Equivalence of Simple Band Representations: Infinite and Finite Space Groups
Comments on the preceding paper

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ABSTRACT

The aim of the preceding paper was exclusively to study carefully the mathematical properties of band representations, like to show the surprising result that all `simple` band representations for infinite space groups are *weakly* equivalent, but not to discuss its impact on the physics. Long discussions during and after the Summer School have motivated the authors to comment on the physical importance of the results of the preceding paper in this short contribution.

1. General Remarks on Band Representations

We shall denote that paper DZD. It recalls carefully the formalism used in solid state physics for the study of bands: Wannier functions and Bloch functions which form respectively a countable orthonormal basis and a continuous (pseudo-) basis for the Hilbert space $L^2(\mathbb{R}^3)$ of functions on our physical space. These two bases are transformed into each other by a generalized Fourier transform. It also makes the comparison with the formalism obtained when one replaces the space group by a finite group, as proposed by Born and von Karman. Then the paper studies some band representations of the space group $\mathbb{G}$, that is the representations induced from an irreducible representation D^α of a *local* group, i.e. the little group $\mathbb{G}_q$ of a point in the action of $\mathbb{G}$ on our space $\mathbb{R}^3$. The strata[1] of this action are called Wyckoff positions in the International Tables of Crystallography (ITC) [15][2] which tabulate them for each space group. The Wyckoff positions are in one to one correspondence with the conjugacy classes of local groups. So there exists among them a partial ordering;

[1]If necessary see in this book L. Michel's lectures for the basic concepts of group actions.
[2]The references given by numbers between square brackets are those of the commented paper.

unhappily it is not given in the ITC. Since $\mathbb{G}_q \subset \mathbb{G}$ does not contain translational subgroups, the restriction of the group homorphism $\mathbb{G} \xrightarrow{\theta} \mathbb{G}/\mathfrak{T} = \mathfrak{P}$ to $\mathbb{G}_q$ is an isomorphism with a subgroup $\mathbb{F}H = \theta(\mathbb{G}_q) \subseteq \mathfrak{P}$ of the point group[3] $\mathfrak{P}$. Beware that several distinct conjugacy classes of $\mathbb{G}_q$ can correspond to the same $\mathbb{F}H$. It is easy to prove that the group generated by $\mathbb{G}_q$ and the translation subgroup $\mathfrak{T}$ is a semi-direct product (= symmorphic) group $\mathfrak{T}\circledS\mathbb{G}_q$. That limits the list of possible $\mathbb{F}H \subseteq \mathfrak{P}$. So a band representation is defined by the local group $\mathbb{G}_q$ (up to a conjugation in $\mathbb{G}$) and one of its representation D^α. We simply denote:

$$\mathsf{D}^{(q,\alpha)\uparrow\mathfrak{G}} = \mathrm{Ind}_{\mathbb{G}_q}^{\mathbb{G}}\ \mathsf{D}^\alpha, \tag{1}$$

where q is the label of a Wyckoff position in the ITC.

We call a band representation *elementary* if it cannot be decomposed into a direct sum of band representations. The possible ones are induced from irreducible representations D^H of maximal finite subgroups[4] [5]. But that necessary condition is not sufficient: some of those representations are not elementary[5]; among the elementary ones, some are equivalent[6]. The classification of the equivalent classes of elementary band representations has been made in [13]. The authors used Frobenius reciprocity theorem: On one side one uses only finite dimensional irreps of $\mathbb{G}$ and of $\mathbb{G}_q$. This well defined side gives a meaning of the ill defined other side that contains the infinite dimensional BR. In general the energy of an elementary band is a multivalued function on the Brillouin zone. The number of energy branches of the band is: "(index $\mathbb{G}_q$ in $\mathfrak{P}$) $\times$ (dim D^H)" (see e.g.[13]). The commented paper studies only the *simple bands*, i.e. those with one branch only. For them $\theta(\mathbb{G}_q) = \mathfrak{P}$ (so $\mathbb{G}$ has to be symmorphic) and $\dim \mathsf{D}^P = 1$. Simple band representations (=SBR) are elementary. Among the 890 of them, [13] proved that only fourteen pairs are equivalent:

$$\begin{array}{llll} \#22 = \mathbf{F}222: & B_{a,\alpha} = B_{b,\alpha},\ B_{c,\alpha} = B_{d,\alpha}, & \alpha = 1,2,3,4 \\ \#196 = \mathbf{F}23: & B_{a,\alpha} = B_{b,\alpha},\ B_{c,\alpha} = B_{d,\alpha}, & \alpha = 1,2,3. \end{array} \tag{2}$$

2. Finite Space Groups

Most solid state physicists use the term *finite space groups* for what we shall call here BvK, since they were first proposed by Born and von Karman [a][7]. That is the case of references [3–10]. DZD studies by this method the case for the non Abelian one dimensional space group, and, in 3 dimensions, $\mathbf{F}222$ and $\mathbf{P}m\bar{3}m$; these three examples are treated correctly, but the general statement in the conclusion is wrong; indeed the authors did not guess the deep cause of the facts they observed.

