# Regular permutations and their applications in crystallography

*Vasily* S. Senashov[1], *Konstantin* A. Filippov[1,2], and *Anatoly* K. Shlepkin[3*]

[1]Siberian Federal University, Krasnoyarsk, Russia
[2]Krasnoyarsk State Agrarian University, Krasnoyarsk, Russia
[3]Siberian State University of Science and Technology, Krasnoyarsk, Russia

**Abstract.** The representation of a group G in the form of regular permutations is widely used for studying the structure of finite groups, in particular, parameters like the group density function. This is related to the increased potential of computer technologies for conducting calculations. The work addresses the problem of calculation regular permutations with restrictions on the structure of the degree and order of permutations. The considered regular permutations have the same nontrivial order, which divides the degree of the permutation. Examples of the application of permutation groups in crystallography and crystal chemistry are provided.

## 1 Introduction

Permutation groups play a significant role in physics, particularly in the context of quantum mechanics and the study of identical particles, such as electrons, protons, or other elementary particles. Here are a few ways in which permutation groups are used in physics [1,2,3].

Identical Particles and Quantum Mechanics: In quantum mechanics, identical particles are particles that cannot be distinguished from one another. For example, all electrons are identical, and the same is true for other particles of the same type. Permutation groups are used to describe the possible ways these identical particles can be arranged in quantum states. The symmetrization or antisymmetrization of the wave function of these particles is described using permutation operators. Bosons have symmetric wave functions, while fermions have antisymmetric wave functions.

Exchange Symmetry: Permutation groups help physicists analyze and understand the exchange symmetry of identical particles. The concept of exchange symmetry is vital in determining the statistics of particles (Bose-Einstein or Fermi-Dirac statistics), and it has important implications for the behavior of systems at the quantum level.

Quantum Mechanics of Systems: Permutation groups also come into play when studying the quantum mechanics of systems with multiple identical particles, such as molecules with identical atoms. These groups help physicists analyze the degeneracy of energy levels and determine the possible quantum states of the system.

* Corresponding author: ak_kgau@mail.ru

Quantum Field Theory: In the context of quantum field theory, which is fundamental to particle physics, permutation groups can be used to understand the statistics and properties of fields that describe particles and their interactions.

Symmetry Groups: Symmetry plays a crucial role in physics, and permutation groups are often used to describe the symmetries of physical systems. These symmetries are used to understand conservation laws, classify particles, and predict the behavior of physical systems.

Overall, permutation groups are a fundamental mathematical tool in quantum mechanics and various branches of physics, allowing physicists to describe the behavior of identical particles and understand the symmetries and properties of physical systems at the quantum level.

## 2 Methods

A powerful method of research in group theory is the study of a group's structure based on its arithmetic parameters. The universality of this method is due to the fact that it works both in finite and infinite groups. In group theory, properties of a group that are determined by its numerical parameters are commonly referred to as 'arithmetic' properties. These parameters include the order of the group, the set of its prime divisors, orders of elements, orders of subgroups, degrees of irreducible representations, orders of conjugacy classes, and so on. With the advancement of computational computer systems and cryptography, fundamental tasks such as studying the arithmetic properties of finite groups and characterizing finite groups using arithmetic parameters have gained special significance in group theory.

Permutation groups are also used in crystallography to describe and understand the symmetries of crystals and to determine their properties. The main methods of applying permutation groups in crystallography and crystal chemistry are as follows [4,5,6,7].

Point Group Symmetry: In crystallography, the point group of a crystal is described by a permutation group that represents the symmetry operations that leave the crystal's structure unchanged. These symmetry operations may include rotations, reflections, and inversions. Permutation groups are used to categorize and describe these operations mathematically.

Space Group Symmetry: Crystals not only have point group symmetry but also exhibit translational symmetry in three-dimensional space. Space groups describe the combination of translational and point group symmetries in crystals. Permutation groups help classify and understand the different space group symmetries by specifying how atoms or ions are transformed within a unit cell under these symmetries.

Generating Symmetry Operators: Permutation groups help generate the symmetry operators used to describe the transformation of points in a crystal's lattice. These operators include rotations, translations, screw axes, and other symmetry operations. By understanding the permutation group associated with a crystal's symmetry, crystallographers can determine how these operations affect the atomic positions in the crystal.

Determining Properties: The symmetries of a crystal can have profound effects on its physical and chemical properties. Permutation groups help identify and predict these properties by analyzing how the crystal's symmetries constrain the behavior of electrons, phonons, and other particles within the crystal lattice.

