simply replace in 3(2) $\chi_G^{(k,\alpha)}$ by its expression given in 1(8)):

$$m_{q,\rho}^{k,\alpha} = \langle \text{Res}_{G_q}^G \text{Ind}_{G_k}^G \chi_{G_k}^{(\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q}. \quad 3(3)$$

⁷ That is less clear for some molecular crystals.

⁸ All strata of the G action on space of the 17, 230 space groups are tabulated in [ITC] under the heading “Wyckoff position”. The G_q selected by Zak are those of the strata with maximal symmetry. They are the maximal finite subgroups of G . The corresponding strata are topologically closed.

⁹ See also P. Zeiner, R. Dirl and B.L. Davies: “Generalized Berry Phases” in these proceedings.

¹⁰ We do not know a relevant mathematical reference justifying this assumption. The usual mathematical theory for the induced representations of locally compact groups is measure theoretic and do not take in account the analyticity properties that we meet in this physical problem.

To find the value of these coefficients we use a relation due to Mackey which tells how to commute *Res* and *Ind* (see e.g. [SER67] §7.4 and §7.5). Before introducing it, we have to recall very elementary facts on groups.

Let H, K be subgroups of a group G . We denote by HK the set of G elements obtained by multiplying any element of H by any element of K . We leave to the reader the easy proof of

Proposition 1. H, K subgroups of G and $HK = KH \Rightarrow HK$ is a subgroup of G .

From the definition of invariant subgroup, $K \triangleleft G, \Leftrightarrow \forall s \in G, sK = Ks$, we have as corollary of proposition 1:

Corollary 1. H subgroup of G , K invariant subgroup of $G \Rightarrow HK = KH$ and, by proposition 1, it is a subgroup of G .

We denote by $G : H$ the set of (left-) cosets of H in G and by $|G : H|$ their number.

For a space group G we will have to use the double cosets of G for G_q and G_k ; they are the subsets $G_q s G_k \subset G$ for arbitrary $s \in G$. We denote by $G_q : G : G_k$ the set of distinct double cosets; to be in the same double coset is an equivalence relation¹¹, so we can choose a set of representative of cosets (with 1 for $G_q G_k$) that we denote by $[G_q : G : G_k]$.

Since $L \triangleleft G$, from corollary 1, $LG_q = G_q L$ is a subgroups of G ; remark that LG_q is itself a symmorphic space group. We also verify easily that $LG_q : G : G_k = G_q : G : G_k$. Finally we remark that if either LG_q or G_k are invariant subgroups¹² of G then $G_q G_k$ is a G subgroup and $LG_q s G_k$ is either $s G_q G_k$ or $G_q G_k s$; i.e; the double cosets become cosets of the subgroup $G_q G_k$ in G .

To permute *Res* and *Ind* in 3(3) we will have first to restrict the representation $\chi_{G_k}^{(\alpha)}$ to a subgroup $K < G_k$ and induce this representation from a conjugate subgroup $s K s^{-1} < G_q$ to G_q . This is possible by choosing successively s in the different double cosets $G_q : G : G_k$. With the definition $K_s = G_k \cap s^{-1} G_q s$, starting from 3(2), Mackey's formula yields:

$$\begin{aligned} m_{q,\rho}^{k,\alpha} &= \langle \text{Res}_{G_q}^G \text{Ind}_{G_k}^G \chi_{G_k}^{(\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q} = \sum_{s \in [G_q : G : G_k]} \langle \text{Ind}_{s K_s s^{-1}}^{G_q} \text{Res}_{K_s}^{G_k} \chi_{G_k}^{(\alpha)} | \chi_{G_q}^{(\rho)} \rangle_{G_q} = \\ &= \sum_s \langle \text{Res}_{K_s}^{G_k} \chi_{G_k}^{(\alpha)} | \text{Res}_{s K_s s^{-1}}^{G_q} \chi_{G_q}^{(\rho)} \rangle_{K_s} = \sum_s |K_s|^{-1} \sum_{g \in K_s} \bar{\chi}_{G_k}^{(\alpha)}(g) \chi_{G_q}^{(\rho)}(s g s^{-1}) \end{aligned} \quad 3(4)$$