Let us recall that Bravais (and Frankenheim), C. Jordan, Schönflies, Fedorov studied only the classification of infinite space groups and their lattices. The study of

[3]The point groups $\mathfrak{P}$ are defined up to a conjugation in the orthogonal group (=geometric class).
[4]It is easy to prove that they are little groups of points of space.
[5]First example found in [10].
[6]First example found in [4].
[7]The reference of his paper are labelled by a letter between square brackets.

finite space groups, whose translation groups are finite, is much more complex [b] than for infinite ones. There exist infinitely many groups that are not correlated to the 230 space groups. So the BvK groups are considered *only* as a finite homomorphic image of the true (i.e. infinite) space groups: $\mathbb{G}_N = \mathbb{G}/(N\mathfrak{T})$ whose number of elements is $|\mathfrak{P}|N^3$ when[8] $N > 0$. As we shall explain, one has to reject many values of N. A mathematical theorem states that if N and $|\mathfrak{P}|$ are relatively prime, then the corresponding BvK group is the semi-direct product $\mathbb{G}_N = Z_N^3 Ⓢ \mathfrak{P}$; so this BvK does not distinguish between the different space groups of an arithmetic class[9]. So non-symmorphic groups could have simple bands! For instance if N is even and not a multiple of 3, $\mathbb{G}_N$ represents both **P3** and the enantiomorphic pair of (isomorphic) space groups $\mathbf{P3_1}$ and $\mathbf{P3_2}$. Notice that this group has only 3 equivalent classes of elementary band representations, depending on the choice of the inducing one dimensional representation of $\mathfrak{P} \sim Z_3$ but independent of the position q, while for N a multiple of 3 (independently of its oddness or evenness), there are 3 distinct Wyckoff positions and therefore 9 simple band representations.

To summarize: The value of N must satisfy the following three conditions:
1. The $\mathbb{G}_N$'s for the different non isomorphic space groups of an arithmetic class, are non isomorphic; that N is not relatively prime with $|\mathfrak{P}|$ is necessary, but not sufficient e.g. for the groups of the arithmetic class **P6**, N must be a multiple of 6.
The homomorphism $\mathbb{G} \longrightarrow \mathbb{G}_N$ must define a bijective (= one to one onto) correspondence between the strata of the respective actions of $\mathbb{G}$ and $\mathbb{G}_N$,
2. on their respective Brillouin zones (= BZ) $\mathcal{S}_1^3$ and Z_N^3
3. i.e. the Wyckoff positions of the respective spaces $\mathbb{R}^3$ and $\mathcal{S}_1^3$.

These conditions are satisfied when N is a multiple of 12 (also stated without explanations in [13]). The number of Wyckoff positions with $\mathbb{G}_q \sim \mathfrak{P}$ for $\mathbb{G}_N$ divides the number of those for $\mathbb{G}$. When the former number decreases, of course the corresponding band representations become equivalent since they become induced from conjugate subgroups of $\mathbb{G}_N$. Notice also that the "good" values of N may imply unwanted properties of $\mathbb{G}_N$. For instance **F222** has no centre and 4 Wyckoff positions with point group symmetry $222 = D_2$; the number of elements of the centre of $\mathbf{F222}_N$ is equal to the number of its Wyckoff positions; that number is 1,2,4 for the respective set of N values: N odd, $N \equiv 2 \bmod 4$, $N \equiv 0 \bmod 4$.

Nearly 60 years ago Wigner and his collaborators explained to us the richness of the use of the true space groups in physics. Let us quote some sentences from the introduction of the paper:

Theory of Brillouin zones and symmetry properties of wave functions in crystals.
L.P. Bouckaert, R. Smoluchowski, E.P. Wigner, Phys. Rev. **50** (1936) 58-67

[8]Remark that $\mathbb{G}_0 = \mathbb{G}$ and $\mathbb{G}_1 = \mathfrak{P}$.

