Applications of group theory in crystallography

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Abstract. Group theory is a powerful tool for studying symmetric physical systems. Such systems include, in particular, molecules and crystals with symmetry. Group theory serves to explain the most important characteristics of atomic spectra. Group theory is also applied to the problems of atomic and nuclear physics. This paper gives examples of the use of the apparatus of group theory in research on crystallography, quantum mechanics, elementary particle physics. In particular, in these studies matrix groups and representations of unitary groups are actively used. For such groups we give an overview of the results on their recognition by the spectrum (by the orders of the elements of the group). This direction has been intensively developed in recent years both in our country and abroad. Recognition of finite simple non-Abelian groups by spectrum has been studied for last thirty years in Yekaterinburg at the Institute of Mathematics and Mechanics of the Ural Division of the Russian Academy of Sciences, in Chelyabinsk Federal University and in the Novosibirsk Institute of Mathematics of Siberian Division of the Russian Academy of Sciences. Some simple non-Abelian groups are not recognizable by their spectra. We have proposed an approach for recognizing groups by the bottom layer. The bottom layer of a group is the set of its elements of prime orders. A group is called recognizable by the bottom layer under additional conditions if it is uniquely restored by the bottom layer under these conditions. The paper considers some examples of simple non-Abelian finite groups that are not recognizable by spectra. For these examples, simultaneous recognition by spectrum and by the bottom layer is proved.

1. Examples of the application of group theory in crystallography and related fields

Many publications have been devoted to applications of group theory to crystallography, quantum mechanics, atomic and nuclear physics, elementary particle physics (see, for example, [1–6]).

Group theory is a powerful tool for studying symmetric physical systems. Such systems include, in particular, molecules and crystals. The monograph [1] examines the application of group theory to the study of the vibrations of atoms that make up a molecule relative to their equilibrium positions.

In 1867, a Russian scientist, academician and professor of the Petersburg Artillery School A.V. Gadolin (1828–1892) gave a clear description of 32 crystallographic groups [2].

In quantum mechanics, the state of a system is completely determined by the wave function or operator. If the set of eigenvalues (operator spectrum) is discrete, we are dealing with the quantization phenomenon when the measured values of the operator are discrete.

The symmetry group $G$ is usually determined by several elements (one or two), raising the latter to a power or multiplying them until new symmetry elements appear. Moreover, it may turn out that the
group constructed in this way is only a subgroup of the complete group $G$. To avoid this, it is necessary to use all available information about the symmetry of the system.

In most cases, rotations, reflections and translations act as elements of $G$. In the presence of system symmetry, group theory provides a convenient method for classifying its eigenfunctions and eigenvalues. If the system has symmetry, then under the action of the group's symmetry operations its eigenfunctions are transformed according to irreducible representations.

A physical system that exists due to the attraction between its components has a ground state with maximum symmetry. Mathematically, this means that the ground state must be invariant with respect to all operations of the group.

Crystals, like molecules, have symmetry. This means that the atoms or ions that make up the crystal are arranged in an orderly spatial lattice.

In the general case, a certain set of atoms with a specific arrangement is associated with each lattice site. Although real crystals are finite, they are nevertheless limited to considering the model of an infinite crystal. The symmetry of an infinite crystal is determined, as already mentioned, by both rotations and translations combining the crystal with itself and forming the so-called crystalline groups.

E. Wigner [3] notes that group theory serves to explain the most important characteristics of atomic spectra. When considering specific problems, group theory allows us to draw conclusions about the behavior of the system without complex calculations using ideas about the symmetry of the system. Such predictions are essential in the study of spectra. If the interaction of electrons is considered as a perturbation, then the spectrum levels are split. Regarding the resulting levels, their symmetry properties are known. They manifest themselves in the transformational properties of the corresponding eigenfunctions with respect to the rearrangement of electrons, rotations, and reflections. Therefore, each level corresponds to three representations: one representation of a symmetric group, one is a group of rotations, and one is a group of reflections.

Most importantly, optical transitions occur only between levels that have certain properties or rules. These rules should follow from quantum mechanics. In the study of atomic spectra, symmetric groups and unitary matrix groups are used. In this case, non-Abelian groups of rotations and reflections are studied. Various representations of unitary groups are also being studied.