For instance on the generic stratum of the BZ , $P_k = 1$ so $G_k = L$ and 3(4) gives simply:

$$b = \text{number of branches of the band} = \frac{|P|}{|G_q|} \dim \chi_{G_q}^{(\rho)}. \quad 3(5)$$

When $\vec{k} = 0$, $P_0 = P$, so $G_0 = G$; the translations are represented trivially, so the allowed unirreps of $G_0 = G$ are simply the P -unirreps. Then 3(3) gives the well known result:

$$\text{with } P_q \stackrel{\text{def}}{=} \theta(G_q) \sim G_q, \quad m_{q,\rho}^{0,\alpha} = \langle \text{Res}_{P_q}^P \chi_P^{(\alpha)} | \chi_{P_q}^{(\rho)} \rangle_{P_q} = \langle \chi_P^{(\alpha)} | \text{Ind}_{P_q}^P \chi_{P_q}^{(\rho)} \rangle_P \quad 3(6)$$

¹¹ Indeed, let us study the double cosets $H : G : K$ with $s, s_1, s_2 \in G, h, h' \in H, k, k' \in K$. If $s_1 = h s k$, then $s = h^{-1} s_1 k^{-1}$; moreover if $s_2 = h' s_1 k'$ then $s_2 = h' h s k k'$.

¹² Equivalently: either $P_q = \theta(G_q)$ or P_k are invariant subgroups of P .

In §5 we will need the case (solved by 3(4)):

$$G_q G_k = G, \quad G_q \cap G_k = 1 \Rightarrow m_{q,\rho}^{k,\alpha} = (\dim \chi_{G_q}^{(\rho)}) (\dim \chi_{G_k}^{(\alpha)}). \quad 3(7)$$

§4. The monodromy over BZ of the unirreps of non-symmorphic space groups.

We refer again to [MIC97] for more details. We want first to give here more equivalent definitions of the *non-symmorphic elements* of a space group. For this we first reproduce here what was said about the Euclidean group. To write the group law of the of the Euclidean group $Eu_n = R^n \rtimes O_n$, we choose an origin o in the Euclidean space \mathcal{E}_n . Then every point $x \in \mathcal{E}_n$ can be labelled by the vector \vec{x} which translates o to x . Then every element of Eu_n can be written as the product of first, an orthogonal transformation A and second, of a translation \vec{s} . We write such an element $\{\vec{s}, A\}$. Its action on the point $x \in \mathcal{E}_n$ is:

$$\{\vec{s}, A\}.\vec{x} = \vec{s} + A\vec{x}. \quad A(1)$$

The group law of the semi-direct product: $Eu_n = R^n \rtimes O_n$ is:

$$\{\vec{s}, A\}\{\vec{t}, B\} = \{\vec{s} + A\vec{t}, AB\}, \quad \{\vec{s}, A\}^{-1} = \{-A^{-1}\vec{s}, A^{-1}\} \quad A(2)$$

To obtain the form of the elements of Eu_n with the origin o' of coordinate we conjugate the elements by the translation $\vec{o}o$. Explicitly the conjugation by the translation \vec{t} gives:

$$\{\vec{t}, I\}\{\vec{s}, A\}\{-\vec{t}, I\} = \{D_A\vec{t} + \vec{s}, A\}, \quad \text{with } D_A = I - A. \quad 4(1)$$

From A(1) we obtain the condition for x to be fixed point of $\{\vec{s}, A\}$:

$$\{\vec{s}, A\}\vec{x} = \vec{x} \Leftrightarrow \vec{s} = (I - A)\vec{x}, \quad \text{i.e. } \vec{s} \in \text{Im } D_A. \quad 4(2)$$

When this condition is satisfied, 4(1) shows that by a change of origin we can transform $\{\vec{s}, A\}$ into $\{0, A\}$. It is a trivial remark to say that any non trivial coset of translations in Eu_n contains elements with fixed points; that is no longer trivial for a space group since the subgroup of translations, L , is discrete and it leads us to make the

Definition: In a space group G , if no elements of a translation coset $gL = Lg$ leaves fix a point of space, the coset elements are called *non-symmorphic*¹³.

