科技资料

Proceedings of the International School on SYMMETRY and STRUCTURAL PROPERTIES OF CONDENSED MATTER

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SYMMETRY and STRUCTURAL PROPERTIES OF CONDENSED MATTER

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Editors

W. Florek

T. Lulek

M. Mucha

Mathematical Physics Division
Institute of Physics
Adam Mickiewicz University

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PREFACE

This volume encloses proceedings of the summer school on theoretical physics, held in Zajączkowo, a village near Poznań, in September (6–12) 1990. The banner title of the school was *Symmetry and Structural Properties of Condensed Matter*. The aim of the school was to give participants a survey of research and achievements associated with a description of some properties of condensed matter structure. The bulk material of these proceedings is arranged within three main subjects:

A. Actions of groups on sets and broken symmetries.

B. Racah–Wigner approach to vibrations, electronic states, correlations and superconductivity in multicentre systems.

C. Crystallography and its extensions: crystals, quasicrystals, incommensurate phases, non-rigid molecules and crystals, structure of line polymers.

Obviously the arrangement of materials is not disjoint since there are various connections and overlaps between these main subjects. In particular, lectures dealing with phase transitions could be assigned either to part A or C. This arrangement was suggested merely by our impression that an adequate description of a structure is associated — perhaps in an inevitable way — with various symmetries, and thus with group actions on sets, broken symmetries, etc. It seems therefore reasonable to start with some methods of symmetry investigations in part A, and then with various selected conceptual applications of these methods in the two other parts. Part B deals with some extensions of Racah–Wigner approach from atomic and nuclear to finite multicentre systems, whereas part C is concerned with some modern concepts in crystallography.

Part A starts with general methods of combinatorial analysis of group actions on finite sets. Prof. Kerber puts a special emphasis on the set Y^X of all mappings $f: X \to Y$ from one set X to another set Y. Such sets frequently appear in physical theories in the context of multiparticle states, magnetic configurations, crystal lattices, etc. Symmetries of physical systems are thus associated with actions of symmetric groups or their appropriate subgroups on the sets X, Y, Y^X. Also various combinatorial relations of such actions, like semidirect or wreath products, exponentation, etc. are useful tools in investigation of properties of physical systems.

A systematic approach to research of symmetry and structure of condensed matter is provided by a recipe proposed by Weyl: if a physical model can be described in terms of an orbit of a group G, referred to as the "obvious" symmetry group, then all intrinsic, structural features of this model can be found by investigation of the group Aut G — the "hidden" symmetry of the model. This recipe is formulated and applied to some "non-rigid" generalizations of simple cubic lattice in the lecture of Dr. Mucha. Its also provides a basis for studying some "fractal" generalizations of structure of polymers in the article of Dr. Kuźma, and rarefied bands in the Heisenberg model of a magnet in the contribution of Dr. B. Lulek.

Some further lectures are associated with the actions of the space groups. Prof. Kopský offers a systematic survey of subperiodic classes of three dimensional space groups, like rod and layer classes. Prof. Dirl describes construction of standard actions in a definitely prescribed form, as well as relations between various non-standard settings, which can differ from the standard one by the choice of, e.g., basis, representatives, conjugated subgroups, etc. Appropriate software packages are in preparation.

The remaining lectures in part A are devoted to symmetry breaking in crystals. Prof. Janovec deals with the domain structure in terms of transitive representations of images of space groups. Prof. Yukalov considers local symmetry breaking in crystals and proposes a method for statistical averaging over heterostructural configurations, which coexist fluctuactionally in some regions of an ordered lattice. Prof. Tolédano describes phase transitions with broken group–subgroup relation, and Dr. Sikora and Dr. Tatarienko deal with incommensurate phases.

Part B is devoted to Racah–Wigner approach. This approach has proven to be very successful in the theory of multielectron atoms. Some general features of this approach for the case of atoms and nuclei are contained in lectures of Prof. Wybourne, Dr. Ross (a collaborator of Prof. Butler), Prof. Louck, and Prof. Chatterjee. An extension of the Racah–Wigner calculus to atoms and ions in a crystalline environment is described by Prof. Kibler.

