THE STRUCTURE OF SPACE - GROUPS' UNITARY REPRESENTATIONS

Louis MICHEL
I.H.E.S.
91440 Bures-sur-Yvette
FRANCE

Jan MOZRYMAS
Institute of Theoretical Physics
University of Wrocław
ul.Cybulskiego 36
50-206 Wrocław, POLAND

ABSTRACT

For systems with a symmetry group G, the description of physical phenomena corresponding to a representation of G, depends only on the image of this representation. The classification of the images of the unirreps (unitary irreducible representations) of the little space groups G_k is remarkably simple. The nearly four thousands inequivalent unirreps corresponding to high symmetry wave vectors k have only 37 inequivalent images.

Unitary representations of space groups are a very useful tool for the study of many problems of crystal physics such as: the structure (and labelling) of electronic levels and energy bands, the vibration spectrum and phonon dispersion relations, the selection rules in transitions between quantum states, the symmetry change in a second order phase transition, etc. Under the influence of Wigner, a systematic study of these representations started nearly fifty years ago[1,2,3,4]. Finally, for the last twenty years, more and more complete (and expensive) tables of space groups unirreps (unitary irdeducible representations) appeared[5,6,7,8,9]. (Each of the 230 spacegroups has an infinity of unirreps, so most of them are labelled by continuous parameters which appear explicitly in the tabulated matrix elements). Thanks to these and associate tables (e.g. Clebsch Gordan coefficients, physicists can compute for each case what they need, as efficiently as they wish. There is a drawback in this situation; it can be best understood by an historical comparison: trigonometric function tables were built to satisfy as efficiently the needs of astronomers, land surveyors, physicists... However, for the progress of science, the knowledge of the trigonometric function values has not been sufficient, another type of knowledge was required: their geometrical meaning, their analytic properties, etc. This lecture is devoted to the "other type of knowledge" physicists need concerning space groups unirreps.

Given a representation Γ of a group G, one must first look for its kernel, Ker Γ, which is an invariant subgroup of G and its image, Im Γ, which is the quotient group Im Γ = G/Ker Γ. For physical phenomena concerning the state-vectors of the carrier space of the representation Γ of the symmetry group G, physics feels only Im Γ and forgets Ker Γ. For example, most macroscopic properties of crystals do not depend on the translation T of the space group G but only on the pointgroup P = G/T. How does the physics formalism implement the underline sentence? All physical properties of a system with symmetry group G must be described in term of invariants and covariants of G; the invariants and covariants built on a representation Γ of G depend only on Im Γ.

A classification of group representation images yields therefore a classification of corresponding physical phenomena. To perform this classification we introduce a new equivalence, much weaker than the usual one, between group representations[11]. Given two linear group representations

$$G \xrightarrow{\Gamma} \mathrm{Im}\,\Gamma \to 1 \ , \quad G' \xrightarrow{\Gamma'} \mathrm{Im}\,\Gamma' \to 1$$

on the carrier spaces E and E', they are weakly equivalent if there exist an inversible linear map $E \xrightarrow{\gamma} E'$ which transform the set of operators (or matrices) of Im Γ into that of Im Γ'

$$\{\mathrm{Im}\,\Gamma'\} = \gamma\{\mathrm{Im}\,\Gamma\}\gamma^{-1} \tag{1}$$

We can also say that $\gamma_o\Gamma$ is a representation of G whose image Im $\gamma\circ\Gamma$ = Im Γ'. Remark that γ defines an isomorphism $1 \to \mathrm{Im}\,\Gamma \xrightarrow{\tilde{\gamma}} \mathrm{Im}\,\Gamma' \to 1$ between the two images. We emphasized that the nature of the physical phenomena "depends only on the image, but the isomorphism $\tilde{\gamma}$ will help us to establish the dictionary for translating the phenomena concerning the state vector of E into those of E'. This two vector spaces need not be distinct: a simple example occurs when $\alpha \in$ Aut G (α is an automorphism of G) and $\Gamma' = \Gamma\circ\alpha$. The two representations Γ' and Γ of the symmetry group G may not be equivalent when Γ is not an inner automorphism, but they are weakly equivalent since their images coincide, ($\gamma = 1$). There is a complete translation (i.e. an isomorphism) between the two sets of physical phenomena described by the carrier space of the two representations Γ' and Γ. This translation is the object of the contribution by R.Dirl[12] in these proceedings.