Since the space groups are subgroups of Eu_n , the orthogonal component A of an element of a space group is defined; it has a finite order ν (it is the smallest positive integer such that $A^\nu = I$). it is useful to introduce the Herbrand operator N_A (acting on the real vector space E_n):

$$\text{order}(A) = \nu, \quad N_A = I + A + A^2 + \dots + A^{\nu-1} = \sum_{j=0}^{\nu-1} A^j; \quad AN_A = N_A = N_A A. \quad 4(3)$$

¹³ That corrects the definition made in [MIC97] before 1(10) which was too weak in some cases.

With D_A defined in 4(2) we have the relations:

$$N_A D_A = 0 = D_A N_A \Leftrightarrow \text{Im } D_A \subseteq \text{Ker } N_A, \text{Im } N_A \subseteq \text{Ker } D_A. \quad 4(4)$$

By definition $\text{Ker } D_A$ is the eigen space of A with the eigenvalue 1; for any vector \vec{v} in this eigenspace $N_A \vec{v} = \nu \vec{v}$, so from 4(4), $\text{Im } N_A = \text{Ker } D_A$. For any linear operator X on E_n we have $\dim \text{Ker } X + \dim \text{Im } X = n$. With 4(4) we can finally write:

$$\text{Ker } D_A = \text{Im } N_A, \quad \text{Im } D_A = \text{Ker } N_A. \quad 4(5)$$

Let $\{\vec{v}(A), A\}$ be an element of the space group G written as an element of the Euclidean group for a choice of origin. Then

$$\text{order}(A) = \nu, \quad G \ni \{\vec{v}(A), A\}^\nu = \{N_A \vec{v}(A), I\} \Leftrightarrow N_A \vec{v}(A) \in L. \quad 4(6)$$

With 4(3) and the last equality of 4(5) we have proven:

Proposition 2. *The element $\{\vec{v}(A), A\} \in G$ has a fix point for its action on the Euclidean space if, and only if $N_A \vec{v}(A) = 0$.*

Indeed if $\{\vec{v}(A), A\}$ has a fix point, it is also fixed for $\{\vec{v}(A), A\}^\nu = \{N_A \vec{v}(A), I\}$; if $N_A \vec{v}(A) \neq 0$, it is a translation and it cannot have a fix point. We can now give a test for determining the non-symmorphic elements of a space group G .

Corollary 2. *The element $\{\vec{v}(A), A\} \in G$ is non-symmorphic if, and only if, $N_A \vec{v}(A) \notin N_A L$.*

Indeed this requires $N_A \vec{v}(A) \neq 0$; assume on the contrary that there exists $\vec{\ell} \in L$ such that $N_A \vec{v}(A) = N_A \vec{\ell}$; that is equivalent to say, from proposition 2 that $\{\vec{v}(A) - \vec{\ell}, A\}$ has a fix point and therefore $\{\vec{v}(A), A\}$ which is in the same L coset, is not non-symmorphic. In the appendix we study the nature of the non-symmorphic elements.

So if a space group has a L -coset of non symmorphic elements, it cannot have a stabilizer isomorphic to the point group P ; hence this space group is non-symmorphic. Indeed, from the definition of a symmorphic group as semi-direct product $L \rtimes P$, it has P as a subgroup and stabiliser. Note that the converse is not true: among the 157 non-symmorphic groups, there exist two: $I2_12_12_1$ and $I2_13$ without non-symmorphic elements.

