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EXOMORPHISM OF GROUP SUBGROUP RELATIONS AND LATTICES OF STABILITY SPACES

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1. Introduction.

The study of subgroups of the space group is an important part of the space group theory, especially in connection with the theory of structural phase transitions, crystallographic twinning, domains and domain walls. The available information on subgroups of space groups [1] is based on the theorem of Hermann [2] (which is a direct consequence of the 'diamond' isomorphism theorem[3]) and consists in listing of maximal equitranslational and equiclass subgroups and conversely of the minimal supergroups..

The purpose of this contribution is to discuss some aspects of the theory of group subgroup relations connected with a new trend in investigations of subgroups of space groups which can and should be opened and which relates the theory of subgroups with the theory of representations. The first step has, in fact, already been done by Ascher [4] who has shown that the problem of a structural phase transition from the symmetry of a space group to its subgroup can always be solved in terms of a certain finite group - the image of the representation of the transition parameter. His epikernels of ireps (here we mean by irep a representation irreducible on the real) are subgroups of primary importance. It can be shown that every subgroup of a finite group can be expressed (perharps in several ways) as an intersection of epikernels of its ireps [5].

We shall, for simplicity, limit our present discussion only to subgroups of finite groups. The results can, however, be applied in consideration of those subgroups of space groups which are themselves space groups of the same dimension. Three points connected with the subduction of identity representation will be discussed here: 1. Exomorphism of group subgroup relations, which is just an equivalence with respect to all aspects of the subduction of identity representation. 2. The stability spaces of subgroups for which we show that they form lattices dual to the lattice of subgroups. 3. The problem of generation of stability spaces, which can also be formulated as a problem of 'faint interactions' in the phase transition theory [6]. There is also a connection of this problem with the theory of extended integrity bases, which is briefly reviewed in another contribution of this meeting.

2. Group lattices.

Subgroups of a given group G form an algebraic structure $\mathcal{L}(G)$ called the group lattice. Since the language of lattice theory is convenient for our purposes, we shall recall some basic notions [3,7].

The lattice is generally defined: (i) either as a partially ordered set with least upper and greatest lower bound for every pair of its elements, or (ii) as a structure with two algebraic operations – union and intersection – which satisfy the idempotent, commutative, associative, and absorption law. It can be shown that both definitions are equivalent and the least upper bound can be identified with union, the greatest lower bound with intersection. Accordingly, we can define isomorphism of two lattices or automorphism of a lattice as mappings which preserve either the inclusion relations or both unions and intersections. Analogously we define duality of lattices as a mapping which reverses all inclusion relations or which interchanges all unions by intersections and vice versa.

The lattice $\mathcal{L}(G)$ of subgroups of the group G is a lattice in which the inclusion relation $\subset$ and the intersection $F \cap K$ of subgroups F and K have the usual set-theoretical meaning, while the union $F \cup K$ is that subgroup of G which contains all possible products of elements of F and K. Each automorphism of the group G defines an automorphism of the group lattice $\mathcal{L}(G)$. Other lattice automorphisms are not of interest for us.

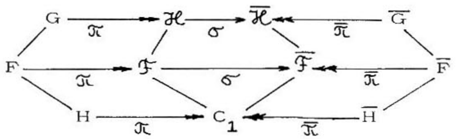
The lattice $\mathcal{L}(G)$ of a space group is an infinite lattice. On the other hand, any subgroup F of G which is a space group of the same dimension is of finite index in G. If F itself is not normal, then there exists a set of conjugate to it groups F_i. The intersection $H = \text{core } F = \bigcap_i F_i$ is normal in G and, in fact, it is the greatest normal subgroup of G contained in F (and hence also in all F_i). The symbol core F means the kernel of the permutation representation of G on cosets of F [4]. The group H is also of the same dimension as G, hence of finite index in G, the factor group $\mathcal{H} = G/H$ is therefore finite and there exists a 'canonical epimorphism' $\pi : G \twoheadrightarrow \mathcal{H}$, which maps any subgroup K of G containing H onto the subgroup $\mathcal{K} = \pi K$ of the factor group $\mathcal{H}$. Vice versa, to each subgroup $\mathcal{K}$ of $\mathcal{H}$ there exists a subgroup K of G which contains H and for which $\pi K = \mathcal{K}$. Hence any subgroup K of G can be embedded into a finite sublattice $\mathcal{L}(G/H)$ of the lattice $\mathcal{L}(G)$, and this sublattice is isomorphic to the lattice $\mathcal{L}(\mathcal{H})$; the canonical epimorphism π maps this sublattice onto the factor group lattice: $\pi\mathcal{L}(G/H) = \mathcal{L}(\mathcal{H})$. The sublattice defined by the normal subgroup H = core F is the least such sublattice in which F can be embedded.