Although our program of classifying the weak equivalence classes of space group unirreps is not completed, we hope that the preliminary results we give here will show its interest. Before explaining our results, we wish to present a relevant remark on the nature of the image of the space group unirrep Γ of G on the vector space E which is involved in the Landau theory[13,14] for the second order phase transition with a spontaneous symmetry breaking from G to its subgroup H. This group H is an isotropy group of the unirrep Γ of G, that of a minimum of a G invariant potential on E. It is easy to show that the Kernel of the representation Γ is the intersection of all G subgroups in $[H]$, the class of G-subgroups conjugated to H . If the transition is to an ordinary crystal state (and not to an incommensurate crystal) H is a space group. This implies that Ker Γ contains a lattice translation group ($\sim Z^3$) so Im Γ is finite. On the contrary, in the case of incommensurate transition, Im Γ is infinite (i.e. enumerable).

We do not need to recall here the notions of group orbits, of cohomology, of free modules since all these notions were used by previous lecturers and no questions were asked concerning their meaning, but it might be appropriate to explain a few basic concepts concerning crystallographic space groups. The translation group T of a space group G is an invariant subgroup isomorphic to Z^3 (and closed in R^3, the translation group of the Euclidean group). Its automorphism Aut T $\sim GL(3,Z)$. A space group G is a discrete closed subgroup of $E(3)$, the 3-dimensional Euclidean group (which is the semi-direct product $E(3) = R^3 \square O(3)$) so the point group $P = G/T$ has to be a finite group. All possible actions of P on T are given by the distinct injections

$$1 \rightarrow P \overset{\Delta}{\rightarrow} GL\ (3,Z) \sim \text{Aut } T \tag{2}$$

i.e. by the conjugation classes of finite subgroups of $GL(3,Z)$. There are 73 such classes and they are called arithmetic classes. For each of the 73 pairs P, Δ one can determine all possible groups extensions G solutions of

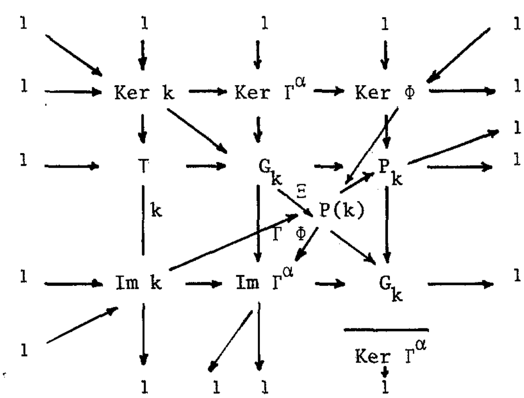
$$\begin{array}{ccccccccc} & & & & & & 1 & & \\ & & & & & & \downarrow & & \\ 1 & \longrightarrow & T & \longrightarrow & G & \longrightarrow & P & \longrightarrow & 1 \\ & & & & & & \downarrow \Delta & & \\ & & & & & & \mathrm{Aut}\ T & & \end{array} \qquad (3)$$

These solutions form an Abelian group $H^2_\Delta(P,T)$, the second cohomolgy group of P in T with action Δ. To the zero element correspond the semi-directproduct $T \overset{\Delta}{\square} P$. (The 73 such semi-direct products are called "symmorphic" in crystallography). Let N(P) be the normalizer of P in Aut T $\sim$ GL(3,Z); since this group acts on P and on T, it acts on $H^2_\Delta(P,T)$. Inequivalent but isomorphic extensions form an orbit of N(P). As a result there are 219 isomorphic classes of 3-dimensional space groups. However the traditional classification of space groups established at the end of last century in crystallography corresponds to the orbits of $N_o(P) = N(P) \cap SL(3,Z)$. Since 11 orbits of N(P) split into pairs of orbits of $N_o(P)$ (the so called enantiomorphic pairs) there are therefore 230 crystallographic classes of space groups.

Remark also that the set of translation lattices T form an orbit $[GL(3,R): GL(3,Z)]$. The action of the subgroup O(n) of GL(3,R) on this orbit yields seven strata (a stratum is the union of all orbits of the same type i.e. with same conjugation class of isotropy groups) corresponding to the seven crystallographic systems. The corresponding seven isotropy groups C_i, C_{2h}, D_{2h}, D_{4h}, D_{3d}, D_{6h}, O_h, are called holohedries and we denote them P_H. They are 14 conjugation classes (respectively 1, 2, 4, 2, 1, 1, 3) of the seven P_H in GL(3,Z). These fourteen actions of P_H of T define the 14 Bravais classes of lattice.