The fact that the power ν of a non-symmorphic element $r \in G$ is a pure translation is the key of the monodromy of the unirreps of G_k when \vec{k} is in the reciprocal direction of $N_A \vec{v}(A) = \vec{t}$. Then G_k is Abelian so its unirreps are one dimensional. We can choose the shortest (up to a sign) lattice vector \vec{b} colinear to \vec{t} as basis vector; the component of \vec{t} is μ satisfying $1 \leq \mu < \nu$. Let k' be the corresponding component of \vec{k} . Then the translation \vec{t} is represented by $\exp(ik'\mu)$ for all the G_k unirreps and r is represented by $\exp i(2\pi\rho + k'\mu)/\nu$ where $\rho \equiv 0, 1, \dots, \nu - 1, \text{mod } \nu$ labels the ν inequivalent unirreps of G_k . When k' goes a full period, parametrizing the circle Γ on BZ , r is represented by $\exp i(2\pi\rho + (k' + 2\pi)\mu)/\nu = \exp i(2\pi(\rho + \mu) + k'\mu)/\nu$. In plain words, after each turn on Γ the ν unirreps of G_k , which are labelled by ρ , have been permuted according to $\rho \mapsto \rho + \mu$. After ν turns the cycle of permutation is closed and the number of permutation orbits is

equal to the greatest common divisor of μ and ν . This monodromy phenomenon for the unirreps of G_k and G over BZ was discovered by Herring in the paper [HER42] in which he made the first computation of the allowed unirreps of G_k and the unirreps of G for two non-symmorphic space groups: that of diamond, $Fm\bar{3}d$, and that of the closed hexagonal packing, $P6_3/mmc$.

This monodromy phenomenon is the essential tool for proving for 155 non-symmorphic groups our conjecture on the connexion of the branches of elementary bands, as we showed on simple examples in the 1996 lectures [MIC97]: the representation of G_k for an elementary band is the direct sum of those belonging to a monodromy orbit. The points of contact are those imposed by time reversal. It is easy to see on the examples we have studied that these symmetry conditions alone are not sufficient for proving the connection of all branches. However, the usual symmetry conditions are sufficient for the proof of the conjecture for the two non-symmorphic space groups without non-symmorphic elements ($I2_12_12_1$ and $I2_13$) as shown in a paper with Zak (to be published in Phys. Rev.).

§5. Proof of the conjecture for the 73 symmorphic groups.

The symmetry under the space group G and time reversal \mathcal{T} are sufficient in some cases. For instance for the bands with $G_q \sim P$; their number of branches is $b = \dim \chi_{G_q}^{(\rho)}$. This is the dimension of the representation of $G_k = G$ at the BZ point $\vec{k} = 0$ (see 3(6), so the b branches meet at this point.

Among the 34 Abelian arithmetic classes, there are 19 corresponding symmorphic groups:

$$\begin{aligned} P1, P\bar{1}, P2, C2, Pm, Cm, P2/m, P222, F222, I222, Pmm2, Amm2, Imm2, \\ Pmmm, P\bar{4}, I\bar{4}, P3, R3, P\bar{6}, \end{aligned} \tag{5(1)}$$

with all maximal stabilizers satisfying $G_q \sim P$. So they have only simple (= one-branch) elementary bands. There are also 8 non-Abelian symmorphic groups with only $G_q \sim P$ maximal stabilizers. They are:

$$I\bar{4}m2, P312, R32, P3m1, R3m, P\bar{6}m2, F23, F\bar{4}3m. \tag{5(2)}$$

The number of branches of each of their elementary bands is $\dim \chi_{G_q}^{(\rho)}$ and these branches meet on BZ at $\vec{k} = 0$. For the 46 other symmorphic space groups we have to study the elementary bands corresponding to their 97 Wyckoff positions with $\theta(G_q) = P_q < P$.