3. Exomorphism of group subgroup relations.

Let us say for brevity 'symmetry descent' $G\downarrow F$ instead of relation of a subgroup F to the group G. We define the following equivalence of symmetry descents:

Definition 1: We shall say that two symmetry descents $G\downarrow F$ and $\overline{G}\downarrow\overline{F}$ are exomorphic , if the following two conditions are satisfied: (i) the factor groups $\mathcal{H} = G/H$ and $\overline{\mathcal{H}} = \overline{G}/\overline{H}$, where $H =$ core F, $\overline{H} =$ core $\overline{F}$, are isomorphic, (ii) among the isomorphisms of these factor groups such isomorphism $\sigma : \mathcal{H} \longrightarrow \overline{\mathcal{H}}$ exists, which maps the factor group $\mathcal{F} = F/H$ onto the factor group $\overline{\mathcal{F}} = \overline{F}/\overline{H} = \sigma\mathcal{F}$.

This definition can be illustrated by the following diagram:



where π and $\overline{\pi}$ are canonical epimorphisms which map the groups G, $\overline{G}$ onto the isomorphic factor groups $\mathcal{H}$ and $\overline{\mathcal{H}}$, and σ is the isomorphism satisfying the condition (ii). Exomorphism is evidently an equivalence in the mathematical sense and can be used to distinguish classes of equivalent symmetry descents - the exomorphic types of symmetry descents. Exomorphism has been first introduced at the Crystallographic Congress in 1978 [8]; consideration of crystal point groups reveals only 44 types of symmetry descents (excluding the trivial one).[9]. To these 44 types belong 212 geometrically inequivalent symmetry descents within the crystal point groups, 1532 within the magnetic point groups and thousands of actual symmetry descents within the space or magnetic space groups.

Application of elements g of G from the left on cosets g_iF of the group F permutes these cosets and defines therefore a permutation representation of the group G with kernel H = core F. It can be shown that the symmetry descents $G\downarrow F$ and $\overline{G}\downarrow\overline{F}$ are exomorphic just if the permutation representations of G on cosets of F and of $\overline{G}$ on cosets of $\overline{F}$ are, as permutation groups, equivalent. It is also worth to mention, that permutation representation of G on cosets of F is just the representation of G induced of the identity representation of the group F.

Let us now look up the situation from the viewpoint of lattices. The first condition of definition 1 requires that groups F, $\overline{F}$ can be embedded into sublattices $\mathcal{L}(G/H)$ and $\mathcal{L}(\overline{G}/\overline{H})$ which are isomorphic in strength of the requirement of the isomorphism of groups $\mathcal{H}$ and $\overline{\mathcal{H}}$. Within the lattice $\mathcal{L}(G/H)$ we find easily all subgroups F_{ij} such that the symmetry descents $G\downarrow F_{ij}$ are exomorphic. To satisfy the second condition of definition 1, we have to apply all automorphisms of the group $\mathcal{H}$ to the subgroup $\mathcal{F}$. This leads to a set of subgroups $\mathcal{F}_{ij}$ (i indicating inner, j an outer automorphism). To groups $\mathcal{F}_{ij}$ then correspond the groups F_{ij} in the lattice $\mathcal{L}(G/H)$.

