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ELEMENTS OF TOPOLOGICAL BAND THEORY IN CONDENSED MATTER PHYSICS

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A b s t r a c t. Band theory of crystals, essentially Bloch theory of periodic systems combined with single-particle approximation, is a scene of detailed and essential analysis of the band topology by means of application of full crystal group symmetry and combinatorial graph theoretical methods, eventually yielding topological classification of gapped band structures. Here we give an introduction to the field by summarizing the symmetry based techniques used in the band topology considerations.

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1. *Introduction*

Over the past decade the research of topological and quantum phases of matter is the most propulsive field of solid state physics. This text is a reminder on the physics of crystals with concepts rooted in the translational symmetry, firstly extended to periodic groups, and then the combinatorial methods of the vector bundles, homotopy theory and K-theory are used in classification of Hamiltonian spectra.

The focus is on the parallel exposition of two dual concepts in the theory of periodic subgroups of Euclidean group E(3), both related to induction of the group representations [1, 2, 3]. The first ingredient assumes group action on the representation torus of the translational invariant subgroup, its stratification and construction of the stabilizers' irreducible (ray) representations, being induced into the irreducible representations of the group. Analogously, the (geometrical) action in $\mathbb{R}^3$ invokes stratification of this space, with the corresponding stabilizers and their irreducible representations, which are induced into the band representations [4]. Finally, decomposition of the band representations over the irreducible ones makes the framework for topological analyses, starting with contraction of the strata to vertices, and exploitation of a homotopy of the energy band structure with the graph obtained.

If $\boldsymbol{G}$ is a group with subgroup $\boldsymbol{F}$, then the coset decomposition (Lagrange theorem) enables to choose a transverzal $\boldsymbol{Z} = \{z_1, \dots, z_{|\boldsymbol{G}|/|\boldsymbol{F}|}\}$, such that $\boldsymbol{G}$ is a disjoint union of the cosets $z_i\boldsymbol{F}$. Then for arbitrary group element g and every z_i, gz_i belongs to some coset, represented by z_j, meaning that there is unique subgroup element $f(h,i)$ such that $gz_i = z_{gi}f(g,i)$. Thus, each element g defines the action of the group on the transverzal, as well as a mapping of the transverzal into subgroup. The action on the transverzal can be reperesented in the matrix form: if E^p_q is standard matrix basis (see Appendix for notation), then $|\boldsymbol{G}|/|\boldsymbol{F}|$-dimensional matrix corresponding to g is $E(g) = \sum_p E^{gp}_p$. This is a permutational matrix (its elements are zeros except for a single unit in each column and each row). As this is the group action, these matrices form the ground representation of the group associated to arbitrary subgroup. Ground representation is a prototypic example of the induced representation, and the basic ingredient in the construction of arbitrary induced representation. In fact, if $d(\boldsymbol{F})$ is representation of the subgroup $\boldsymbol{F}$, the induced representation $D(\boldsymbol{G}) = d(\boldsymbol{F}) \uparrow \boldsymbol{G}$ is defined by:

$$D(g) = \sum_{q=1}^{|\boldsymbol{G}|/|\boldsymbol{F}|} E^{Gq}_q \otimes d(f(g, z_q)). \tag{1}$$

A manifestation of the Frobenius theorems is the modified group projector expression [5] for frequencies f^μ_D of the irreducible representations $D^{(\mu)}(\boldsymbol{G})$ in $D(\boldsymbol{G})$:

$$f^\mu_D = \frac{1}{|\boldsymbol{F}|}\mathrm{Tr} \sum_{f\in\boldsymbol{F}} d(f)D^{(\mu)^*}(f). \tag{2}$$

For the symmetry groups of crystals, i.e. for the *periodic groups*, the induction from the translational invariant subgroup is a way to get the irreducible representations (as explained in Section 2.), the elementary building blocks of all the group representations (here, only unitary representations are used). On the other hand, induction from stabilizers of the points in Euclidean space give band representations (Section 3.), and in particular *elementary band representations* [6], as basic ingredients of all the band representations.

Quantum mechanical description of crystals in the single particle model assumes a Hilbert state space carrying a band representation of the symmetry group, while the dynamics of the system is described by Hamiltonian, hermitian operator of energy. Commutation of these two has strong impact on the energy eigenvalues of the Hamiltonian. Namely, the spectrum is organized in bands, making a real vector bundle over the (Brillouin zone) torus counting irreducible representations of translations. Additional symmetry enables further Brillouin zone reduction to irreducible domain. With the help of homotopy (contraction) the band structures can be transformed into graphs (Section 4.), the analyzes which gives insight to the band topology characteristics, and eventually get the topological classification of matter.

The discussion and the notation are given at the end of the text.

2. *Irreducible representations of periodic groups*

Crystals are studied for many centuries, and their symmetry is among the first observed characteristics. After giving definition of these symmetry groups, the periodic groups, the construction of their irreducible representations will be reviewed.

2.1. Translations and periodic groups

We consider real vector space $\mathbb{R}^N$ and its Euclidean group $E(N)$ with elements $g = (G\,|\,\boldsymbol{g})$ (with $G \in O(N)$ and $\boldsymbol{g} \in \mathbb{R}^N$) defined by the action $g\boldsymbol{r} = G\boldsymbol{r} + \boldsymbol{g}$. A subgroup $\boldsymbol{G} < E(N)$ is called *$\wp$-periodic* if there is a set $\boldsymbol{A} = \{\boldsymbol{a}_1, \dots, \boldsymbol{a}_\wp\}$ of independent vectors from $\mathbb{R}^N$ generating abelian invariant subgroup (*lattice*) $\boldsymbol{T}(\boldsymbol{A}) = \boldsymbol{T}(\boldsymbol{a}_1) \otimes \cdots \otimes (\boldsymbol{a}_\wp)$ of *translations*. The factor group $\boldsymbol{G}/\boldsymbol{T}(\boldsymbol{A}) = \boldsymbol{P}$ is called *isogonal point group*, and it is naturally isomorphic to a point group (subgroup of $O(N)$) obtained by setting $\boldsymbol{g} = 0$ in all group elements $(G\,|\,\boldsymbol{g})$. Clearly, $\wp \leq N$, and for $\wp < N$ the groups $\boldsymbol{G}$ are called *subperiodic*. It will be assumed that $N = 3$, as this is the only interesting case in the solid state physics; then, for $\wp = 1, 2, 3$ the corresponding periodic groups are known as line, layer and space groups. Note that $\boldsymbol{T}(\boldsymbol{a}_i)$ is infinite cyclic group generated by $(\mathbb{1}\,|\,\boldsymbol{a}_i)$. Only in the case of the line groups we allow also helical group, generated by $(R\,|\,\boldsymbol{a})$, where $R(\phi)$ is a rotation for ϕ around the $\boldsymbol{a}$-axis; in fact, for π/ϕ irrational, the helical group does not contain translations, and it is called incommensurate (in this sense such a group is not crystallographic). The helical group can be treated in the same way as the translations, and in the following text there will be no more reference to this subtlety.