Other lectures in part B deal with some extensions to multicentre systems. An application of duality between symmetric and unitary groups to configuration interaction calculations of electronic structure of molecules, based on symmetric group approach, is presented by Prof. Karwowski. Lectures of Dr. Szopa and Prof. T. Lulek propose an extensions of Racah–Wigner formalism to multicentre systems, based on substitution of irreducible by transitive representations, and of Clebsch–Gordan decomposition by Mackey theorem. The report of Prof. Lehmann is an application Racah–Wigner formalism to classification of energy bands in complex garnet structures.

Part C starts with the lecture of Prof. Janner on definition of crystals and quasicrystals. He points out one feature common to both kinds of ordering: the Fourier transform of the density of a crystal or quasicrystal can be described in terms of an n-dimensional module over the ring Z of integers; $n = 3$ for crystals and $n > 3$ for quasicrystals. Moreover, in addition to "classical" Euclidean symmetries, quasicrystals exhibit also some scaling symmetry operations (e.g. those leading to a Fibbonachi sequence), which are compatible with hyperbolic rather than euclidean geometry. Another application of hyperbolic geometry, in the context of solitons and superstrings, is shown in the lecture of Prof. Mozrzymas. He uses symplectic group instead of orthogonal one in constructing appropriate space groups as extensions. Some non-crystallographic symmetries of spatially one-dimensional solitons (associated intrinsically with the set Y^X rather than X or Y) are reported by Prof. Błaszak. The lecture of Prof. Kopský provides review of various applications of group theory to phase transitions, based on group actions on sets (lattices of subgroups, epikernels, strata, extended integrity bases, etc.). In particular, he expresses some critical remarks on colour groups. The theoretical and model considerations presented on School were nicely encouraged by the lecture of Prof. Łukaszewicz, who gave a review of history of crystallography and pointed out the crucial role of "badly behaved" materials. Just these "bad" materials stimulated (since 1960) further development of crystallography as a science, which otherwise could fell into a push-button routine. Dr. Florek considers in his lecture finite space groups with the wreath product structure. His procedure yields irreducible representations of point groups as exact quantum numbers, in addition to the quasimomentum resulting from purely translational symmetry. Dr. Mulder considers various intermediate phases between a liquid and solid crystal. Appropriate order parameters are determined by symmetry breaking bifurcations. Dr. Ziemczonek deals with symmetries of phonon modes in hexagonal ice. Prof. Gorzkowski demonstrates a nice pattern of a quasiperiodic structure having seven-fold symmetry.

One of the aims of the school was also a review of mathematical tools, used in description of structure of matter. We observe, on the basis of lectures presented here, that such a description involves various branches of mathematics, like group theory and group representations over various fields or rings, elements of modern algebra (homology, Galois theory), fiber bundles and other topics from differential geometry and algebraic topology, etc. It suggests an increasing role of sophisticated modern mathematics in explanation of structural properties of condensed matter (despite still alive "gruppenpest"-type prejudices). Specially now, when the structure of various new "badly behaved" materials has not been explained and remains to be a challenge for modern crystallography.

On behalf of organizers, we would like to thank all participants for their contributions and creation of a specific climate during the school. Special thanks are due to all lecturers for their presentations, tireless discussions, and preparation of manuscripts.

Poznań, 20 October 1990

Wojciech Florek
Tadeusz Lulek
Michał Mucha

CONTENTS

Part B. Racah–Wigner approach to vibrations, electronic states, correlations and superconductivity in multicenter systems

Part C. Crystallography and its extensions: crystals, quasicrystals, incommensurate phases, non-rigid molecules and crystals, structure of line polymers

Supplement: Abstracts of not submitted manuscripts

Part A

Action of groups on sets and broken symmetries

GROUP ACTIONS, CONFIGURATIONS AND FINITE STATES*

A KERBER[†], B LULEK[‡] and T LULEK[‡]

[†]*Department of Mathematics, University of Bayreuth Bayreuth, Germany*

[‡]*Institute of Physics, Adam Mickiewicz University Poznań, Poland*

ABSTRACT

This review article starts with a short description of the theory of finite group actions. The basic notions and methods are introduced and applied in particular to configurations on which there is an action of a symmetry group (particular cases are spin configurations like these of a Heisenberg magnet, but also graphs, switching functions, chemical isomers and many other structures in mathematics and sciences). For more details and proofs see the given references.