We begin first by a simplest case of two branch bands for which time reversal is sufficient for requiring a contact between them. We consider the space group $p4$ in 2 dimensions. The point group is the cyclic group $Z_4(R)$ with $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ (the rotation by $\pi/2$). The maximal stabilizers and the corresponding Wyckoff positions are:

$$Z_4(R) : a = \begin{pmatrix} 0 \\ 0 \end{pmatrix}; \quad Z_4(\beta) : b = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}; \quad Z_2(\gamma) : c = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \quad c' = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$$

$$\beta = \{\vec{\ell}, R\}, \gamma = \{\vec{\ell}, R^2\}, \vec{\ell} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad 5(3)$$

To the Wyckoff position c correspond two elementary bands: (c, ζ) with $\zeta(\gamma) = \pm 1$ which labels the two representations ¹⁴ of the stabilizer $G_c = Z_2(\gamma)$.

Similarly the points of maximal symmetry on BZ and their stabilizers G_k (which are space groups) are:

$$G_A = p4 : A = \begin{pmatrix} 0 \\ 0 \end{pmatrix}; \quad G_B = p4 : B = \begin{pmatrix} \pi \\ \pi \end{pmatrix}; \quad G_C = p2 : C = \begin{pmatrix} \pi \\ 0 \end{pmatrix}, \quad C' = \begin{pmatrix} 0 \\ \pi \end{pmatrix}. \quad 5(4)$$

As we know from 3(6), the allowed unirreps of $G_A = G$ are the four unirreps of the point group. We label them by $\rho \equiv 0, 1, 2, 3, \text{mod } 4$ and define them by $\rho(R) = \exp i2\pi\rho/4 = i^\rho$. Since the translations are trivially represented, $\rho(\gamma) = \rho(R^2) = (-1)^\rho$ we deduce that the two branches of the elementary band $(c, 1)$ have the G_k symmetry $\rho = 0, 2$ and that of the elementary band $(c, -1)$, the G_k symmetry $\rho = 1, 3$. By time reversal these two complex representations $\rho = 1, 3$ form a unique corepresentation, which implies the contact of the two branches of $(c, -1)$ at the point $\vec{k} = 0$ of BZ .

The 4 allowed representations of G_B have the same translation part and we keep for them the same label ρ ; it is easy to compute

$$\vec{t} = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix}, \quad \rho(\vec{t}) = (-1)^{n_1+n_2}, \quad \rho(R) = i^\rho \Rightarrow \rho(\gamma) = -(-1)^\rho. \quad 5(5)$$

The two bands of the elementary band representation $(c, 1)$ have the symmetry of the complex conjugate G_k representations $\rho = 1, 3$: so they meet on BZ at the point B of coordinates (π, π) . That concludes the proof for the group $p4$. To transpose the proof to the space group $P4$ in 3 dimensions, is trivial. Instead of points, the Wyckoff positions are axes parallel to the third basis axis; but the stabilizer G_q does not depend on the third coordinate of q . Similarly, on the Brillouin zone, the high symmetry strata are circles instead of points, e.g. $A = (0, 0, k_3)$, $B = (0, 0, k_3)$. The same results are obtained for $k_3 = 0$ or π (that is sufficient for the proof) while, for the other values of k_3 time reversal does not require contact between the two branches of one of the (c, ζ) bands.

We emphasize the phenomena of change of sign of ζ between A and B is quite general. It is due to the fact that $\gamma \in G_c$ contains the translation $\vec{\ell}$. To contain a translation has to be so for some elements of every stabilizer G_q when q is not the origin; the change of sign also depends on the choice of the pairs of \vec{k} on BZ .

We will treat now an exemple which seems hopeless from the knowledge of occurrence of degeneracies recalled in §2: P is Abelian so all $P(\vec{k})$ are Abelian, hence all G_k allowed unirreps are one dimensional; moreover they are all real at the BZ points $2\vec{k} = 0$ and no time reversal degeneracy appears. However, we will establish the proof by the only use of the compatibility relations 2(1) explained in [BOU36]; remark that we will use them not only “locally” but also “globally” .

¹⁴ We can choose arbitrarily one point of a Wyckoff position; the other points give the same results.