Beside these, purely geometrical groups, also their extensions to the spin-half spaces (essentially double covering of the subgroup $SO(3)$ to spin group SU(2)) and groups constructed by inclusion of the time reversal transformation (grey and black-and-white) are considered too. In quantum mechanical applications of symmetry only norm preserving operators are important, and by Wigner's theorem this means that the unitary representations of ordinary (single and double) groups, as well as unitary co-representations (with antiunitary coset action) of grey and black-and-white groups are looked for. Therefore all (co-)representations can be decomposed into irreducible components, and the first task is to find them.

2.2. Irreducible representations

Since $\boldsymbol{T}$ is product of (infinite) cyclic groups, its irreducible representations are $\Delta^{(\boldsymbol{k})}(\,\mathbb{1}\,|\,\boldsymbol{t}\,) = \mathrm{e}^{\mathrm{i}\boldsymbol{kt}}$ with momentum vector $\boldsymbol{k}$ from Brillouin zone $\mho(\boldsymbol{A}) = (-\pi,\pi]^{\times\wp}$ (torus $T^{\wp}$). Then, it should be noted that conjugation $g(\,\mathbb{1}\,|\,a\,)g^{-1}$ of the translations by arbitrary group element $g = (\,G\,|\,\boldsymbol{g}\,)$ gives, via g-conjugation of irreducible representations of $\boldsymbol{T}(\boldsymbol{A})$, the group action on $\mho$ as $\wp$-dimensional polar-vector representation $u(\boldsymbol{G}) = G_{\wp}$ (reduction of G in the subspace spanned by $\boldsymbol{A}$):

$$\Delta_g^{(\boldsymbol{k})}(\mathbb{1}\,|\,\boldsymbol{t}) = \Delta^{(\boldsymbol{k})}(g(\mathbb{1}\,|\,\boldsymbol{t})g^{-1}) = \Delta^{(g\boldsymbol{k})}(\mathbb{1}\,|\,\boldsymbol{t}) = \Delta^{(G_{\wp}\boldsymbol{k})}(\mathbb{1}\,|\,\boldsymbol{t}).$$

This action stratifies Brillouin zone: orbit of $\boldsymbol{k}$ is called star, denoted as $\boldsymbol{k}^*$, and representatives of all the stars form the irreducible domain $\mho_{\boldsymbol{G}}$. Strata $\mho_{\boldsymbol{G}}^K$ are subdomains with conjugated stabilizers, and their intersection with irreducible domain will be called ID-strata (making partition of ID). According to the basic topological theorem [7], the interior (dense in $\mho_{\boldsymbol{G}}$) $\mho_{\boldsymbol{G}}^{\mathrm{i}}$ is *generic stratum*, which is surrounded by the boundary $\mho_{\boldsymbol{G}}^{\mathrm{b}}$, consisted of the special planes and lines and isolated special points. Obviously, the translations fix arbitrary $\boldsymbol{k}$; hence, each stabilizer (*little group*) $\boldsymbol{F}^{\boldsymbol{k}}$ has the translational invariant subgroup (it is also a $\wp$-periodic group; the properties to be discussed refer both to strata and to ID-strata, unless specified otherwise). Since it is fixed (up to the conjugation along the orbit) for the whole stratum, it will be denoted as $\boldsymbol{F}^K$; consequently, the factor group $\boldsymbol{P}^K = \boldsymbol{F}^K/\boldsymbol{T}$ (sometimes called *small stabilizer*) is a subgroup of $\boldsymbol{P}$ and a supergroup of the generic stratum small stabilizer $\boldsymbol{P}^{\mathrm{i}}$. Thus $|\boldsymbol{k}^*| = |\boldsymbol{G}|/|\boldsymbol{F}^K| = |\boldsymbol{P}|/|\boldsymbol{P}^K|$, and elements of stabilizer $\boldsymbol{F}^K$ (fixing $\boldsymbol{k} = \boldsymbol{k}_1^*$) are $f^{\boldsymbol{k}^*} = (P\,|\,\boldsymbol{p})$, with P from $\boldsymbol{P}^K$.

Irreducible representations of $\boldsymbol{G}$ are obtained by induction procedure, using this stratification. The symmetry group $\boldsymbol{G}$ decomposes into the cosets of $\boldsymbol{F}^K$, with the transverzal $\boldsymbol{Z}^K = \{z_q^K = (\,Z_q^K\,|\,\boldsymbol{z}_q^K\,)\,|\,q = 1,\ldots,|\boldsymbol{k}^*|\}$ (conventionally $(\,Z_1\,|\,\boldsymbol{z}_1\,) = (\,\mathbb{1}\,|\,0\,)$): $Z_q^{\boldsymbol{k}^*}$ maps $\boldsymbol{k} = \boldsymbol{k}_1$ into $\boldsymbol{k}_q = Z_q^{\boldsymbol{k}^*}\boldsymbol{k}$, and the group permutes the elements of the star: relation $\boldsymbol{k}_{Gq} = G\boldsymbol{k}_q (= g\boldsymbol{k}_q)$ associates to q the Gq-th star point, and the corresponding permutational matrices form $|\boldsymbol{k}^*|$-dimensional *ground* representation $E(\boldsymbol{P})$ of the isogonal group (also of the whole group $E(\boldsymbol{G})$) over

