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Приложения теории графов и теории групп в химии, физике

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Аннотация. Работа посвящена рассмотрению приложений математики, в частности, теории графов и теории групп в химии и физике. Химия была одной из первых, кто воспринял идеи теории графов. Математическая химия является разделом теоретической химии, в котором изучается применение математики к химическим задачам. Возможность формализации молекул на языке структурной химии с помощью графов позволяет методами теории графов определять число различных изомеров. Основным инструментом в математической химии является математическое моделирование с использованием вычислительной техники. Методы теории графов активно применяются в трех областях химии: структурная химия, химическая кинетика, химическая физика полимеров. Теория групп нашла применение во многих областях физики. Теория групп служит для объяснения важнейших характеристик атомных спектров. Теория групп дает возможность единообразного подхода к большому числу задач физики твердого тела. В этих исследованиях активно используются матричные группы и представления унитарных групп. Неприводимые представления групп используются для классификации колебательных и электронных состояний кристалла. Методы теории групп применяются к моделям задач классификации электронных состояний кристалла. В кристаллографии много внимания уделяется приложениям методов теории групп к изучению колебаний атомов, входящих в состав молекулы, относительно их положений равновесия. Результаты могут быть полезны при кодировании информации в сеансах космической связи.

Ключевые слова: математическая химия, атомная физика, кристаллография, теория графов, теория групп, приложения.

Applications of graph theory and group theory in chemistry, physics

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Abstract. The work is devoted to the consideration of applications of mathematics, in particular, graph theory and group theory in chemistry and physics. Chemistry was one of the first to adopt the ideas of graph theory. Mathematical chemistry is a section of theoretical chemistry that studies the application of mathematics to chemical problems. The possibility of formalizing molecules in the language of structural chemistry using graphs allows one to determine the number of different isomers using graph theory methods. The main tool in mathematical chemistry is mathematical modeling using computer technology.

The methods of graph theory are actively used in three areas of chemistry: structural chemistry, chemical kinetics, and chemical physics of polymers. Group theory has found application in many areas of physics. Group theory serves to explain the most important characteristics of atomic spectra. Group theory provides an opportunity for a uniform approach to a large number of problems in solid state physics. Matrix groups and unitary group representations are actively used in these studies. Irreducible group representations are used to classify vibrational and electronic states of a crystal. Methods of group theory are applied to models of problems of classifying electronic states of a crystal. In crystallography, much attention is paid to applications of group theory methods to the study of vibrations of atoms that make up a molecule relative to their equilibrium positions. The results can be useful in encoding information in space communications sessions.

Keywords: Mathematical chemistry, atomic physics, crystallography, graph theory, group theory, applications.

Introduction

The work is devoted to the applications of mathematics in physics and chemistry. Graph theory methods emerged in the 18th century thanks to L. Euler. Group theory originated in the 17th century from the manuscript of E. Galois then transformed into an elegant theory in the works of L. Euler, K. Gauss, J. Lagrange, N. Abel.

Graph theory and group theory began to be actively applied in chemistry and physics in the second half of the 20th century.

In this review, we will present the applications of graph theory and group theory in such areas of mathematical chemistry as structural chemistry, organic chemistry, chemical kinetics, and the chemical physics of polymers. The applications of graph theory in chemistry are covered in a review book edited by R. King [1].

Graph theory is indispensable in the study of metal-organic frameworks, which belong to coordination polymers-compounds consisting of repeating units that recur in one, two, or three dimensions.

The Tutte polynomial provides important information about the structure of a graph. Tutte polynomials contribute to a better understanding of the properties of chemical structures and have potential applications in chemistry and materials science.

Graph theory has become an essential approach for studying the complex behavior of interactions in protein systems.

In mathematical physics, applications of graph theory and group theory will be presented in particle physics, crystallography, crystal physics, the study of atomic vibrations, and the theory of atomic spectrum. Applications to quantum mechanics problems, such as atomic theory, solid-state theory, and the classification of vibrational and electronic states of a crystal will be considered.

The theory of group representations is used for the classification of states of a many-electron atom. An application of group theory to quantum mechanics is the establishment of selection rules in various aspects of quantum mechanics. Point groups of rotations and reflections, which leave a certain point invariant, find application in quantum physics.

Group theory finds application in molecular, atomic physics, and the physics of elementary particles.