The simplest such example is the 2-dimensional space group $cmm2$: in the basis of two vectors of the same norm, we list the matrices of the four elements of the point group P and their characters for the four 1-dimensional unirreps of this Abelian group:

$$I_2, -I_2, cm = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, cm' = -cm; \quad \rho(I_2) = 1, \quad \rho(-I_2) = \xi, \quad \rho(cm) = \eta, \quad \rho(-cm) = \xi\eta; \\ \xi^2 = 1 = \eta^2; \quad 5(6)$$

i.e. the four unirreps ρ are labelled by a pair of signs ξ, η . The only Wyckoff position generating multi-branch elementary bands is labelled c in [ITC]:

$$c = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \quad c' = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \quad G_c = Z_2(\gamma), \quad \gamma = \{\vec{\ell}, -I_2\}, \quad \vec{\ell} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad 5(7)$$

We label the two elementary bands (c, ζ) where $\zeta(\gamma) = \zeta = \pm 1$; each one has two branches. In BZ with the dual basis (see 1(3)), we will use the two points A, B whose coordinates mod 2π are $A : (0, 0)$, $B : (\pi, \pi)$ and two closed curves $M : (k, k)$ and $M' : (k, -k)$ which correspond to the 2 symmetry axes of the lattice and of the reciprocal lattice. These curves meet¹⁵ at A and B . The corresponding P_k 's are $P_A = P_B = P$, $P_M = Z_2(cm)$ and $P_{M'} = Z_2(-cm)$. We denote by σ, σ' the unirreps of $P_M, P_{M'}$ and label them by the value ± 1 of $\sigma = \sigma(cm)$, $\sigma' = \sigma'(-cm)$. We recall from 1(7) that the unirreps of G_k are given by $\text{Im } \vec{k}$ for the translations and by those of P_k . By the restriction of the unirreps of G_k for A, B we obtain that the two branches of the elementary band (c, ζ) belong to the unirreps

$$\text{at } A : (\xi = \zeta, \eta), \quad \text{at } B : (\xi = -\zeta, \eta). \quad 5(8)$$

On the axes M and M' , we are exactly on the case $G_q G_k = G$, $G_q \cap G_k = 1$, studied in 3(7), so $m_{c, \zeta}^{M, \sigma} = 1$, i.e. the two unirreps σ of P_M and σ' of $P_{M'}$ are the symmetry of the two branches over these lines of BZ , for each elementary band (c, ζ) . But σ and σ' must satisfy the compatibility conditions 2(1); we use 5(6)) for the notations and incorporate the results of 5(8):

$$\text{at } A : \sigma = \eta, \quad \sigma' = \xi\eta = \zeta\eta; \quad \text{at } B : \sigma = \eta, \quad \sigma' = \xi\eta = -\zeta\eta. \quad 5(9)$$

The change of sign for σ' is the crux of the proof; indeed in table 1 we follow each branch for each elementary band $(c, \pm 1)$ by giving the value of their quantum numbers.

Table 1 shows that for each of the two elementary bands $(c, \pm 1)$, each branch starts from one state at the point A of BZ and after a full turn on the closed path (A, M, B, M', A) it reaches the other state at A ; so *their must be a point of the cycle at which the two bands cross. That proves the connexion of the two branches.* A second turn completes the full cycle.

¹⁵ Moreover we can check that the closed curve $AMBM'A$ cannot be shrunk to a point by continuous deformation.

band	A	M	B	M'	A	M	B	M'	A
(c, ζ)	$\xi\eta$	σ	$\xi\eta$	σ'	$\xi\eta$	σ	$\xi\eta$	σ'	$\xi\eta$
$(c, 1)$	++	+	-+	-	+-	-	--	+	++
	+-	-	--	+	++	+	-+	-	+-
$(c, -1)$	-+	+	++	+	--	-	+-	-	-+
	--	-	+-	-	-+	+	++	+	--

Table 1. Connexion of the two branch elementary bands of $cm\bar{m}2$.

For each of the two elementary bands $(c, \pm 1)$ each branch starts from one state at the point A of BZ and after a full turn on the closed path (A, M, B, M', A) it reaches the other state at A ; so *their must be a point of the cycle at which the two bands cross*. A second turn completes the full cycle.