Since T is isomorphic to Z^3, its dual T^*, (i.e. its group of character) is isomorphic to $U(1)^3$ and has the topology of a 3-dimensional torus. T* is the Brillouin zone and its elements are the wave-vectors usually denoted k. (Beware that the use in physics of the wave-vectors may not be always equivalent to their use here as characters of T). The coordinate of k in $U(1)^3 = T^*$ are traditionally given by three real numbers modulo one and the group law of T* is noted additively. Wigner taught us the Frobenius method for determining the unirrep of a group with one Abelian invariant subgroup. In the case of G of (3), consider an orbit G.k of G on T*. Let G_k be an isotropy group of this orbit and Γ^α one of its unirrep. By induction to G one obtains an unirrep $\Gamma^{\alpha}_{G_k}\uparrow G$ of G and this method yields the whole set of inequivalent G unirreps. Theseare therefore labelled by the orbits (physicists say the stars) of G on T^* and the inequivalent irreps of the corresponding G_k. All quoted tables leave the induction $\Gamma^{\alpha}_{G_k}\uparrow G$ to be performed by the users. Here also we discuss only the unirreps Γ^{α} (Remark that each G_k is a space group and any space group can be a G_k, e.g. $G = G_o$ for $k = 0$; then the corresponding G unirrep has T in its kernel and is therefore a unirrep of P).

We denote by Ker k, Im k, the kernel and the image of the unirrep k of T. Given the unirrep Γ^{α} it is natural to apply the Noether isomorphism theorems to G_k and its two invariant subgroups Ker Γ^{α} and Ker k. All results are summarized (and visualized) in the commutative Diagram 1 of exact sequences.



<u>Diagram 1</u>

On this diagram, aligned arrows define an exact sequence of group homomorphisms.

We have used the notation $P_k = G_k/T$ for the "little point group" (i.e. the isotropy group of k in the action of P on T*). Very naturally we are led to consider the quotient group

$$P(k) = G_k/\mathrm{Ker}\ k = \mathrm{Im}\ \Xi \qquad (4)$$

which seems to have been first introduced by Herring[4] and is sometimes called the "extended little point group".

We note that Im Γ^{α}, the image of the representation Γ^{α} of G_k is also the image of the irrep Φ of P(k); indeed $\Gamma = \Phi \circ \Xi$. It is easy to check that P(k) is a central extension of P_k by Im k

$$P_k = P(k)/\mathrm{Im}\, k, \quad \mathrm{Im}\, k < \text{Center of } P(k) \tag{5}$$

For a given arithmetic class, the set of P(k) form the cohomology group $H_o^2(P_k, \mathrm{Im}\, k)$. To the map $T \overset{k}{\to} \mathrm{Im}\, k$ corresponds the functorial homomorphism

$$H_\Delta^2(P_k, T_m) \xrightarrow{\tilde{k}} H_o^2(P_k, \mathrm{Im}\, k) \tag{6}$$

This defines a method of computation of the P(k)'s. Before giving the results of these computation, we wish to make several remarks:

i) Only the images Im Φ of "allowed" irreps Φ_a of P(k) yields Im Γ = Im Φ. These allowed irreps are characterized by "Im k is a subgroup of Im Φ = Im Γ^α" or equivalently

$$\text{"}\Phi \text{ is allowed"} \iff \mathrm{Ker}\, \Phi \cap \mathrm{Im}\, k = \{1\} \tag{7}$$

In the literature, the construction of G_k irreps is usually based on the study of projective representation of P_k. Indeed to the irreps $\mathrm{Im}\, k \xrightarrow{r} U(1)$ of the Abelian group corresponds the homomorphism $T \xrightarrow{r\circ k} U(1)$ and the functorial homomorphism $H_\Delta^2(P_k, T) \xrightarrow{\tilde{r}\circ\tilde{k}} H_o^2(P_k, U(1))$. In our opinion, this traditional method inspired from the old Clifford paper[15] is awkward; since $\tilde{r}\circ\tilde{k}$ factorizes we do believe that our method based on $\tilde{k}$ and P(k) is preferable.