$\boldsymbol{k}^*$. An irreducible representation is then obtained by induction [8]:

$$D^{(K\boldsymbol{k}\kappa)}(g) = \sum_{q=1}^{|\boldsymbol{k}^*|} E_q^{Gq} \otimes d^{(\boldsymbol{k}\kappa)}(f^K(g, z_q^K)) = \sum_{q=1}^{|\boldsymbol{k}^*|} E_q^{Gq} \otimes \Delta^{(\boldsymbol{k})}(\mathbb{1}\,|\boldsymbol{p}_q) d^{(\kappa)}(P_q)$$
$$= \sum_{q=1}^{|\boldsymbol{k}^*|} E_q^{Gq} \otimes \mathrm{e}^{\mathrm{i}G\boldsymbol{k}\cdot(G\boldsymbol{z}_q+\boldsymbol{g}-\boldsymbol{z}_{Gq})} d^{(\kappa)}(P_q). \tag{3}$$

Here, the orbit representative $z_{Gq}^K = z_{gq}^K$ (since q stands for $\boldsymbol{k}_q$, and in Brillouin zone $g\boldsymbol{k} = G\boldsymbol{k}$) and the little group elements $f^K(g, z_q^K) = (P_q|\boldsymbol{p}_q)$ are defined by $gz_q^K = z_{gq}^K f^K(g, z_q^K)$:

$$P_q = Z_{Gq}^{-1} G z_q \in \boldsymbol{P}^{\boldsymbol{k}}, \quad \boldsymbol{p}_q = Z_{Gq}^{-1}(G\boldsymbol{z}_q + \boldsymbol{g} - \boldsymbol{z}_{Gq}). \tag{4}$$

Further, $d^{(K\boldsymbol{k}\kappa)}(P|\boldsymbol{p}) = \Delta^{(\boldsymbol{k})}(\mathbb{1}|\boldsymbol{p}) d^{(K\kappa)}(P)$, is irreducible representation of $\boldsymbol{F}^K$, obviously *allowed* (subduces $|\kappa|\Delta^{(\boldsymbol{k})}(\boldsymbol{T})$). In fact, this is provided by condition

$$d^{(\kappa)}(P) d^{(\kappa)}(P') = c(P, P') d^{(\kappa)}(PP'), \quad c(P, P') = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(P\boldsymbol{p}'-\boldsymbol{p}')}, \tag{5}$$

giving the algorithm of its construction: $d^{(K\kappa)}(\boldsymbol{P}^{\boldsymbol{k}})$ is a projective irreducible representation of $\boldsymbol{P}^K$, with factor system $c(P, P')$, and it is extended to the (allowed) representation $d^{(K\boldsymbol{k}\kappa)}(\boldsymbol{F}^K)$.

Note that the phase $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(P\boldsymbol{p}'-\boldsymbol{p}')}$ is independent of κ, and only specifies the point in Brillouin zone, thus it is the same for all irreducible representations associated to $\boldsymbol{k}^*$. In fact, since P is from $\boldsymbol{P}^{\boldsymbol{k}}$, this phase is trivial (and the irreducible representation $d^{(\kappa)}(\boldsymbol{P}^{\boldsymbol{k}})$ is linear) whenever $\boldsymbol{k}$ is in the interior of $\mho$: relation $P\boldsymbol{p}' \sim \boldsymbol{p}'$ allows $P\boldsymbol{p}' \neq \boldsymbol{p}'$ only at the boundary (and only for nonsymorphic groups). For each point $\boldsymbol{k}$ of $\mho_{\boldsymbol{G}}^K$ complete set (counted by κ) of the nonequivalent irreducible projective representations of $\boldsymbol{P}^{\boldsymbol{k}}$ with the factor system (5) defines the set of associated irreducible representations (3) of $\boldsymbol{G}$; collection of these over $\mho_{\boldsymbol{G}}$ is complete set of nonequivalent unitary irreducible representations of $\boldsymbol{G}$, with finite dimension $|D^{(K\boldsymbol{k}\kappa)}| = |\kappa||\boldsymbol{G}|/|\boldsymbol{F}^{\boldsymbol{k}}|$. Further, since the (small) stabilizer is common for the whole stratum, the (projective) representation $d^{(K\kappa)}(\boldsymbol{P}^K)$ is the same along the strata, and each stratum K defines the set of *associated* irreducible representations $D^{(K\boldsymbol{k}\kappa)}(\boldsymbol{G})$, such that for fixed κ a series parameterized by $\boldsymbol{k}$ has the matrices of the same form (differing in the $\boldsymbol{k}$-value only).

Taking all the representations (3) for each stratum K, each $\boldsymbol{k}$ from the ID-strata K and the corresponding nonequivalent irreducible (ray) representations of the small stabilizer, one gets complete set of irreducible representations of $\boldsymbol{G}$. Thus, irreducible representations of $\boldsymbol{G}$ are parameterized by quantum numbers $\mu = (K\boldsymbol{k}\kappa)$: $\boldsymbol{k}$ is quasi-momentum vector $\boldsymbol{k}$ from Brillouin zone (and the representation involves the whole star), while κ comprises the isogonal group quantum numbers (angular momentum and/or parities originating in O(3)), counting representations (5) of the small stabilizer $\boldsymbol{P}^{\boldsymbol{k}}$. Precisely, for each $\boldsymbol{k}$, there is a choice $\kappa_{\boldsymbol{k}}$ of the compatible orthogonal quantum numbers. The representations associated to the same stratum $\mho_{\boldsymbol{G}}^{K}$ are κ-series differing in $\boldsymbol{k}$ (with the same κ): in Γ-point ($\boldsymbol{k} = 0$) these are representations of $\boldsymbol{P}^{\Gamma} = \boldsymbol{P}$; for generic stratum with trivial $\boldsymbol{P}^{\mathrm{i}}$ (in all space and layer groups without horizontal mirror symmetry), there is single series with unit representation of the small stabilizer.