4. Subduction of identity representation and stability spaces.

If $\chi_\alpha(G)$ is the character of an irep of G and F the subgroup of G, then the branching rules:

$$\chi_\alpha(G)\downarrow F = \sum_\gamma (\alpha\gamma)_F \, \chi_\gamma(F)$$

inform us, how many times an irep $\chi_\gamma(F)$ of F is contained in the representation $\chi_\alpha(G)\downarrow F$ of F subduced of the irep $\chi_\alpha(G)$. Let us denote by $s_\alpha(F) = (\alpha 1)_F$ the subduction coefficients for the identity irep of F; $s_\alpha(F)$ is therefore the number of times the irep $\chi_\alpha(G)$ subduces the identity irep of F. Further we introduce a G-module L_o which contains just once a $\chi_\alpha(G)$-module L_α for each irep $\chi_\alpha(G)$.

Definition 2.1: The subspace of L_o which envelopes all vectors of L_o, invariant under the subgroup F, is called the stability space of F and will be further denoted by $L_1(F)$.

Definition 2.2: If L_n is any G-module, we call its subspace, on which F acts trivially, the stability space of F in L_n and denote it by $L_{n1}(F)$. Particularly, the spaces $L_{\alpha 1}$ will be the stability spaces of F in minimal $\chi_\alpha(G)$-modules L_α. The dimension of these spaces is evidently just $s_\alpha(F) = \dim L_{\alpha 1}(F)$ and their direct sum is the stability space $L_1(F)$.

Theorem 1: The subduction coefficients $s_\alpha(F)$ satisfy the relation:

$$\sum_\alpha s_\alpha(F).d_\alpha = [G:F],$$

where $d_\alpha = \dim L_\alpha$ and $[G:F]$ is the index of F in G.

Proof: According to Frobenius reciprocity theorem, the subduction coefficients $s_\alpha(F)$ give also the number of times the identity irep $\chi_1(F)$ induces the irep $\chi_\alpha(G)$. The dimension of the latter is just d_α and hence the left-hand side of the relation gives the dimension of the space on which the representation of G induced of $\chi_1(F)$ is realized. Since this representation is also equivalent to the permutation representation of G on cosets of F, its dimension must be $[G:F]$.

Each subgroup F of G can be characterized by the set of subduction coefficients $s(F) = (s_1(F)=1, s_2(F), \ldots\ldots, s_\alpha(F), \ldots\ldots)$. The sum of these coefficients is evidently the dimension of the stability space $L_1(F)$. If L_n is any $\chi(G)$-module, n_α the multiplicity with which $\chi_\alpha(G)$ is contained in $\chi(G)$, then the sum $\sum_{\alpha} s_{\alpha}(F).n_{\alpha}$ is the dimension of the stability space $L_{n1}(F)$ of F in L_n. The stability space of the group G itself is simply the space $L_1(G) = L_1$ which contains only a representative of invariants of G; accordingly the $L_{n1}(G)$ is the subspace of invariants of G in L_n. If $K \subset F \subset G$ (the inclusion relation referring to proper subgroups), then from the definition of stability spaces and from the relation of theorem 1 follows $L_1(G) = L_1 \subset L_1(F) \subset L_1(K)$, where the inclusion relations refer here to proper subspaces. We may consider this inclusion relation as a defining relation for the ordered set of stability spaces, obtaining at once the following conclusion:

Theorem 2: Stability spaces $L_1(F)$ of subgroups F of G form a lattice which is dual to the lattice $\mathcal{L}(G)$ of subgroups of G.

Notice, that the theorem does not hold generally for stability spaces of F in any L_n, but holds certainly for all L_n which contain L_o.

5. The lattices of stability spaces.

The theorem 2 follows from the fact that the inclusion relations for stability spaces are reversed in comparison with inclusion relations in the lattice $\mathcal{L}(G)$. It means, accordingly, that unions and intersections are exchanged, so that:

$$L_1(F \cup K) = L_1(F) \cap L_1(K), \quad L_1(F \cap K) = L_1(F) \cup L_1(K).$$

So far we have to consider these relations as formal ones and it is necessary to reveal the meaning of the union and intersection in the lattice of stability spaces in terms of linear spaces, or rather in terms of these spaces as G-modules.

We have already made a natural choice of the meaning of inclusion relation and it is quite straightforward to show that the intersection of stability spaces has also the ordinary meaning of intersection of linear spaces which coincides with set-theoretical meaning of the intersection.