Group theory studies the properties of symmetry and the resulting conservation laws, which allow to obtain statements used in solid state physics. At the beginning of the twentieth century, this rapidly developing field was even called the “group plague”, threatening the theory of solid state.

Considerations of group symmetry in quantum mechanics help classify and describe the transformational properties of wave functions.

Application of Graph Theory and Group Theory in Chemistry

According to chemists, chemistry was one of the first to embrace the ideas of graph theory. The molecule of a chemical substance began to be represented as a graph, with atoms as the vertices and the bonds between atoms as the edges. The ability to formalize molecules in the language of structural chemistry using graphs allows the methods of graph theory to determine the number of different isomers. In 1874, this allowed mathematician A. Cayley to solve the classic problem of structural chemistry regarding the enumeration of hydrocarbon isomers [2].

Mathematical chemistry is a branch of theoretical chemistry that studies the application of mathematics to chemical problems.

The basis of mathematical chemistry is the mathematical modeling of possible chemical processes. In mathematical chemistry, the dependence of these processes on the properties of atoms and the structure of molecules is also studied.

In mathematical chemistry, it is possible to construct models without involving quantum mechanics. The criteria of truth in mathematical chemistry are mathematical proof, computational experiment and comparison of results with experimental data [2]. The main tool in mathematical chemistry is mathematical modeling using computational technology.

Graph theory is applied in the study of metal-organic frameworks [3], which are interesting due to their complex structures and their practical significance in enhancing the efficiency of various technologies. They find applications in energy storage technologies and catalysis. In work [3], the spectral graph energies and entropies of metal-organic frameworks were calculated using graph theory methods.

Metal-organic frameworks are a class of porous polymers composed of metal clusters. Coordination networks, including metal-organic frameworks, are also referred to as coordination polymers, that is, coordination compounds consisting of periodically repeating coordination units and extended in one, two or three dimensions [4].

In 1995, O. Yagi demonstrated the crystallization of metallo-organic structures [Omar]. This was a breakthrough that paved the way for the creation of stable and crystalline porous materials, allowing to precise construction and increased mechanical stability, which enabled metallo-organic frameworks to maintain their porosity under industrial conditions.

Group theory is widely applied in organic chemistry, and graph theory is used to predict the properties of complex organic molecules [6]. Methods of graph theory are actively applied in three areas of chemistry: structural chemistry, chemical kinetics, and the chemical physics of polymers.

Recently, group theory has found another application in the field of chemical reactions, which is based on the principle of conservation of orbital symmetry proposed by R. Woodward and R. Hoffman (the latter was awarded the Nobel Prize in Chemistry) [7].

In chemical kinetics, specialists depicted the kinetic scheme of reactions using arrows connecting substances and recorded the mechanism reaction by reaction, thereby drawing a graph of a complex chemical reaction.

New types of graphs have emerged: for molecular transformations, substances were considered as vertices and elementary reactions as edges; for some graphs, substances and reactions served as vertices.

Symmetry is a very common phenomenon in chemistry: almost all known molecules either possess some form of symmetry themselves or contain certain symmetrical fragments [8]. Group theory is an effective tool for studying symmetric systems.

The Tutte polynomial is a classical polynomial graph invariant that provides important information about the structure of a graph. Tutte polynomials are used for silicate molecular networks and benzenoid systems. H. Chen derived formulas for polycyclic chemical graphs and determined explicit analytical expressions for the number of trees, connected subgraphs, and orientations of these chemical polycyclic graphs. Tutte polynomials contribute to a better understanding of the topological properties of chemical structures and have potential applications in chemistry and materials science [9].

A cut of a graph is a set of edges forming a subgraph, the removal of which divides the graph into two or more components. The cut method has proven to be extremely useful in the chemical graph theory. In article [10], the cut method is extended to hypergraphs and applied to cubic hypergraphs and hypertrees. The authors of the article have also developed extensions of the method to hypergraphs that arise in chemistry [10].

Feynman diagrams used in theoretical physics have proven effective in chemical kinetics and in the chemical physics of polymers.