2.3. Decomposition of representations

Any representation $D(\boldsymbol{G})$ (in the space $\mathcal{S}$) decomposes into the irreducible components with frequency numbers $f_D^{K\boldsymbol{k}\kappa}$:

$$D(\boldsymbol{G}) = \sum_{K\boldsymbol{k}\kappa} f_D^{K\boldsymbol{k}\kappa} D^{(K\boldsymbol{k}\kappa)}(\boldsymbol{G}). \tag{6}$$

Then the symmetry adapted basis (with standard basis $\{|\kappa a\rangle\}$ of $d^{(\kappa)}(\boldsymbol{P}^{\boldsymbol{k}})$)

$$\{|(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (p,a)\rangle \mid \boldsymbol{k} \in \mho_{\boldsymbol{G}}^{K};\ t_\kappa^{K\boldsymbol{k}} = \overline{1, f_D^{K\boldsymbol{k}\kappa}};\ p = \overline{1,\ |\boldsymbol{k}^*|};\ a = \overline{1, |\kappa|}\} \tag{7}$$

consists of the multiplets $\{|\,(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (1,a)\rangle \mid p = \overline{1,\ |\boldsymbol{k}^*|};\ a = 1,\dots,|\kappa|\}$, and in the view of (3), the basis transformation rule is:

$$D(g)\ |(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (p,a)\rangle = \sum_{a'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{g}_p} d_{a'a}^{(\kappa)}(G_p)\ |(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (Gp,a')\rangle. \tag{8}$$

The space $\mathcal{S}^{\boldsymbol{k}}$ (Bloch space introduced in Subsection 3.) corresponding to the point $\boldsymbol{k}$ includes only $\boldsymbol{k}$-parts (fixed p) of a multiplet associated to $K\boldsymbol{k}$; the rest is from the spaces of the other points in the star. Hence $\mathcal{S}^{\boldsymbol{k}}$ is not invariant for $\boldsymbol{G}$, but the invariant space is the sum over $\boldsymbol{k}^*$.

In particular, stabilizer elements $f = (P|\boldsymbol{p})$ act as

$$D(f)\ |(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (1,a)\rangle = \sum_{a'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{p}} d_{a'a}^{(\kappa)}(P)\ |(\boldsymbol{k},\kappa), t_\kappa^{K\boldsymbol{k}}, (1,a')\rangle.$$

With notation accommodated to the counters $K\boldsymbol{k} = \boldsymbol{k}^*$ and $q = \boldsymbol{k}_q$ of stars and star points, (3) provides the form

$$D(g) = \sum_{K\boldsymbol{k}} E_{K\boldsymbol{k},q}^{K\boldsymbol{k},gq} \otimes d^{\boldsymbol{k}}(f^{\boldsymbol{k}}(g,q)) \quad d^{\boldsymbol{k}}(f) = \sum_{\kappa} \sum_{t_\kappa^{K\boldsymbol{k}}=1}^{f^{K\boldsymbol{k}\kappa}} d^{(K\kappa)}(f). \tag{9}$$

This manifests once again that the subspace invariant under the whole group join star of the point fibres. This also justifies that irreducible domain generates all the irreducible representations.

3. *Band theory*

Hamiltonian, as quantum mechanical represent of energy, governs the dynamics of any system. In crystalline matter it has special spectral properties imprinted by symmetry.

3.1. State space and Bloch theory

In a single particle problem the state space is infinite dimensional separable Hilbert's space $\mathcal{S}$, with Lebesgue's space $\mathcal{L}(\mathbb{R}^3)$ as its coordinate representation. This space is tensor product of three spaces $\mathcal{L}(\mathbb{R})$. Each irreducible representation $\Delta^{(\boldsymbol{k})}(\boldsymbol{T})$ of the full translational subgroup of the Euclidean group appears once in this space, with symmetry adapted basis $|\boldsymbol{k}\rangle$ (eigenbasis of the momentum operator). For $\wp$-periodic discrete translational group $\boldsymbol{T}(\boldsymbol{A})$ the representations $\Delta^{(\boldsymbol{k})}(\boldsymbol{T}(\boldsymbol{A}))$ are from Brillouin zone $\mho(\boldsymbol{A})$, and the vectors $|\,\boldsymbol{k}\rangle$ differing for a vector $\boldsymbol{K}$ of inverse lattice (spanned by basis $\boldsymbol{a}^i$ such that $(\boldsymbol{a}^i, \boldsymbol{a}_j) = 2\pi\delta^i_j$) transform according to the same representation. Hence, each representation occurs infinitely many times, and the vectors can be relabeled: $|\,\boldsymbol{k}, \boldsymbol{K}\rangle = |\,\boldsymbol{k} + \boldsymbol{K}\rangle$ ($\boldsymbol{k} \in \mho(\boldsymbol{A})$, $\boldsymbol{K} = \sum z_i \boldsymbol{a}^i$, $z_i \in \mathbb{Z}$); with fixed $\boldsymbol{k}$, these vectors are basis of infinite-dimensional isotypic space $\mathcal{S}^k$. Generalizing, the action of $\wp$-periodic discrete translational group $\boldsymbol{T}(\boldsymbol{A})$ in the space $\mathcal{S}$ introduces natural decomposition $\mathcal{L}(\mathbb{R}^3) = \mathcal{L}(\mathbb{R}^\wp) \otimes \mathcal{L}(\mathbb{R}^{3-\wp})$ into the space over the periodic coordinates, and the complementary space. Taking arbitrary basis $|\,i\rangle$ in the second factor, the symmetry adapted basis gets form $|\,\boldsymbol{k}, \boldsymbol{K}\rangle \otimes |\,i\rangle$, where $\boldsymbol{k}$ is from Brillouin zone $\mho(\boldsymbol{A})$ and $\boldsymbol{K}$ counted by $\mathbb{Z}^\wp$. Hence, the isotypic spaces $\mathcal{S}^{\boldsymbol{k}}$ are infinite-dimensional, with basis containing symmetry adapted vectors with fixed $\boldsymbol{k}$.