The meaning of the union of stability spaces is more complicated. A rigorous analysis requires introduction of linear operators Ω which project G-modules onto the $\chi_o(G)$-module L_o, leaving the transformation properties of vectors invariant, so that $\Omega(gx) = g\Omega(x)$. The union $L_1(F) \cup L_1(K)$ can then be interpreted as a projection, by such an operator, of the space of all tensors formed on the direct sum of $L_1(F)$ and $L_1(K)$. We shall discuss this conclusion in connection with generation of stability spaces.

6. Stability spaces of normal subgroups and their generation.

Let $H \triangleleft G$ be a normal subgroup of the group G and $\mathcal{H} = G/H$ the corresponding factor group. Then the stability space $L_1(H)$ can be identified with the space $L_o(\mathcal{H})$, which contains just once each $\chi_\gamma(\mathcal{H})$-module L_γ for the irep $\chi_\gamma(\mathcal{H})$. Each $\chi_\gamma(\mathcal{H})$-module L_γ can be interpreted as a $\chi_\gamma(G)$-module, where $\chi_\gamma(G)$ is the irep of G engendered of the irep $\chi_\gamma(\mathcal{H})$ of $\mathcal{H}$. Thus the stability space is simultaneously a G-module and a $\mathcal{H}$-module and it contains all G-modules L_γ the vectors of which are invariant under H.

According to the representation generating theorem [10], a faithful representation $\chi_\alpha(G)$ of the group G generates all ireps $\chi_\gamma(G)$ in the sense, that each irep $\chi_\gamma(G)$ is contained in some finite power of $\chi_\alpha(G)$. The theorem can be narrowed: each $\chi_\gamma(G)$ is contained in some finite symmetrized power of $\chi_\alpha(G)$. Let now $H_\alpha = \ker \chi_\alpha(G)$, so that H_α is normal in G, and let $\mathcal{H}_\alpha =$ $= G/H_\alpha$ be the corresponding factor group. As an irep of $\mathcal{H}_\alpha$ the $\pi\,\chi_\alpha(G) =$ $\chi_\alpha(\mathcal{H}_\alpha)$ is faithful and hence it generates all ireps $\chi_\gamma(\mathcal{H}_\alpha)$ each of which engenders an irep $\chi_\gamma(G)$. In the language of spaces it means, that the $\chi_\alpha(G)$-module L_α generates the whole stability space $L_1(H_\alpha)$ in the sense, that among tensor spaces (or even spaces of symmetrized tensors) on the space L_α we shall find $\chi_\gamma(G)$-modules for each irep $\chi_\gamma(G)$ for which L_γ is a part of $L_1(H_\alpha)$. In the language of polynomials we arrive to a conclusion that there exist polynomial $\Gamma_\gamma(G)$-covariants $p^{(\gamma)} = (p_{\gamma 1}, p_{\gamma 2}, \ldots, p_{\gamma d_\gamma})$, in components of vectors $x \in L_\alpha$, to each irep $\Gamma_\gamma(G)$ engendered of the irep $\Gamma_\gamma(\mathcal{H}_\alpha)$. Finally, in the language of 'faint interactions' of the phase transition theory, where vectors of L_α play the role of the transition parameter, it means that there exists the faint interaction $\sum_j x_{\gamma j} p_{\gamma j}$ for all variables $x_{\gamma j}$ which can onset at the symmetry descent from G to H_α – the $x_{\gamma j}$ are just the components of vectors from the stability space of H .

If $H \lhd G$ is not a kernel of an irep, then it is a kernel of some composed representation and at the same time the intersection of kernels of ireps which enter this representation. The situation is quite analogous to the previous case, instead of the minimal $\chi_\alpha(G)$-module we have, however, to start with a direct sum of minimal G-modules.

Let us now consider the meaning of the union of stability spaces in case of normal subgroups. If $F = \ker \chi_a(G)$ and $K = \ker \chi_b(G)$, then $F \cap K =$ $= \ker (\chi_a(G) \oplus \chi_b(G))$. According to representation generating theorem, the corresponding spaces L_a, L_b generate the stability spaces $L_1(F)$, $L_1(K)$, and the direct sum $L_a \oplus L_b$ generates the stability space $L_1(F \cap K)$ which is just the union $L_1(F) \cup L_1(K)$. It is therefore not necessary to use the direct sum of the full spaces $L_1(F)$ and $L_1(K)$ to generate the union; it suffices to use only the direct sum of their generating spaces.