The stability of a crossing under perturbation in quantum theory has been studied by von Neumann and Wigner [NEU29]; the instability is due to the possibility of an off diagonal term between the two bound states. In the present case the two states have opposite parity, so the crossings are stable.

We emphasize that this contact is imposed by symmetry but its position on the closed cycle is not determined by symmetry. By varying the potential in the Schrödinger equation, **this contact can be moved but it cannot be removed!** This is a completely new concept in band theory.

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§6. References.

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§7. Appendix: Non-symmorphic elements.

The aim of this appendix is to establish the list of non-symmorphic elements in dimension 2 and 3. As elements of the Euclidean group, these elements can be written $\{\vec{v}(A), A\}$. From Corollary 2 they must satisfy:

$$L \ni N_A \vec{v}(A) \notin N_A L. \quad A(1)$$

This requires $N_A \vec{v}(A) \neq 0$. From 4(4) and 4(2) this is impossible if $\text{Im } N_A \subseteq \text{Ker } D_A = 0$ which is the case when A has no eigenvalue $=1$. From the list of arithmetic elements given in [MIC95] equ. 2(31), 4(5) this eliminates (outside the trivial elements $p1, P1$) the rotations $p2, p3, p4, p6$ for $d = 2$ and $P\bar{1}, P\bar{3}, P\bar{4}, P\bar{6}, R\bar{3}, I\bar{4}$ for $d=3$; indeed, each of these arithmetic elements does not leave invariant a vector $\neq 0$.

Equation A(1) eliminates also $cm, C2, R3$. For cm : $N_{cm} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$; then the vectors $N_{cm} \vec{v}(cm)$ are of the form $\begin{pmatrix} m \\ m \end{pmatrix}$ with m integer. But these vectors are in $N_{cm} L$; indeed $N_{cm} \begin{pmatrix} 0 \\ m \end{pmatrix} = \begin{pmatrix} m \\ m \end{pmatrix}$. For $C2, R3$:

$$C2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad L \cap \text{Im } N_{C2} = \left\{ \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}, m \in \mathbb{Z} \right\}, \quad N_{C2} \begin{pmatrix} m \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}. \quad A(2)$$

So, for instance, the arithmetic classes $C2, C2/m$ have no non-symmorphic space groups. Note that in the non-symmorphic space group $C222_1$ which contains 3 rotations by π around three orthogonal axis, the first two are of C type but the last one is the non-symmorphic elements $P2_1$. The space groups of Bravais classes I contain $C2$ but the two whose symbols contains 2_1 , i.e. $I2_12_12_1$ and $I2_13$ have none non-symmorphic elements; that was a (non explicitly explained) way for the [ICT] to signal that these groups had no

fixed point $G_q = P$ so there is no origin for which all $\vec{v}(A)$ can be simultaneously removed (note that $I2_13$ is automorphism group of $I2_12_12_1$).

$$R3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad L \cap \text{Im } N_{R3} = \left\{ \begin{pmatrix} m \\ m \\ m \end{pmatrix}, m \in Z \right\}, \quad N_{R3} \begin{pmatrix} m \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m \\ m \\ m \end{pmatrix}. \quad A(3)$$

So the only arithmetic elements which can produce non-symmorphic elements are $pm, P2, P3, P4, P6, I4, Pm, Cm$ (8 out of $7+16=23$). Let us begin by the first five of them. They have a 1-dimensional eigenspace with the eigenvalue 1, i.e; $\text{Im } N_A = \text{Ker } D_A$ are an axis. It contains a 1-dimensional sublattice generated by the lattice vector \vec{b} (we choose arbitrarily its sign); so $N_A \vec{v}(A) = \mu \vec{b}$. For these p, P lattices, this axis of fix points is orthogonal to $\text{Ker } N_A = \text{Im } D_A$; by a choice of origin of coordinates we can bring to zero the component of $\vec{v}(A)$ in $\text{Im } D_A$, so it becomes $\vec{v}(A) = \nu^{-1} \mu \vec{b}$. On the other hand $N_A L = \{\nu m \vec{b}, m \in Z\}$. So we obtain the complete solutions of A(1) for these five cases:

$$A = pm, P2, P3, P4, P6, \quad \vec{v}(A) = \frac{\mu}{\nu} \vec{b}, \quad 0 < \mu < \nu. \quad A(4)$$

