

Quantum mechanics and quantum biomolecular science

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The questions of contemporary trends in the development of the biological sciences were the subject of discussions in the Management of the Academy. Justifiably some of our scientists well-grounded the opinion about the necessity of an accelerated development of molecular biology. This is entirely in the spirit of the new tendencies in the development of this science in the advanced countries. We want, however, to introduce a supplement to the concept of molecular biology — an attitude which we expressed at the time of these discussions: for the proper understanding and foretelling of the extraordinarily complicated biological processes one should start from the atomic level. In basic lines we also explained this question in the report on "Quantum and classical mechanics" before the 3rd National Congress on Theoretical and Applied Mechanics in 1977 in Varna. During the time of my visit to France at the end of the last year I had the possibility to get acquainted with French scientists, who share the same opinion and have succeeded in this direction.

Biological matter has a mechanical, physical, chemical and biological form of motion, the biological form of motion not existing separately from the first three forms. These forms of motion are continuous and inseparable. They are found in a unity. The investigations comprise different levels of motion, beginning with the investigation of the atoms, molecules, tissues, fluids, the individual organs, subsystems, the entire biological system and so on.

The investigations at atomic and molecular level should be performed with the help of the quantum mechanical laws. The significance of quantum mechanics, wave mechanics respectively, is obvious from the following thought of the prominent French scientist R. Dodelle (1): "Wave mechanics gives a conception of the microworld, where there is a harmonious combination of continuity and discontinuity, the wave and the particle, the undetermined and determined."

Another prominent French scientist, B. Pullman, remarks [2] that while in 1950 a great many considered molecule biology as the most significant advanced front of biological sciences, then the well-known Nobel prize winner Albert Szent-Gyorgyi stated and proved the necessity of "submolecular biology". He underlined that the molecular properties are determined at submolecular level and that they arise from the combined effects of the elementary particles. For the deep understanding of the molecular world the internal play of electrons and nuclei should be unraveled, provided the way to these particles and the way

from them to the properties of the organized compounds, which are subject to scientific investigations, could be found. A. Szent-Gyorgyi believed that the deep knowledge of the laws of biology should be looked for at electronic level. Hence it follows that for him submolecular biology meant essentially quantum biology.

Quantum biology finds its expression through the application of quantum mechanical methods in the investigation of different forms of motion of the atoms and the molecules of biological matter. One of the most developed at present quantum sciences of the geneological tree of quantum biomolecular sciences is quantum biochemistry. A great merit for this have the students of the founder of wave mechanics Louis de Broglie, R. Daudel, B. Pullman and others. A great part of the investigations in quantum biochemistry during the first stage has been carried on mainly for the investigation of the distribution of electrons and the biomolecular properties. During the last 3—4 years the investigations developed in the direction of theoretical study of the conformational basis of biological structures and mechanisms.

Ten years ago the International Academy of Quantum Molecular Sciences was founded in France with the aim to promote and support the development and applications of wave mechanics in the investigation of molecular phenomena. R. Daudel was elected as first president of this Academy (in 1967) and later on (in 1973) — B. Pullman.

At the opening of the International Conference on Electronic Aspects of Biochemistry in 1969 B. Pullman mentioned that the appellation "quantum biochemistry" is still disturbing, but inspite of that recently it started entering the scientific vocabulary. Besides this B. Pullman defines also the major problem of biochemistry in the application of the general ideas and methods of wave mechanics in investigating the electronic structure of biological molecules with respect to their behaviour as substances of life, i. e. their part in the biochemical and biophysical processes, characteristic of living matter.

Quantum biophysical chemistry and quantum pharmacology are being formed as the newest branches of quantum biomolecular sciences. They represent a new field for scientific investigations — these are the questions, connected with the mechanism of the activity of the pharmacological compounds.

During the last few years the conformations of pharmacological molecules and the pharmacological activity of medicines have been subject to wide theoretical and experimental investigations.

In connection with the world-wide cancer problem on the forefront of scientific investigations since a quarter of a century stand the quantum mechanical investigations of large molecules. The special question about the possible relations between the electronic structure of different classes of large organic molecules and their cancerogenous force is studied. It is supposed that there is a connection between the appearance of tumours and the existence of certain specific electron distributions.

Following the logical internal structure of the quantum interdisciplinary biomolecular sciences, the legality of the existence also of quantum biomechanics must be assumed. Its subject is the investigation of the mechanical motion of biological atoms and molecules.

The advantages in the use of the quantum mechanical methods in biochemistry are that a complete information on the biodynamical structural properties of the investigated atomic and molecular system can be obtained. In a number of cases the obtaining of experimental data is particularly difficult, while the quantum mechanical calculations allow us to discover and foretell new mecha-

nical, physical and chemical properties and mutual relations between the structure and the phenomenological events.

The knowledge of the molecular wave function ψ allows the exact calculation of the electrostatic potential $v(r_i)$, formed in the surrounding space by the nuclear charges and the electronic distribution. With the help of this potential the interaction energy of the molecular distribution with an external point charge can be determined and the chemical reactivity and the influence of an external reagent investigated.

One of the fundamental problems of quantum biomechanics, biophysics and biochemistry is the investigation of the bioenergetic problem of the transformation of the energy of active molecules in muscles or membranes into mechanical work. Probably the fast and large region of motion of the excited electrons has a significant part in this process. This can be understood on the basis of quantum mechanics of crystals and the influence of the delocalized electrons on the supermolecular structure [3].

Some authors [4] underline that at the present time analytical investigations in biology are carried on, which descend to the level of the molecules and atoms and ascend to the investigation of the subconscious psychic processes. In the same way synthetic investigations are made which more and more persistently pose the questions of the nature of life and the fate of the biosphere.

Those authors are right, who underline that it is not enough to know the specific electronic states of the atoms in order to reach the phenomenological and ecological events, to explain the various properties and the transfer of the inherited information of the living organisms.

These difficulties should be solved with the help of the quantum biomolecular sciences, with the help of the quantum and classical statistical mechanics and other sciences, which will make it possible to connect the phenomena at a microlevel with those at a macrolevel. It is necessary to consolidate the conviction that the investigation of the microstructure of matter, generally, and, more specifically of biological matter, will be the basis of submolecular biology will help for the deepening of the knowledge about the molecular foundations of life, will decipher the general principles of the elementary processes at a microstructural level.

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