ii) It is true that some authors have considered "auxiliary" groups for building the irreps of G_k (e.g.)[9] where 92 auxiliary groups are used). However these auxiliary groups are not systematically obtained and not all of them are P(k)'s.

iii) We see that "Im $\Gamma^\alpha_{G_k}\uparrow G$ is finite" $\iff$ "Im Γ^α finite" $\iff$ "Im k finite". Moreover, from Artin's theorem dim $\Gamma^\alpha_{G_k}$ = dim Φ divides the order of "P(k)/Center of P(k)" which divides $|P_k|$, the order of P_k = P(k)/Im k. So the dimension of the induced representation divides $|P|$ (which divides 48), a well known result.

iv) If P_k is cyclic (there are ten cyclic groups among the 32 point groups) its central extension (e.g. P(k)) are Abelian. When it is possible, it is interesting to decompose the P(k)'s into a direct product

$$P(k) = A(k) \times S(k) \tag{8}$$

where A(k) is an Abelian group and S(k) does not contain Abelian factors (we will call it the skeleton of P(k)). Indeed the unirreps of the Abelian groups are one-dimensional and easy to determine: their images are cyclic when the Abelian group is finite. As an example of the simplification introduced by (8) note that for trivial extensions of $H^2_o(P_k, \mathrm{Im}\, k)$ and this includes the symmorphic groups and all G_k in the kernel of $\tilde{k}$, $P(k) = \mathrm{Im}\, k \times P_k$ and the 32 P_k's themselves lead to only 4 non-isomorphic skeletons (isomorphic to D_3, D_4, T, O). The unirreps of P(k) are those of S(k) multiplied tensorially by the one dimensional unirreps of A(k).

v) Finally, not only Im k and P_k are the same for all G_k of the same arithmetic class, but there is a strong correlation between P_k and Im k. For a given P_k, and independently of its Bravais class, the structure of Im k is fixed up to few alternatives. We did not find these simple geometrical relations in the literature. They were published with B. Stawski as a poster of the Austin conference[16]. It is useful to reproduce them here (Table 1). Note that for the 22 non-polar groups P_k the image Im k is finite, cyclic and its order divides 6. For the ten polar P_k's, Im k is infinite only if it contains a factor Z^δ with $\delta = 1,2,3$; it is the number of (relatively) irrational components of k in $T^* \sim U(1)^3$.

Here are some results we have already obtained. The zero dimensional strata in the action of the seven P_H on the T* of the 14 Bravais lattice contain 80 orbits which contain 128 k's, the "high symmetry wave vectors" of Herring. They yield 1370 P(k)'s and more than 3800 inequivalent unirreps of C_k's. However these P(k)'s fall into 68 isomorphic classes and there are only 26 distinct skeletons S(k) of order.

order	6	8	12	16	24	32	48	96	Total	
nb of S(k)	1	2	2	6	4	5	4	2	26	(9)

Finally these nearly four thousand tabulated G_k unirreps have only 37 <u>inequivalent images</u>.

TABLE 1: Possible Im k's corresponding to a given P_k (independently from its Bravais lattice); d = dimension of the stratum in the action of the holohedry P_H of P_k on the Brillouin zone T*. The 10 cyclic P_k are underlined. m is an arbitrary positive integer. Z_m is the cyclic group of order m, Z the infinite cyclic group.

d	nb of P_k		P_k	Im k
0	22	13	$\underline{C_i}, C_{2h}, C_{4h}, D_{2h}, \underline{S_6}, C_{6h}, D_{3d}, D_{4h}, D_6, D_{6h}, T_h, O, O_h$	$\{0\}, Z_2$
		6	$D_2, D_{2d}, \underline{S_4}, D_4, T, T_d$	$\{0\}\ Z_2, Z_4$
		3	$D_3, \underline{C_{3h}}, D_{3h}$	$\{0\}, Z_2, Z_3, Z_6$
1	8	2	$C_{6v}, \underline{C_6}$	Z_m, Z
		2	$C_{3v}, \underline{C_3}$	$Z_m, Z, Z_3 x Z$
		4	$C_{4v}, \underline{C_4}, C_{2v}, \underline{C_2}$	$Z_m, Z, Z_2 x Z$
2	1		$\underline{C_s}$	$Z_m, Z_m x Z, Z^2, Z_2 x Z^2$
3	1		$\underline{C_1} = \{1\}$	$Z_m, Z_m x Z, Z_m x Z^2, Z^3$

Their dimension is

dimension	1	2	3	4	6	
nb of images	7	20	6	3	1	(10)

It is worthwhile to compute the isotropy groups of these 37 images and give the generators of their free module of invariants. This is nearly completed. Only for the four P_k's (C_{nv}, n = 2,3,4,6) of one dimensional strata will there appear new skeleton of non Abelian P(k)'s. They are infinite in number but fall into few families, all characterized in reference[17].