When describing hydrocarbons, molecular graphs allow for the assessment of the number of possible isomers. Using graph theory, it is shown that compounds of hydrogen and carbon atoms with the formula $C_n H_{2n+2}$ allow only two non-isomorphic variants for $n = 4$, which correspond to two different hydrocarbon molecules: butane and isobutane. For $n = 5$ there are three isomers and as n increases the number of isomers increases sharply. For example, when $n = 20$, the existence of 366,319 isomers is possible [2]. That is, in the study of molecular graphs, computational technology plays an increasingly important role.

As a fundamental tool, graph theory, as a mathematical formalism in mathematical chemistry, has become an essential approach for studying the complex behavior of interactions in protein systems, including methods developed to access protein functions and their applications in disease biology. The definition of structures is based on graphs, as well as methodologies developed at the node, subgraph, and path levels. Graphs are used to solve problems in a multilayer network, which is more realistic in the biological world [11].

Application of Graph Theory and Group Theory in Physics. In addition to chemistry, graph theory has found new applications: theoretical physics and crystallography.

In the twentieth century, physicists began to actively apply mathematical methods, particularly the methods of group theory.

Group theory has found applications in many areas of physics. In modern particle physics, unitary groups are actively used. The groups $SU(3)$ are groups of spin and isotopic transformations, and they are also the basic subgroups of the groups of weak interaction transformations. In particular, matrix groups and representations of unitary groups are actively used in these studies. The unitary group $SU(3)$ is the basis of the unitary symmetry model [12].

Applications of group theory are intensively used in crystallography [12–17]. Monograph by L. V. Kartonova [14] considers the application of group theory methods to the study of the vibrations of atoms that are part of a molecule, relative to their equilibrium positions. A. V. Gadolin, using graph theory methods, provided a clear description of thirty-two crystallographic groups [14].

The structure of a regular periodic crystal can be described by its unit cell, in which a specific distribution of atoms is defined, and which is then replicated throughout the entire space using a subgroup of three-dimensional translations. Modern crystallophysics studies quasicrystals, whose structure can be described similarly, but instead of a single unit cell, a group of cells is used, and iterative algorithms are employed to fill the entire space with cells [18].

Group theory is used to explain the most important characteristics of atomic spectra [15]. When considering specific problems, group theory allows conclusions to be drawn about the behavior of the system without using complex calculations, based only on the concept of the system's symmetry. Such predictions are significant in the study of spectra. As for the obtained levels, their symmetry properties are known. Therefore, each level corresponds to three representations: one representation of the symmetric group, one of the rotation group, and one of the reflection group.

The interconnection between mathematics and physics is illustrated by the scientific activity of I. Kepler. So, in the field of astronomy, he established and mathematically described the basic laws of celestial mechanics.

Group theory finds applications in quantum mechanics problems such as atomic theory, solid-state theory and quantum chemistry [19].

The main principles of applying group theory in quantum mechanics were formulated in the 1930s. However, after a period of skepticism towards group theory as a mean of studying physical systems, it was only the middle of the last century when the active application of group theory began [15]. As E. Wigner wrote, the exact solution of quantum mechanical equations is so difficult that only very rough approximations to the exact solutions can be obtained through direct calculations. Therefore, it often proves useful to derive a significant portion of quantum mechanical results from the consideration of the fundamental symmetry properties of such equations [15].

The most important for quantum mechanics are the groups of coordinate transformations (symmetry groups) and permutation groups. Permutation groups are used for systems with a finite number of elements. The symmetry groups of nonlinear molecules are discrete and finite, while the symmetry groups of atoms and linear molecules are continuous and infinite. The groups describing the translational symmetry of atoms in crystals are discrete and infinite [7].

Irreducible representations of groups are used to classify the vibrational and electronic states of a crystal.

In these representations, the crystal is considered as a system of material particles that perform small vibrations relative to their equilibrium positions. If it is assumed that the equilibrium positions of the particles form a configuration possessing the symmetry of group G , then the Cartesian components of the particle displacements transform according to some reducible representation of this group.

When studying the normal vibrations of a crystal, in addition to considerations of symmetry, one can rely on the properties of the spectrum of its natural frequencies.

When classifying the electronic states of a crystal, it is additionally assumed that the atomic nuclei are fixed at the lattice points.

Methods of group theory are applied to simplified models of the classification problems under consideration.

The main method of approximate consideration is the self-consistent field method. In this method, the problem of interacting electrons is reduced to a single-electron problem, where the interaction with an electron is approximately replaced by interaction with a certain field possessing the symmetry of the crystal. The question of how good the solutions obtained with the help of group theory are is resolved by comparison with practice.