Explicitly this gives the following 13 non-symmorphic elements in the notation of [ITC]:

$$pg, Pc, P2_1, P3_1 \sim P3_2, P4_1 \sim P4_3, P4_2, P6_1 \sim P6_5, P6_2 \sim P6_4, P6_3. \quad A(5)$$

The case of the arithmetic element Pm is similar: $\text{Im } N_{Pm} = \text{Ker } D_{Pm} \perp \text{Ker } N_{Pm} = \text{Im } D_{Pm}$ but $\dim \text{Im } N_{Pm} = 2$. Hence $L \cap \text{Im } N_{Pm}$ is a two dimensional lattice; we say that a vector $\vec{\ell}$ of this lattice is *visible* if no vector $m^{-1} \vec{\ell}$, $1 < m \in Z$ is a lattice vector; in other words $\vec{\ell}$ belong to the $GL_2(Z)$ orbit of vectors which can be basis vectors. Then $\vec{v}(Pm) = \frac{1}{2} \vec{\ell}$. This non-symmorphic element is denoted by Pc but also one of the following: Pa, Pb, Pd, Pn ; indeed if the point group has more than two elements, the direction of the glide vector $\vec{v}(Pm)$ is constrained by the preferred directions of the other point group elements. We refer to [ICT] for the definition of the symbols a, b, c, d, n following P .

Case Cm :

$$Cm = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad L \cap \text{Im } N_{Cm} = \left\{ \begin{pmatrix} m \\ m \\ n \end{pmatrix}, m, n \in Z \right\}, \quad N_{Cm} \begin{pmatrix} m \\ 0 \\ n \end{pmatrix} = \begin{pmatrix} m \\ m \\ 2n \end{pmatrix}$$

$$\Rightarrow \vec{v}(Cc) = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}. \quad A(6)$$

Indeed this non-symmorphic element is labelled Cc in [ITC]. For instance the non-symmorphic space groups of the arithmetic class $Cmm2$ are $Cmc2_1$ and $Ccc2$ (indeed the two reflections belong to the Cm class while the rotation is of the $P2$ class. There is another arithmetic class (of the same geometric class¹⁶ $mm2$), denoted by $Amm2$; its rotation is

¹⁶ This geometric class $mm2$ is the one which has the biggest number of corresponding arithmetic classes: 5 of them. They are denoted by: $Pmm2, Cmm2, Amm2, Fmm2, Imm2$.

of the $C2$ class and the two reflections belong to the different classes Pm, Cm . The three non-symmorphic space groups are $Abm2, Ama2, Aba2$. The reflections Cm occur also in the I classes (where they are denoted by Ca, Cb, Cc) and the F class (where they are denoted by Fd).

The last case to be considered is the arithmetic element $I4$:

$$I4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix}, \quad L \cap \text{Im } N_{I4} = \left\{ \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}, m \in Z \right\}, \quad N_{I4}L = \left\{ \begin{pmatrix} 2m \\ 2m \\ 0 \end{pmatrix}, m \in Z \right\}$$

$$\Rightarrow \vec{v}(I4_1) = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}. \quad A(7)$$

Indeed this non-symmorphic element is denoted by $I4_1$ in [ITC]; its square is symmorphic (it is $C2$ up to a lattice translation). Beware to distinguish it from $P4_1$ whose square $P2_1$ is non-symmorphic. The non-symmorphic space group $I4_1$ is sub-space group of six of them in the I -tetragonal Bravais class and two of them in the cubic crystallographic system: $F4_132, I4_132$.

These notes will be published in the Proceedings of the School without the appendix.