It is of utmost importance that the irreducible representations of $\boldsymbol{T}(\boldsymbol{A})$ are equally populated in the single particle state space: the frequency number $f^{\boldsymbol{k}} = |\mathcal{S}^{\boldsymbol{k}}| = |\mathbb{Z}^\wp||\mathcal{L}(\mathbb{R}^{3-\wp})|$, though infinite, is $\boldsymbol{k}$-independent, i.e. the isotypic spaces $\mathcal{S}^{\boldsymbol{k}}$ are of the same dimension $|\mathcal{S}^{\boldsymbol{k}}| = |\mathcal{S}^0|$. This gives rise to the natural, $\boldsymbol{k}$-dependent isomorphism between $\mathcal{S}^0$ (space of invariants under $\boldsymbol{T}(\boldsymbol{A})$) and $\mathcal{S}^{\boldsymbol{k}}$, realized by Bloch theorem: $\mathcal{S}^{\boldsymbol{k}} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}}\mathcal{S}^0$. Hence, $\mathcal{S}$ becomes a fiber bundle with base manifold $\mho(\boldsymbol{A})$ and fibre $\mathcal{S}^0$. Hamiltonian H, commuting with translations is reduced in each of the spaces $\mathcal{S}^{\boldsymbol{k}}$ into $h(\boldsymbol{k})$, and natural isomorphism gives Bloch Hamiltonians $H(\boldsymbol{k}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}}h(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}}$ acting in $\mathcal{S}^0$; they make operator field over $\mho(\boldsymbol{A})$.

3.2. Inductive models

In the effective physical models, the approximate single particle spaces are constructed as a sum of the mutually equivalent subspaces associated to elementary cells: $\mathcal{S} = \oplus_{\boldsymbol{t}}\mathcal{S}_{\boldsymbol{t}}$, where $\mathcal{S}_{\boldsymbol{t}}$ (with a basis $\{|\,\boldsymbol{t}i\rangle \mid i = \overline{1, |\mathcal{S}_0|}\}$ of "orbitals") is associated to the cell $\boldsymbol{t} = (t_1, \ldots, t_\wp)$. The only translation fixing the cell is identity (stabilizer is trivial $\{e\}$). Hence, the state space carries the representation induced from the $|\mathcal{S}_0|$-dimensional unit representation $\mathbb{1}_{\mathcal{S}_0}$ of (trivial) stabilizer. Expression (2), after substituting $d(\boldsymbol{F}) = \mathbb{1}_{\mathcal{S}_0}$, becomes $f_D^{\boldsymbol{k}} = |\mathcal{S}_0|$. This result justifies that the inductive state space preserves the full state space fiber bundle picture; only the fiber $\mathcal{S}^{\boldsymbol{k}}$ is finite dimensional with symmetry adapted basis $|\boldsymbol{k}i\rangle = \sum \mathrm{e}^{\mathrm{i}\boldsymbol{kt}}\,|\boldsymbol{t}i\rangle$.

Concerning total symmetry group, it has been shown that only the star spaces $\mathcal{S}^{\boldsymbol{k}^*} = \oplus_{\boldsymbol{k}\in\boldsymbol{k}^*}\mathcal{S}^{\boldsymbol{k}}$ are invariant for $\boldsymbol{G}$, since group maps $\boldsymbol{k}$ into the whole star $\boldsymbol{k}^*$. Hence, the irreducible domain, with single $\boldsymbol{k}$ from each star, with corresponding fibres completely define the whole state space, also inheriting the bundle structure. Note further, that in this case $d^{\boldsymbol{k}}(\boldsymbol{F}^{\boldsymbol{k}})$ defined in (9) is of the fixed ($\boldsymbol{k}$-independent) dimension $d = |\mathcal{S}^{\boldsymbol{k}}|$, although the stabilizer depends of $\boldsymbol{k}$; it is called *Bloch representation*.

3.3. The Bloch Hamiltonian – bands

Hamiltonian, the quantum mechanical operator H associated to energy, by definition commutes with the symmetry group $\boldsymbol{G}$, meaning that it commutes with all representative operators $D(\boldsymbol{G})$. In particular, commutation $D(\boldsymbol{T}(\boldsymbol{A}))H = HD(\boldsymbol{T}(\boldsymbol{A}))$ with translational subgroup implies that H reduces in the spaces $\mathcal{S}^{\boldsymbol{k}}$ into Bloch Hamiltonians $h(\boldsymbol{k}) = h^{\boldsymbol{k}}_{\boldsymbol{k}}$:

$$H = \sum_{\boldsymbol{k}\in\mho} E^{\boldsymbol{k}}_{\boldsymbol{k}} \otimes h(\boldsymbol{k}). \tag{10}$$

Commutation, with help of (9), shows that Bloch Hamiltonians within a star are related by Bloch space representation of stabilizer $d^{\boldsymbol{k}}(\boldsymbol{F}^{\boldsymbol{k}})$ (sum of the allowed components associated to $\boldsymbol{k}$):

$$h(g\boldsymbol{k}) \quad = \quad d^{\boldsymbol{k}}(f^{\boldsymbol{k}}(g,\boldsymbol{k}))h(\boldsymbol{k})d^{\boldsymbol{k}^{-1}}(f^{\boldsymbol{k}}(g,\boldsymbol{k})) \tag{11}$$

it is assumed that $\boldsymbol{k}^*$ is generated by $\boldsymbol{k} = \boldsymbol{k}_1^*$ from irreducible domain. In particular, in two cases, when g is from $\boldsymbol{F}^{\boldsymbol{k}}$, and when it is a transverzal element, one obtains:

$$h(\boldsymbol{k}) \quad = \quad d^{\boldsymbol{k}}(f^{\boldsymbol{k}})h(\boldsymbol{k})d^{\boldsymbol{k}^{-1}}(f^{\boldsymbol{k}}), \tag{12}$$

$$h(\boldsymbol{k}_p) \quad = \quad d^{\boldsymbol{k}}(f^{\boldsymbol{k}}(z_p,\boldsymbol{k}))h(\boldsymbol{k})d^{\boldsymbol{k}^{-1}}(f^{\boldsymbol{k}}(x_p,\boldsymbol{k})) = h(z_p\boldsymbol{k}). \tag{13}$$