We will publish elsewhere, with all relevant details these results on the structure of all G_k unirreps when they will be completed. The complete realization of this program will require to perform the induction $\Gamma^{\alpha}_{G_k} \uparrow G$. Not only, as we will show, the present sets of long tables can be replaced by a sequential set of few short tables easy to implement in computers, but we hope it becomes clear that the "other type of knowledge" about space group unirreps can be useful for a deeper understanding and, in the same time, a simplification of the study of the related physics phenomena.

Another comparable example concern the knowledge of the invariants of a given symmetry group G. With computer help physicists are producing more and more tables of G invariants (for point groups and spacegroups). They can only be incomplete (since there is an infinity of polynomial invariants). However we know since Hilbert[18] that the ring of polynomial invariants of a finite group image is finitely generated. This extend to compact images: this is the case of the topological closure of the non-finite image of space groups (we remark that their smooth invariants are those of this closure). Very recently it can be proven that the smooth invariant - or covariant - functions on the m dimensional carrier space of Im Γ form a <u>free finite dimensional module</u> on a smooth function ring generated by m algebraically independent invariant polynomials[19]. The knowledge of such m polynomials and those of the free module basis gives a much more important knowledge for physicists than any table listing invariant polynomials.

ACKNOWLEDGEMENTS

One of us (L.M.) is very grateful to the organizers of this colloquium for its very stimulating atmosphere.

J.Mozrzymas has not been able to read the last version of this manuscript and is not responsible for the errors it could contain.

REFERENCES

1- F.Seitz, Z.Kristallogr. Kristalgeom. <u>88</u> (1934) 433, <u>90</u> (1935) 289, <u>91</u> (1935) 336, <u>94</u> (1930) 100.

2- L.P.Bouckaert, R.Schmoluchowski, E.P.Wigner, Phys.Rev. <u>50</u> (1936) 58.

3- F.Seitz, Ann.Math. <u>37</u> (1936) 17.

4- C.Herring, J.Franklin Institute <u>233</u> (1942), 525.

5- D.K.Faddeyev, Tables of the principal unitary representations of the Fedorov groups Acad.Sci. USSR, Translation Pergamon, New York, 1946.

6- O.V.Kovalev, Irreducible representation of space groups, Izd.Akad. Nauk. Ukraine hoj USSR, translation-Gordon Breach, New York, 1965.

7- S.C.Miller, W.F.Love, Irreducible representations of space groups. Pruett, Boulder Colorado 1967.

8- J.Zak, P.Casher, M.Gluck, Y.G.Gur, The irreducible represenations of space groups, Benjamin, New York 1969.

9- C.J.Bradley, A.P.Cracknell, The mathematical theory of symmetry in solids, Clarendon Press, Oxford 1972.

10- A.P.Cracknell, B.L.Davies, S.C.Miller, W.F.Love, General introduction and Tables of irreducible representations of space groups, Plenum Press, London 1979.

11- L.Michel, J.Mozrymas, Match 10 (1981) 223.

12- R.Dirl, These Proceedings.

13- L.D.Landau, Phys.Z.Soviet 11 (1937) 26, 545.

14- L.D.Landau, E.M.Lifschitz, Statistical Physics, translation Pergamon Oxford 1965.

15- A.H.Clifford, Ann.Math. 38 (1937) 533.

16- L.Michel, J.Mozrymas, B.Stawski, Lecture Notes Phys. 94 (1979) 86, Springer 1979.

17- H.S.M.Coxeter, W.O.J.Moser, Generators and Relations for discrete groups, Springer (1957).

18- D.Hilbert, Math.Ann. 36 (1890) 473.

19- M.Jaric, L.Michel, R.T.Sharp, These Proceedings p. and to appear.