1 Introduction

A *configuration* of a set X, say of the set of nodes of a Heisenberg magnet, is a mapping from X into a set Y. This means that to each element $x \in X$ we associate a certain $y \in Y$, say a spin or a color. But a problem arises since usually symmetry groups are involved, so that *different* configurations can be interrelated by symmetry group operations, and hence the configurations fall into classes of *equivalent* configurations under the symmetry group in question. There may in fact be a symmetry group of X, the cyclic group on the set of nodes of the magnet, say, and moreover, there may be also a symmetry group of Y come into play, so that these two groups define a symmetry group on the set of all the configurations, and it is this group which gives rise to the decomposition of the total set of configurations into the *symmetry classes of configurations* which was just mentioned.

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Hence question like the following arise: How many symmetry classes of configurations do exist? Moreover, we would like to know how many classes of configurations are there with certain prescribed properties (say 3 of the nodes carry a spin which is directed upwards, while the other spins are directed downwards). And we might even ask for a way of constructing a complete set of configurations belonging to pairwise different classes, so that we can really check the properties of all the possible situations. Moreover, if such a construction is not possible, we might look for a method which allows a generation at random of configurations that are distributed over the symmetry classes of configurations uniformly at random.
Let us add a second example: interacting particles. Consider n particles, say. A state of these, or, if you prefer, an interaction model, is a mapping from the set X, consisting of all the pairs of particles, into the set $Y := \{0, 1\}$, where the pair $x \in X$ is mapped onto 1 if and only if this pair of particles is assumed to be *interacting* (e.g. the Heisenberg magnet with exchange interactions between nearest neighbours only). Again there may be a symmetry group of the set of the particles, and hence the analogous problems arise here, too.
This shows clearly that configurations, interaction models and the theory of group actions are closely related. Let us therefore begin with a brief review of finite group actions, which we shall then apply to configurations and interaction models in particular. The enumeration methods are discussed in detail and particular emphasize is laid on the application to configurations and their symmetry classes. A paradigmatic example is the Heisenberg magnet.

2 Finite Group Actions

An *action* of a group G on a set X is described by a mapping of the following form:

$$G \times X \to X: (g, x) \mapsto gx, \text{ such that } g(g'x) = (gg')x, \text{ and } 1x = x.$$

We abbreviate this by writing

$$_GX,$$

since G acts from the left on X, and we shall assume in the following that both X and G are *finite*.
Such an action defines various important structures on X and G:

$$G(x) := \{gx \mid g \in G\}, \text{ the } \textit{orbit} \text{ of } x \in X,$$

$$G_x := \{g \in G \mid gx = x\}, \text{ the } \textit{stabilizer} \text{ of } x \in X,$$

$$X_g := \{x \in X \mid gx = x\}, \text{ the } \textit{set of fixed points} \text{ of } g \in G.$$

Many notions of mathematics and sciences can be defined as orbits, stabilizers or fixed point sets, so that the methods we are going to describe can be applied in all these cases. The main properties of actions, orbits and stabilizers are contained in the following items:

- For $g \in G, x, x' \in X$ we have

$$gx = x' \iff x = g^{-1}x'.$$

- Two orbits $G(x)$ and $G(x')$ are either equal or disjoint. Hence a transversal T of the set

$$G\backslash\!\backslash X := \{G(x) \mid x \in X\}$$

of all the orbits yields a partition of X:

$$X = \bigcup_{t \in T} G(t).$$

- The mapping $\varphi: gx \mapsto gG_x$ is a bijection between the orbit $G(x)$ and the set

$$G/G_x := \{gG_x \mid g \in G\}$$

of all the left cosets of the stabilizer of x.

An important consequence of the last item is, that the length of an orbit is equal to the index of the stabilizer of each of its elements, which is the quotient of the order $|G|$ of G and $|G_x|$ of the stabilizer. This is a very strong condition. It allows an easy proof of the following basic lemma which says that the total number of orbits is the average number of fixed points:

2.1 The Cauchy–Frobenius Lemma:

$$|G\backslash\!\backslash X| = \frac{1}{|G|}\sum_{g \in G} |X_g|.$$

This lemma has several refinements, which we are going to describe next.

2.2 The Cauchy–Frobenius Lemma, weighted form: *If $w: X \to R$ is a mapping from X into a commutative ring R, which contains the field $\mathbb{Q}$ of natural numbers as subring, then, for each transversal T of the set $G\backslash\!\backslash X$ of orbits, we have:*

$$\sum_{t \in T} w(t) = \frac{1}{|G|}\sum_{g \in G}\sum_{x \in X_g} w(x).$$