7. Epikernels and generation of stability spaces for any subgroup.

Epikernel F of an irep $\chi_\alpha(G)$ is defined as a stabilizer of a vector x from the $\chi_\alpha(G)$-module L_α. We can analogously define epikernels of composed representations, but here we shall use the term only for ireps. Every irep has at least two trivial epikernels – the whole group G, which is the stabilizer of null vector, and the kernel $H_\alpha = \ker \chi_\alpha(G)$. The nontrivial epikernels appear in sets of conjugate groups F_i and the group $H_\alpha = \bigcap_i F_i = \text{core } F$ is the kernel of the same irep $\chi_\alpha(G)$. The stability space $L_1(F)$ is the subspace of $L_1(H_\alpha)$ and the spaces $L_{\gamma 1}(F)$ are subspaces of $L_{\gamma 1}(H_\alpha)$. The subduction coefficients $s_\gamma(F)$ are the same for all conjugate epikernels and the subduction coefficient $s_\alpha(F)$ is smaller than d_α. There is a simple criterion (an analogue to the 'chain subduction criterion' [11]), which enables us to determine from subduction coefficients, whether a group F is an epikernel of $\chi_\alpha(G)$:

Criterion: A group F is an epikernel of $\chi_\alpha(G)$ if and only if the relation $s_\alpha(K) < s_\alpha(F)$ holds for every group K which contains F.

For a given epikernel of $\chi_\alpha(G)$, we can choose such form of matrix ireps and hence such bases of $\chi_\gamma(G)$-modules L_γ, that just the first $s_\gamma(F)$ vectors form the basis of $L_{\gamma 1}(F)$. Let us have a polynomial $\Gamma_\gamma(G)$-covariant $p^{(\gamma)} = (p_{\gamma 1}, p_{\gamma 2}, \ldots, p_{\gamma s_\gamma(F)}, \ldots, p_{\gamma d_\gamma})$ and let the vector x run the space L_α. We know, that the polynomial $\Gamma_\gamma(G)$-covariants $p^{(\gamma)}$ in x exist for all ireps $\chi_\gamma(G)$, for which the $\chi_\gamma(G)$-modules belong to stability space of H_α. Now, the first $s_\gamma(F)$ components of such covariant are invariants of the group F, while the remaining are not. If the region, in which x varies, is restricted to the stability space $L_{\alpha 1}(F)$, then the polynomials $p_{\gamma j}$, which were originally polynomials in $x_{\alpha i}$, $i = 1,2, \ldots, d_\alpha$, turn into polynomials of the first $s_\alpha(F)$ variables $x_{\alpha i}$ only. Since each of these variables itself is invariant under F, the polynomials must also be invariant under F. Hence the polynomials $p_{\gamma j}$, for which $j = s_\gamma(F)+1, \ldots, d_\gamma$, must vanish on $L_{\alpha 1}(F)$. This result could be interpreted as generation of the stability space $L_1(F)$ by $L_{\alpha 1}(F)$, if we ascertain that the polynomials $p_{\gamma j}$, $j = 1,2, \ldots, s_\gamma(F)$ do not vanish. Actually, some of these polynomials may also vanish for a given covariant $p^{(\gamma)}$. An inspection of extended integrity bases, which have been so far calculated, shows, that there always exist such covariants, for which these polynomials do not vanish. A question about the general validity of this conclusion has been raised in connection with the problem of 'faint interactions' [6]. This problem is of rather principal character in phase transition theory, where $x_{\alpha i}$ represent the transition parameter and $x_{\gamma j}$ the other onsetting variables – faint variables (for example the components of polarization in 'improper ferroelectric transitions' [12]). Let us outline the proof of the positive answer:

The group F acts trivially on the whole $L_1(F)$. The normalizer $N_G(F)$

of the group F in G leaves the space $L_1(F)$ invariant, i.e. $L_1(F)$ is a $N_G(F)$-module. In fact, this normalizer is the greatest group which sends the vectors of $L_1(F)$ again into $L_1(F)$. The factor group $N_G(F)/F$ can be defined, because F is normal in $N_G(F)$ and, since F is an epikernel of $\chi_\alpha(G)$, this factor group acts faithfully on $L_{\alpha 1}(F)$. Hence the polynomials in variables $x_{\alpha i}$, $i = 1,2, \ldots, s_\alpha(F)$ realize all representations of the factor group $N_G(F)/F$. On the other hand, the variables $x_{\gamma j}$, $j = 1,2, \ldots, s_\gamma(F)$, which correspond to the whole stability space $L_1(F)$ also realize only representations of this factor group.