[9]An arithmetic class is a conjugacy class of a finite subgroup of $GL_n(Z)$. It defines an action of $\mathfrak{P}$ on the lattice $\mathfrak{T}$. For all n Jordan proved that the number of arithmetic classes is finite. For $n = 3$ it is 73; hence the existence of 73 symmorphic groups. The international symbols (in ITC) for the non symmorphic space groups of an arithmetic class are obtained from the symbol of the symmorphic ones by adding indices in the figures (skew rotations) and//or replacing some letters m (representing reflections) by a, b, c, d, n (different types of glide reflections). The international symbol of a space group gives its group law: the (older) Schönflies symbols are inferior; they should be obsolete.

Thus far the group theory of the B-Z is not different from the group theory of any other system. But while in atoms, molecules, etc., the characteristic values of (1) [= the eigenvalues of the Schrödinger equation for bound states] *are well separated, the characteristic values of (1) for a crystal form a continuous manifold....*[for instance the energy E is a function over the B-Z].

Thus a certain topology for the representations must exist and it will be shown that part of this topology is independent of the special B-Z. [...]

[The introduction ends with the sentence]:

The investigation of the "topology" of representations will be essentially the subject of this paper, from the mathematical point of view.

This paper never mentions the Born-von Karman method. It is worth quoting its footnote 10a: *The case of accidental degeneracy will be treated in a paper by C. Herring, to appear shortly* [Phys. Rev. **52** (1937) 365-367]. *We wish to thank Mr C. Herring for interesting discussions on this subject.*

3. Infinite (True) Space Groups

The simplest way to extend the study of SBR from BvK groups to infinite space groups is to do it in the Wannier basis; one passes from the $N^3 \times N^3$ matrices to infinite matrices in an enumerable basis. DZD do it first for the simplest possible case: the space group in one dimension containing the inversion through the origin. They obtain a very striking result: when N is even, there are four inequivalent SBR; but, in the Wannier basis, they are all equivalent for the corresponding infinite group! That is a particular case of the general theorem they prove:

Theorem. *For each (true) space group, all SBR are weakly equivalent.*

The notion of *weak equivalence* that DZD introduced, means equivalence by a unitary matrix (denoted by $\mathbf{S}$) in the Wannier basis, but in the continuous Bloch basis, the function $F(\mathbf{k})$, which represents the diagonal intertwinig matrix has to vanish on a subset of the the higher symmetry strata of BZ (it is modulus one on the generic - open dense - stratum). Since the union of non generic strata has zero measure that pathology of $F(\mathbf{k})$ has no effect on the value of the integral (27) which defines $\mathbf{S}$ from $F(\mathbf{k})$.

4. Critical Comments and Outlook

The Mackey theory [10] of induced representations of locally compact groups applies to the very particular case (from its point of view) of space groups; since it is a measure theoretic formalism, it also forgets the (zero measure) non generic strata of BZ; so it yields the more general theorem: For each true space group, BR with the same number of branches are equivalent! That theory is useless to physics, just as the weak equivalence studied by DZD.

In that paper the authors point out that in the basis transformed by the matrix $\mathbf{S}$ of a weak equivalence, the Wannier functions are no longer (exponentially) localisable.

Their paper also proves that for weak equivalence, $F(\mathbf{k})$ *cannot be continuous.* In [12] it had been shown (using limits of BvK groups) that it is also the case for the equivalence (found in [13]) inside the 14 pairs (given here in (2)) of SBR. The proof of DZD is better and it shows that this non continuity of $F(\mathbf{k})$ is compatible with $|F(\mathbf{k})| = 1$ everywhere on BZ.

It was proved by Kohn [c] in one dimension and by Nenciu [d] in 3 dimensions, that the Wannier functions of SBR can be chosen to be analytic functions. Instead of using a Hilbert space of square integrable functions, one may wonder that physics might require Hilbert spaces of analytic functions (first used by Bargmann [e]), although nothing is known about the analyticity of Wannier functions for the BR with several branches.

It was first shown by Herring [f], that the matrix elements of some representations of two non symmorphic groups could not be analytic on BZ, but only on a multiple covering; that is true for *any* non symmorphic group. That is an example of *a certain topology for the representations* predicted by the quoted BSW paper. Indeed, when one makes closed loops on BZ, some sets of $\mathbb{G}$ unirreps have their elements permuted. However, for the direct sum of the unirreps in such a set, one can make analytic the matrix elements of such reducible representation of the space group. For BR it is worth pursuing the problem of *topology for these representations.*

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