4. *Band graphs and band topology*

Due to the reduction of H in Bloch spaces $\mathcal{S}^{\boldsymbol{k}}$, the eigenvalues of Bloch Hamiltonians form energy bands: they are functions $E_i(\boldsymbol{k})$ $(i = \overline{1,d})$ over Brillouin zone, in accordance with (10). Topological properties of these bands are to a large extent determined by symmetry. The first step in this direction is to represent the bands as graphs, which will be classified afterwards. This is achieved by contraction of strata and band-patches over them; contraction as a special type of homotopy, preserves some of the topological properties of the band structures. Therefore, counting possible band-graphs is important to understand topology of energy bands, and this is the main subject of the section. Precisely, possible diagrams of bands can be classified by symmetry, in the following procedure based on compatibility relations and monodromies.

4.1. Irreducible domain graph

As it has been explained, the group action partitions Brillouin zone into strata. Taking a single representative from each orbit, and grouping the equivalent orbits, the irreducible domain is obtained, with strata (of representatives) of dimensions varying from 0 to $\wp$. Among them there is a $\wp$-dimensional *generic* stratum (its stabilizer is minimal, though not necessarily trivial), and the strata of lower dimension and higher symmetry (larger stabilizers) are on its boundary. In fact, the strata of lower dimension are at the boundary of the strata of gretaer dimension. Generally, the strata are partially ordered set, following supergroup-subgroup relation of the stabilizers. This order has important property: if stratum B is on the boundary of stratum A, then the stabilizers are ordered as $\boldsymbol{F}^A < \boldsymbol{F}^B$. Just the last relation is used to define *ID-graph* (graph of the irreducible domain): the vertices are different strata (each contracted to a point); each vertex (stratum) is connected to the vertex corresponding to its boundary strata, with edges oriented from higher to lower symmetry, i.e. from boundary to the interior stratum.

4.2. Band graph

Further, it is intuitively clear that arbitrary band structure can be in the same way contracted into a graph. Namely, each band is a surface over Brillouin zone, partitioned into subbands corresponding to strata (patches over strata). Contracting the patches along with the strata in irreducible domain, each band is converted to a band-graph over (projected into) ID-graph. The vertices of band-graph are (associated to stratum) irreducible representations assigning the patches over stratum, while the edges of the band graph are projected into ID-graph edges, i.e., they connect, as prescribed by compatibility relations, different irreducible representations assigned to the connected strata; in addition, monodromy can impose "vertical" edges, connecting representations associated to the same stratum (of the nonzero dimension). Connections (crossings) of different bands are realized in the high symmetry strata (with more dimensional allowed representations) via compatibility relations.

In other words, there is a bundle with ID-graph as a basis, and fibre in each vertex (stratum) being set of the irreducible representations associated to the stratum. Then band-graph is a sort of a section of this bundle: to a stratum K corresponds an associated irreducible representation $D^{(K\boldsymbol{k}\kappa)}(\boldsymbol{G})$ (and allowed representations $\delta^{(K\kappa)}(\boldsymbol{F}^K)$ of the stabilizer) assigning band patch. However, some of the bands may be connected, and a band structure separated from other bands is in general multivalued function (several sections) over ID-graph; still, recall that the that the band degeneracy is constant, which gives restriction to possible sections.

4.2.1. Compatibility relations. The theorem that more symmetric strata are on the boundary of the less symmetric ones enables to transfer partial order among the subgroups to the neighboring strata: if the stratum B is on the boundary of the stratum A (consequently $\boldsymbol{F}^A < \boldsymbol{F}^B$ and for the factor groups $\boldsymbol{P}^A < \boldsymbol{P}^B$). Therefore, allowed representations of $\boldsymbol{F}^B$ can be subduced to $\boldsymbol{F}^A$:

$$d^{(B\beta)}(\boldsymbol{F}^B \downarrow \boldsymbol{F}^A) = \sum_{\alpha} f^{A\alpha}_{B\beta}(\boldsymbol{F}^A) d^{(A\alpha)}(\boldsymbol{F}^A). \tag{14}$$

Compatibility relations are determined by the frequencies $f^{A\alpha}_{B\beta}(\boldsymbol{F}^A)$: a band patch assigned by β (on B) is continued (and perhaps split) by all of the $f^{A\alpha}_{B\beta}(\boldsymbol{F}^A)$: band patch(es) assigned by the irreducible representations α (associated to A). Note that this, compatibility rule automatically preserves the degeneracy.

4.2.2. Monodromy. Induction of irreducible representations shows that nonsymmorphic elements of the group are represented by $\boldsymbol{k}$-dependent matrices, with matrix elements and eigenvalues depending on some fraction $\boldsymbol{k}/C$ of $\boldsymbol{k}$. Thus, these are subperiodic functions, which do not return to the initial value after change of $\boldsymbol{k}$ for full range of Brillouin zone, but only after C turns around it. In fact, periodic group $\boldsymbol{G}$ is an extension of (isogonal) point group $\boldsymbol{P}$ by translational group $\boldsymbol{T}$, meaning that $\boldsymbol{T} \lhd \boldsymbol{G}$ and $\boldsymbol{G}/\boldsymbol{T} \cong \boldsymbol{P}$. Therefore, all symmorphic and nonsymmorphic groups with the same factors $\boldsymbol{P}$ and $\boldsymbol{T}$ are different extensions and they are classified by the cohomology groups $\boldsymbol{H}^2(\boldsymbol{P},\boldsymbol{T})$ and $\boldsymbol{H}^3(\boldsymbol{P},\boldsymbol{T})$ (note analogy to representations of double groups, i.e. of group extensions, e.g. SU(2) as a covering of SO(3)). This is manifested by the energy bands: every turn of $\boldsymbol{k}$ around torus of Brillouin zone gives another band connected with the previous, and after C turns bands are returning to the initial value (energy). This is called monodromy (of the nonsymmorphic) elements, and causes C-connectivity of the bands.