Group theory has now found application in many fields of physics [4]. In particular, group theory has applications in elementary particle physics. The main role in modern particle physics is played by the unitary groups. These groups are the groups of spin and isotopic transformations, and also forms the basis of the transformation groups of weak interactions. The unitary group $SU(3)$ is the basis of the unitary symmetry model.

Thus, the issue of particle classification is closely related to the representations of unitary groups.

Other important examples of the specific application of group theory and their representations are examples of calculations of such important characteristics of elementary particles as magnetic moments and axial-vector coupling constants in a unitary symmetry model [5].

Group theory is also applied to the problems of atomic and nuclear physics. One of the main tasks of atomic physics and nuclear physics is to determine the energy levels of a system of equivalent particles. Since it is impossible to precisely solve this problem for a system of interacting particles, one has to resort to perturbation theory methods. In this case, the perturbation will consist of some part of the field of one particle plus the interaction between the particles. If the particles are identical, then the interaction operator will be symmetric over all particles.

Another point of view is as follows. The wave function is considered as a vector in $n$-dimensional space spanned by basis vectors. If the basis vectors are subjected to a unitary transformation, we get another basis for the same vector space. In addition, unitary transformations can be made unimodular. As a result, we can assume that the space spanned by functions gives us a basis for representing the unitary unimodular group $SU(n)$ [6].

2. The study of simple non-Abelian groups using their spectra

Recognition of finite simple non-Abelian groups by their spectra has been studied for last thirty years in Yekaterinburg at the Institute of Mathematics and Mechanics, in Ural Branch of the Russian
The spectrum \( \omega(G) \) of a finite group \( G \) is called the set of all element orders of \( G \).

In other words, a natural number \( n \) is in \( \omega(G) \) if and only if there is an element of order \( n \) in \( G \).

Definition. A finite group \( G \) is called recognizable by its spectrum if any finite group whose spectrum coincides with the spectrum of \( G \) is isomorphic to \( G \) [16].

Among the results on recognizability of simple non-Abelian groups, a typical result is the following theorem of A.V. Vasiliev:

Let \( G \) be a finite simple group \( L_6(3) \) and \( H \) be a finite group with the property \( \omega(H) = \omega(G) \). Then \( H \) is isomorphic to \( G \) or \( H \) is isomorphic to \( G(\gamma) \), where \( \gamma \) is a graph automorphism of the group \( G \) of order \( 2 \). In particular, \( h(G) = 2 \) [9].

We say that for a finite group \( G \) the recognition problem is solved if we know the value of \( h(\omega(G)) \) (for brevity, \( h(G) \)).

More precisely, \( G \) is said to be recognizable by its spectrum in such designations if \( h(G) = 1 \), almost recognizable by spectrum if \( 1 < h(G) < \infty \), and nonrecognizable by spectrum if \( h(G) = \infty \).

Almost all simple non-Abelian groups are recognizable by their spectra. But there are exceptions: different groups of this set have the same spectra.

3. The study of simple non-Abelian groups using the bottom layer

Recognition of groups by bottom layer has been studied in Krasnoyarsk for last five years by author.

We will show the possibility of recognizing by the bottom layer for such simple non-Abelian groups with the same spectrum on the example of the groups \( S_6(2) \) and \( O_8^- (2) \).

Groups \( S_6(2) \) and \( O_8^- (2) \) are unrecognizable by their spectra [9].

Definition. The bottom layer of a group is the set of its elements of prime orders.

Previously, recognizability by the bottom layer of groups in the class of infinite groups with additional finiteness conditions was considered by the author together with I.A. Parashchuk. As additional restrictions to the task by the bottom layer of the group, the completeness of the group and its layer-finiteness were used [23].

Recall that a group is called layer-finite if it has a finite number of elements of each order [24].

In this paper, instead of such finiteness conditions, we consider the simplicity of a group, non-Abelianity and its finiteness.