Hence the space $L_1(F)$ is generated by $L_{\alpha 1}(F)$, if F is the epikernel of $\chi_\alpha(F)$. We can proceed in the same way as in the preceding section to show, that the stability space $L_1(K)$ of any group K is generated by the direct sum of spaces $L_{\alpha 1}(K)$ which has the property that K is stabilizer of a vector of this sum. And finally, we can show, that the meaning of the union of two stability spaces is the projection of tensor product spaces formed by generating spaces of the original stability spaces.

8. Exomorphism and stability spaces.

Let us now consider two exomorphic symmetry descents $G \downarrow F$ and $\overline{G} \downarrow \overline{F}$. Since the factor groups $\mathcal{H}$, $\overline{\mathcal{H}}$ are isomorphic, we can choose the same labelling for their ireps and the same complete set of linear spaces L_α, which are at the same time $\chi_\alpha(\mathcal{H})$- and $\chi_\alpha(\overline{\mathcal{H}})$-modules. The direct sum of these spaces: $L_o(\mathcal{H}) = L_o(\overline{\mathcal{H}})$ can be interpreted as well as the stability space $L_1(H)$ as the stability space $L_1(\overline{H})$. In view of the choice of the isomorphism σ, the groups $\mathcal{H}$ and $\overline{\mathcal{H}}$ act in precisely the same way on $L_1(H)$ and, since the isomorphism maps $\mathcal{F} = F/H$ onto $\overline{\mathcal{F}} = \overline{F}/\overline{H}$, the groups F, $\overline{F}$ act also in precisely the same way on $L_1(H)$. Generally, there is a one-to-one correspondence between groups of the lattices $\mathcal{L}(G/H)$, $\mathcal{L}(\overline{G}/\overline{H})$, $\mathcal{L}(\mathcal{H})$, and $\mathcal{L}(\overline{\mathcal{H}})$ such, that groups corresponding to each other have the same stability spaces, are either together epikernels of the same ireps or intersections of the same epikernels etc. It can be shown, that the exomorphic symmetry descents are also quite equivalent as concerns the mathematical features of corresponding phase transitions - particularly, they lead to the same structure of orbits (domains) and, up to the choice of instability, to the same form of thermodynamic potential.

Finally we shall consider the case, when the subgroup F is an epikernel of irep $\chi_\alpha(G)$. The corresponding group $\mathcal{F}$ is then an epikernel of $\chi_\alpha(\mathcal{H}_\alpha)$. The irep $\chi_\alpha(\mathcal{H}_\alpha)$ is a faithful irep of $\mathcal{H}_\alpha$ or, in other words, a matrix group. This matrix group is the image Im $\Gamma_\alpha(G)$ of the matrix irep $\Gamma_\alpha(G)$. To consider epikernels, it is therefore sufficient to study the irreducible matrix groups. All epikernels of such matrix group Im $\Gamma_\alpha(G)$ = Im $\Gamma_\alpha(\mathcal{H}_\alpha)$ will then correspond to epikernels of ireps of any group G which is an extension of any group H_α by the factor group $\mathcal{H}_\alpha$, namely to those ireps which are engendered of the irep $\Gamma_\alpha(\mathcal{H}_\alpha)$.

9. Conclusion.

The typing of symmetry descents for crystal point groups as well as for the magnetic point groups has already been performed [5,9]. This typing also naturally includes all group subgroup relations between space group for the equitranslational case. As a first step in an analogous study of space groups we have to consider the epikernels of their representations – in the first instance it means the determination of epikernels of images of their ireps. A problem which goes in hand with this determination is the calculation of fundamental algebras for these ireps.

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