Full monodromy is found in generic stratum, while in the special strata it may be reduced (and completely absent in special points). As some generic bands can be joined in the same band over special strata, the compatibility relations diminish the number of bands linked only by monodromy in high symmetry strata.

For line groups, nosymmorphic elements (helical axes and glide planes) form abelian invariant subgroup, which can be used instead of translations in the induction procedure. This results in "helical" Brillouin zone (and quantum numbers), which is C times greater than the standard one. It is clear that the band over "helical" Brillouin zone gives the connected C standard bands: therefore, with helical Brillouin zone there is no monodromy, while it appears over linear Brillouin zone. Analogous procedure can be performed for diperiodic groups, but it is less transparent, since the groups generated by the nonsymmorphic generators may not be abelian.

4.3. Elementary band representations

For each subgroup of Euclidean group there is a finite number of nonequivalent strata in $\mathbb{R}^3$. These are classified according to the conjugation class of their stabilizers $\boldsymbol{F}_P$. *Band representation* (BR) $D(\boldsymbol{G})$ is any induced representation:

$$D(g) = \sum_P D^P(g), \quad D^P(g) = \left(\sum_p E_{Pp}^{P,gp} \otimes \delta^P(f^P(g,p)) \right). \qquad (15)$$

If D has not a band subrepresentation it is called *elementary band representation* (EBR).

It is important to note that the stabilizers in the Euclidean space $\mathbb{R}^3$ have only trivial translation, i.e. $\boldsymbol{F}_P \cap \boldsymbol{T}(\boldsymbol{A}) = \{(\mathbb{1}\,|\,0)\}$. Therefore, (3) shows that reduction of the induced representations (realized on the stabilizer by (2)) gives $\boldsymbol{k}$-independent frequencies of the representations in the series κ over stratum K. Thus, the reduction of band representation has the form:

$$D(\boldsymbol{G}) = \sum_{K\kappa} f_D^{K\kappa} \sum_{\boldsymbol{k}\in K} D^{(K\boldsymbol{k}\kappa)}(\boldsymbol{G}). \qquad (16)$$

Therefore, finite-dimensional vectors $\boldsymbol{f}_D$, with coefficients being nonnegative integers $f^{K\kappa}$ define different band representations. Thus, if each irreducible (ray) representations of all strata (R denotes their total number) are taken as standard vectors (absolute basis), then they span (representation) module $\mathbb{Z}^R$.

Several simple observations reduce classification of band representations.

1. Any representation (15) involving more than one orbit has subrepresentations $D^P(\boldsymbol{G})$, which are BRs themselves. Hence, EBRs are induced from a single stabilizer.

2. If in (15) with single orbit (with stabilizer $\boldsymbol{F}$) a reducible

$$\delta(\boldsymbol{F}) = \delta_1(\boldsymbol{F}) + \delta_2(\boldsymbol{F})$$

is used, then the representations induced from δ_1 and δ_2 are subrepresentations of BR induced from δ, and D is not elementary.

3. Due to transitivity of induction, if $\boldsymbol{F} > \boldsymbol{F}'$, then the representation induced from irreducible representation of $\boldsymbol{F}'$ can be seen as induced to $\boldsymbol{F}$ at first (this is possibly not an irreducible representation of $\boldsymbol{F}$), and then to $\boldsymbol{G}$ from $\boldsymbol{F}$. Hence, each BR obtained from $\boldsymbol{F}'$ can be obtained from $\boldsymbol{F}$ (those being not irreducible at the mid-step are a priori not elementary). This allows to consider only maximal stabilizers. Namely, the stabilizers are not totally ordered: maximal stabilizer is a stabilizer which is not a subgroup of any other stabilizer. In the case of periodic groups, several maximal stabilizers may occur since no $\mathbb{R}^3$ orbit is fixed by the whole group.

Accordingly, all EBRs form a subset in the set of BRs obtained as induced IRs of all maximal stabilizers:

$$E^{\mu}_{\boldsymbol{M}}(\boldsymbol{G}) = \delta^{(\mu)}(\boldsymbol{M} \uparrow \boldsymbol{G}) = \sum_{K\boldsymbol{k}\kappa} f^{K\boldsymbol{k}\kappa}_{\boldsymbol{M}\mu} D^{(K\boldsymbol{k}\kappa)}(\boldsymbol{G}). \tag{17}$$

On the right, the decomposition into irreducible components is given. It should be noted that there are *exceptional cases* when such a representation is not an EBR, i.e. each irreducible representation of a maximal stabilizer gives an EBR, with some exceptions (usually listed explicitly). In other words, the band representations form abelian group (extended by Grothendieck's construction from the semigroup of induced representations) $\boldsymbol{AI} = \mathbb{Z}^A$ spanned by A independent induced irreducible representations of maximal stabilizers. To apostrophize, these BRs may be dependent, and if some of them is a combination of others, it is an exception.

While the induction procedure (maximal stabilizer and its irreducible representations) define the decomposition (17), it does not completely define EBR, in the sense that the same induced representation, i.e. the same set of frequency numbers may lead to different band topologies, each corresponding to a single EBR; these topological variations are allowed by compatibility rules and monodromies.

4.4. Compatibility relations induced graphs – paths

Compatibility relations and monodromies sublimate local band connectivity, and gathering these local requirements in consistent way gives one possible band graph. Namely, assume that B is a stratum on the boundary of A, thus with $\boldsymbol{F}^B$ being a supergroup of $\boldsymbol{F}^A$. Compatibility relations (14) mean that a group of $f^{A\alpha}_{B\beta}$

bands $E_j^{A\alpha}(\boldsymbol{k})$ over the low symmetry stratum A joins at the boundary B (of higher symmetry) into a single band-patch $E_i^{B\beta}(\boldsymbol{k})$ assigned to $\delta^{(B\beta)}$; the same, with another group of A-bands, is valid for each $i = \overline{1, f_D^{B\beta}}$.

In general, provided the compatibility relations and monodromies, it remains to start from the high symmetry strata B, and for each appearing irreducible representation associated to them, draw the possible continuations/splittings into bands over all nearby lower-symmetry strata.

