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The symmetry method as a way to visualize the interaction of an ultrashort pulse with matter, using the example of RNA molecules, DNA and diamond crystals

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To date, the European free electron laser is actively used to determine the structure of many materials [1,2]. The advantage of such a laser over other research methods is the ability to generate short beams that make it possible to study the structure without radiation exposure[3]. At the same time, the exposure time of such a pulse is commensurate with the characteristic atomic time, which makes it possible to study molecules without additional preparation, crystallization, etc. This was a revolution in structural biology and not only [4]. However, the difficulty of obtaining and decoding diffraction patterns stops the use of a laser. The complexity of data processing and decoding, namely the phase problem, prevents the widespread use of ultrashort laser pulses to work with molecules[5]. It is necessary to search for new ways to decrypt the received data in order to create an effective three-dimensional visualization method. In the previous work, the method proposed as the basis for decoding experimentally obtained diffraction patterns was described [6]. The method is based on a theoretical description of the interaction of an ultrashort pulse with the substance under study, using numerical modeling and using the Dirac–Hartree-Fock-Slater model. To simplify the decoding of molecular structures, it is proposed to conduct theoretical modeling of the interaction in order to obtain a reference diffraction pattern. In [7], the method was changed, it was proposed to simplify the calculation if there were symmetries or repeating sections in the structure under study. In this paper, the proposed method is tested in more detail on different structures, on a DNA molecule (a larger site), an RNA molecule, and a diamond crystal. All these substances are of great interest in structural biology, medicine and physics. Their research at the atomic level is still difficult, which prompts the development of similar methods of their analysis. The use of the symmetry method will allow calculations to be carried out at the analytical level and reduce processing time. The spectra of the interaction of an ultrashort pulse with molecules and a crystal will be obtained in the article, the proposed theory will be verified by calculating the interaction spectra on these objects. The interaction spectra obtained here will be compared with previous results.

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