Sometimes group representations cannot fully explain some of the observed properties. For example, it was found that symmetry breaking occurs when an external magnetic field is applied. In this particular case, it was suggested that the wave function of the electron transforms under rotations according to a different group representation. The properties of representations of the groups $S(n)$, $O^+(3)$, $U(n)$ and their subgroups find applications.

The results obtained in representation theory are used for the classification of states of a multi-electron atom.

One of the important applications of group theory to quantum mechanics is the establishment of selection rules, which are understood as criteria that allow one to determine whether the matrix element of a certain operator can be non-zero, given the representations of the considered group under which this operator and the wave functions transform. In radiation theory, this criterion is applied to the matrix element of the interaction operator with the electromagnetic field and is used to determine the probability of a quantum mechanical system transitioning from one stationary state to another [20]. Selection rules are developed for the study of light scattering by molecules, and the absorption and emission of light by atoms [21].

A comprehensive review of the application of group theory in molecular, atomic physics, and particle physics is contained in the book by L. Michelle and M. Schaaf [22]. Physical applications allow mathematicians to learn which mathematical concepts play the most significant role in modern physics. At the same time, the applications provide physicists with the opportunity to present the fundamentals of the theory in a somewhat unusual aspect for them, using the most modern mathematical language. M. Schaaf's review from the second part of the book [22] is dedicated to the

most important group for particle physics and quite interesting from a mathematical point of view - the group of motions of four-dimensional pseudo-Euclidean space (the inhomogeneous Lorentz group, or the Poincaré group). M. Schaaf examines the irreducible unitary representations of the Poincaré group and its subgroups.

To describe hadrons in the first approximation, the symmetry $SU(3)$ and higher symmetries, such as the direct product $SU(3) \times SU(3)$ are used. This symmetry becomes exact if the mass of O^- mesons is neglected. This approximation corresponds to the subgroup

$$SU(2) \times SU(2) \times U(1) \text{ groups } SU(3) \times SU(3) [10].$$

The approximation method takes into account the most characteristic and important properties of the system, which include symmetry properties and the resulting conservation laws. Many statements used in solid-state physics are essentially based solely on them. When narrowing a physical problem to the study of the symmetry that forms its basis, it is possible to examine only partial information about the substance. However, the information obtained in this case will be accurate depending on the precision of our understanding of the symmetry. A well-developed section of symmetry theory is precisely called group theory. In the thirties of the twentieth century there was a discussion about a "group plague" threatening the theory of solid bodies [23].

Point groups of rotations and reflections, which leave a certain point invariant, find application in quantum physics. All axes of rotation intersect at this point, and all planes of reflection contain it. The cyclic group C_n is used to consider rotations by an angle $2\pi/n$. The group D_n is obtained from the group C_n by adding to it a second-order axis perpendicular to the n -fold axis [23].

Group theory provides a unified approach to a large number of problems in solid state physics, in which the properties of translational and rotational symmetries of the lattice are important.

Group theory provides an exact mathematical language for describing symmetry and classifying the properties of complex systems.

Considerations of symmetry in quantum mechanics help classify states and describe the transformational properties of wave functions [24].

Many molecular systems possess some form of spatial symmetry. This circumstance allows for a significant simplification of the process of solving the Schrödinger equation by using the apparatus of group theory. The application of group theory in solving the Schrödinger equation is based on identifying those aspects and features of the solutions that are determined solely by the symmetry of the system, the symmetry of the field in which the electrons move. Consistent consideration of symmetry is necessary for the classification of single-electron states and the state of the entire system. This classification is based on the theory of group representations. Group theory plays a particularly important role in establishing selection rules for transitions between different states and when considering the splitting of terms, when a symmetric system is exposed to external disturbances that have lower symmetry [25].

Mathematical models are actively used for research in modern aviation science. To solve problems of strength, study elastic and plastic deformations of aircraft structural elements, methods of group theory, equations of mathematical physics, differential equations, complex analysis, and computational mathematics are useful. The task of solving differential equations that describe natural phenomena, including by numerical methods, is central to the interaction between physics and mathematics.

Conclusion

Applications of mathematics, in particular, graph theory and group theory in physics and chemistry, are considered.

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