Structure Analysis: Permutation groups are used to analyze crystallographic data, including X-ray diffraction patterns, to determine the arrangement of atoms in a crystal. Understanding the symmetry of the crystal is crucial for identifying the unit cell and solving the crystal structure.

In summary, permutation groups are a fundamental mathematical tool in crystallography, enabling the classification of crystal symmetries, the description of symmetry operations, and the prediction of various properties and behaviors of crystalline materials. They are instrumental in the study of crystal structures and the development of crystallographic techniques for materials analysis.

## 3 Results and discussion

The concepts mentioned below, namely permutations, regular permutations, permutation degrees, and permutation orders, are widely known. Representing a group G in the form of regular permutations is extensively used to investigate the structure of finite groups, especially for parameters such as group density function, group spectrum, and the Cayley graph of the group [8,9,10]. This is related to the increased capabilities of computer technologies for conducting computations. Quantitative characteristics of regular permutations were discussed at the Algebraic Seminar of Siberian Federal University. During the discussion of regular permutations, G.P. Egorichev proposed several independent proofs of a well-known formula for calculating the number D_n of regular permutations of degree n.

Let$k$beanaturalnumber, $p, q, r$ – pairwise distinct prime numbers, $w = pqr$. The number of regular permutations of degree $n = w^k$, of order$w$, we will denote as $R(n, p, k)$.

**Theorem.** Let$x, y, z$– be a natural numbers, such that$xp + yq + zr = w^k$ and $I$– the set of all such distinct triples. Then:

$$R(n, w, k) = \sum_I \left(\frac{A_n^x}{p^x x!} \times \frac{A_n^y}{q^y y!} \times \frac{A_n^z}{r^z z!}\right).$$

Proof scheme. For the number of possible combinations for the first cycle $\left(i_1^{(1)} \dots i_p^{(1)}\right)$ is equal to

$$n \cdot (n-1) \cdot \dots \cdot (n-p+1).$$

Considering that the cycle remains the same as a permutation when elements are shifted in a "circular" manner, we have

$$\frac{n \cdot (n-1) \cdot \dots \cdot (n-p+1)}{p}.$$

The number of possible combinations for the second cycle $\left(i_1^{(2)} \dots i_p^{(2)}\right)$ is

$$(n-p) \cdot \left(n-(p+1)\right) \cdot \dots \cdot (n-(2p-1)).$$

With the same consideration that the cycle remains unchanged under circular shifting of elements, we have

$$\frac{(n-p) \cdot \left(n-(p+1)\right) \cdot \dots \cdot (n-(2p-1))}{p}.$$

By following a similar approach for the last cycle$\left(i_1^{(x)} \dots i_p^{(x)}\right)$ with number *x*, we obtain

$$\frac{(n-(n-p)) \cdot \left(n-\left(n-(p-1)\right)\right) \cdot \dots \cdot (n-(n-(p-(p-1))))}{p}.$$

The product of the number of combinations for all cycles is

$$\frac{n!}{p^x}.$$

Since the cycles are commutative, for p, it is enough to divide the above value by *x!*. We get

$$\frac{n!}{p^x \cdot x!} = \frac{A_n^x}{p^x \cdot x!} -$$

the number of cycles corresponding to *p*. Similarly,

$$\frac{n!}{q^x \cdot y!} = \frac{A_n^y}{q^y \cdot y!} -$$

the number of cycles corresponding to $q$, and

$$\frac{n!}{r^z \cdot z!} = \frac{A_n^z}{r^z \cdot z!} -$$

the number of cycles corresponding to *r*. To complete the proof, multiply the obtained values and sum over *l*.

$$R(n, w, k) = \sum_{I} \left( \frac{A_n^x}{p^x x!} \times \frac{A_n^y}{q^y y!} \times \frac{A_n^z}{r^z z!} \right).$$

The theorem is proven.

## 4 Conclusion

The permutation representation of an abstract group is one of the effective methods in group theory research. In this context, a significant role is played by the so-called regular representations of an abstract group, where the elements of the group are represented as regular permutations of fixed power. In cases where this power is finite, we have a situation where we establish properties of a finite group in terms of regular permutations whose degree coincides with the order of the group being studied.

The main task that arises in this context is to determine, from all regular permutations of the specified degree (this classical problem has been solved), those that form a group whose order matches the degree of the permutations. This problem is solved on a case-by-case basis in each specific situation. Within the scope of this article, this problem is addressed with additional restrictions on the structure of the order of the group under investigation (the number of prime divisors of the order and the exponent of their inclusion in the order of the group). The next step is the development of a multiplication algorithm for regular permutations based on the principles of enumerating regular permutations as developed in this work.

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