Definition. A group is called recognizable by the bottom layer under additional conditions if it is uniquely restored by the bottom layer under these conditions. A group \( G \) is said to be almost recognizable by the bottom layer if there are a finite number of pairwise non-isomorphic groups with the same bottom layer as in the group \( G \). A group \( G \) is said to be unrecognizable by the bottom layer if there exist an infinite number of pairwise non-isomorphic groups with the same bottom layer such as in the group \( G \) [23].

By the bottom layer of a group, you can sometimes recognize a group, sometimes you can say something about the properties of such a group. Among the results of groups recognized by the bottom layer with the additional condition, that the groups without a unit element coincide by the bottom layer are the following:

- if the bottom layer of the group consists of elements of order 2 and the group does not have non-identity elements of other orders, then \( G \) is an elementary Abelian 2-group;
- if the bottom layer consists of elements of orders 2, 3, 5 and the group has no nonidentity elements of other orders, then A. S. Kondratiev and V. D. Mazurov proved that this is a group of even permutations on five elements [21].
Many results for groups with a given bottom layer describe only some of the group properties. For example, V. D. Mazurov proved that a group with a bottom layer consisting of elements of orders 2, 3, 5, in which all other non-identity elements are of order 4 with the additional condition that the groups coincide without an identity element with the bottom layer, is locally finite [22].

The almost recognizable by bottom layer groups in the class of infinite layer-finite groups are the groups in the following example. V. P. Shunkov proved that if the bottom layer in an infinite layer-finite group consists of one element of order 2, then the group $G$ is either a quasicyclic or an infinite generalized group of quaternions [25].

We will show that the groups $S_6(2)$ and $O_{8^+}(2)$ are recognizable simultaneously by the spectrum and by the bottom layer.

The group $O_{8^+}(2)$ is simple, it has order $174182400 = 2^{12} \cdot 3^5 \cdot 5^2 \cdot 7$. Using the GAP application package, it was established that it has 69615 involutions (elements of order 2) and 24883200 elements of order 7.

The group $S_6(2)$ is simple, it has order $1451520 = 2^9 \cdot 3^4 \cdot 5 \cdot 7$. Using the GAP application package, it was found that it has 5103 involutions (elements of order 2) and 207360 elements of order 7.

That is, these groups differ in the bottom layer, but do not differ in the set of orders of elements.

As established by A. V. Vasiliev [9], a finite simple group $U_4(5)$ is not recognizable by its spectrum. In this regard, we prove that simultaneous recognition of this group by spectrum and bottom layer is possible.

Let $G$ be the finite simple group $U_4(5)$ and $H$ a finite group with the property $\omega(H) = \omega(G)$ and the bottom layer is the same as that of the group $U_4(5)$. Then $H$ is isomorphic to $G$. That is, the group $U_4(5)$ is unique with such a spectrum and a bottom layer.

Indeed, let $G$ be the finite simple group $U_4(5)$ and $H$ be a finite group with the property $\omega(H) = \omega(G)$. By the theorem of A. V. Vasiliev [9], in addition to the group $U_4(5)$, there is only one such group $H$ isomorphic to $G(\gamma)$, where $\gamma$ is a field automorphism of the group $G$ of order 2. The groups $U_4(5)$ and $H$ have the same spectrum, at the same time these groups have different bottom layers, which differ at least by an element of order 2.

Thus, we have established that the group $U_4(5)$ is unique with such a spectrum and a bottom layer.

### 4. Conclusion

The paper gives some examples of applications of finite groups in crystallography, quantum mechanics, atomic and nuclear physics, elementary particle physics. A small review of the results on the recognition of simple non-Abelian groups by their spectra is presented. Previously, recognizability of the bottom layer groups in the class of infinite groups with additional finiteness conditions was considered. In this paper, instead of such finiteness conditions, we consider the simplicity of a group, non-Abelianity and its finiteness. The recognizability of some simple non-Abelian groups by both their spectra and their bottom layer for groups that are not recognizable by their spectra is established. In particular, we proved that the groups $S_6(2)$ and $O_{8^+}(2)$ which can not be recognized by spectrum alone can be recognized by the combination of their of their spectrum and bottom layer. The same is proved for the group $U_4(5)$.

These results will find applications in the study of finite groups, in particular, matrix groups. Matrix groups, in turn, find application in crystallography, atomic and nuclear physics and elementary particle physics.

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