Consequently, if A is such a (lower symmetry) stratum, then its bands must obey the compatibility relations for all the surrounding (higher symmetry) strata, i.e. they are glued/split bands at all these boundaries. All of these split bands on the boundaries of A are to be connected (identified) in all possible ways over A, each possibility being an element of a different connectivity class. If there are even less symmetric strata, A is in the boundary of some of them, and the process is repeated (with A in the role of high symmetry stratum). This is continued down to the generic stratum, giving possible connectivity graphs of the band structures with representation $D(\boldsymbol{G})$. When for each A all choices are made a path over whole ID graph is obtained. This complements the information given by frequencies $f^{K\kappa}$ in (17) (vertices) to a band-graph over ID-graph, which represents a possible band structure.

This procedure can be performed for all EBRs. However, there are cases when there are many possibilities, and the task become intractable even for computer techniques (in layer groups there are seveal cases when the number of possibilities is of the order of 10^{31}). It can be observed that this number increases as a factoriel function with the frequencies of the representations associated to the generic stratum. Anyway, the nonequivalent band-graphs are important to find typical topologies of band structures. Two graphs are band-equivalent if they coincide when one of them is subjected to a permutations of vertices within the groups of $f^{K\kappa}$ identical irreducible representations.

4.5. Connectivity and symmetry indicators

In general, there are connected and unconnected EBRs [9, 10]. This refers to the standard path-connectivity: in connected EBRs each two points are path connected. In unconnected EBRs, there may be connected components which are EBRs themselves, but also some of them are not, i.e. at least one connected component is not the EBR. However, this procedure assumes construction of all paths, decomposition on the connected components, and attempt to find if all the components are band-graph-equivalent to some other connected EBR. Due to number of paths, the procedure may be intractable in this form, but there is a tractable ID-subgraph which allows equivalent connectivity calculations with tractable reduction to band-subgraphs.

Since the connected components of subgraphs correspond to representations which are not induced, but share the properties of constant degeneracy, satisfied compatibility relations and monodromy based continuations, unconnected graphs arouse more general treatment. In fact, these three properties can be written as a system of homogeneous linear equations in frequencies $f^{K\kappa}$: summing on the boundaries, circular path around Brillouin zone and sum of the allowed representations' dimensions in various $\boldsymbol{k}$-points:

$$f_D^{A\alpha} = \sum_{\beta} c_{B\beta}^{A\alpha} f_D^{B\beta}, \tag{18a}$$

$$f_D^{K\kappa} = f_D^{K\kappa\boldsymbol{\kappa}}, \tag{18b}$$

$$(\forall K, K') \quad \sum_{\kappa} |d^{K\kappa}| f_D^{K\kappa} = \sum_{\kappa'} |d^{K'\kappa'}| f_D^{K'\kappa'}. \tag{18c}$$

Frequency vectors, satisfying this system are in the null-space of the matrix of the system. Therefore, if the dimension of this null-space is B, the abelian group $\boldsymbol{BS}$ of *band structures* module of such representations (which are not necessarily induced!) is abelian group with the same dimension A, but may have also some finite factors (this is shown for all periodic groups by direct calculations). Therefore, there is X such that $\boldsymbol{SI} = \boldsymbol{BS}/\boldsymbol{AI} = \boldsymbol{Z}_{C_1} \otimes \cdots \otimes \boldsymbol{Z}_{C_X}$, where $\boldsymbol{Z}_{C_i}$ is cyclic group of order C_i.

While the induced representations, by construction, describe systems with electrons localized in particular Wyckoff positions, the components are topological, with delocalized electrons. The same holds also for representations from the cosets of $\boldsymbol{SI}$. In some cases addition of trivial bands trivialize the whole band structure (e.g. connected component with other components being EBRs); there are different cases, when two or more connected components are not EBRs, or band representations is found independently as the coset representative of $\boldsymbol{SI}$. This is the task of K-theory, intensively developed in the field. As the group $\boldsymbol{AI}$ is with localised electrons associated to particular atoms, in the limit of infinitely separated atoms the band structure is essentially atomic spectrum, these band structures are called *atomic insulators*, and the factor group over them of the band structures group $\boldsymbol{BS}$ is called group of *symmetry indicators* [11].

5. *Conclusions*

A brief review of the actual analyses of the topology of the energy bands of crystals is given. It is shown that symmetry alone suffices to give a list of possible band graphs. Taking into account that these graphs are homotopy image of the energy band structures, it becomes clear that homotopy preserved topological invariants can be found by the analysis of the obtained graphs.

Unfortunately, there are groups and band representations for which the combinatorial problem of construction of possible graphs is technically intractable. Therefore, the problem of classification cannot be totaly resolved. In fact, for line groups all graphs are found [12, 13]: there is no unconnected graphs, and all symmetry indicator groups are trivial. For the layer groups, symmetry indicator groups show that there are topologically nontrivial band structures; except for around fifty intractable elementary band representations, all the graphs (more than twelve thousands of them) are found.

Appendix: Notation

- Bold: Sets, groups ($\boldsymbol{G}$, $\boldsymbol{F}$, $\boldsymbol{R}$, $\boldsymbol{S}$), vectors of any dimension ($\boldsymbol{r}$, $\boldsymbol{s}$).
- Calligraphic: vector spaces ($\mathcal{S}$, $\mathcal{A}$).
- Absolute value has contextual meaning: the dimension of the vector space ($|\mathcal{S}|$), cardinality of sets ($|\boldsymbol{G}|$, the order of the group $\boldsymbol{G}$, $|\boldsymbol{Z}|$ for the order of transversal), dimension of the matrices and representations ($|\mu|$, $|D(\boldsymbol{G})|$, $|M|$).
- $\mathbb{1}$: the identity operator with indices specifying the space ($\mathbb{1}_3$, $\mathbb{1}_\delta$), or the unit representation, $\mathbb{1}(\boldsymbol{G})$.
- E^i_j is the matrix with elements $(E^i_j)_{pq} = \delta_{pi}\delta_{jq}$.

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