Contribution ID: **54** Type: **Lecture**

Conformational solitons in DNA macromolecule

Wednesday, 23 December 2020 12:00 (45 minutes)

Accuracy of genetic information implementation in living cells is largely due to the peculiarities of the structure and variability of DNA double helix. The regulation of genetic activity, stability and security of genetic texts, reading and translation of genetic information, all of these important biological processes take place because of the unique properties of the DNA double helix, which distinguish them from other cellular molecules. One of the key properties of DNA molecule is the polymorphism of its double helix, through which this molecule has the ability to change the structure on some definite sites under the influence of external factors or depending on the nucleotide sequence. Arising in this case localized deformations can have a sufficiently large amplitude of structural element deviations from their equilibrium positions in the double helix and are the conformational solitons by their nature. Such localized deformations cannot be understood within the framework of the elastic rod model, which is suitable for studying DNA mechanics in a harmonic approximation. On the other hand, the all-atomic modelling cannot frequently explain the mechanism of DNA double helix deformations due to the complex character of macromolecule structure changes and many degrees of freedom of the double helix.

The report presents an approach for the consideration of conformation-dependent deformations in DNA macromolecule. The transformation of the DNA structure is considered in the frame of the two-component model. One model component (external) describes the macromolecule deformation as in the model of the elastic rod, another component (internal) - the conformation changes of the macromolecule monomer units. Both components are considered as interconnected on the paths of certain conformational transformation. The approach provides the possibility to predict the sizes and energies of local deformations of the double helix and explained the appearance of solitary excitations in the DNA chain at the location of some definite nucleotide sequences.

The results obtained make it possible to uniformly interpret the long-range soliton effects in the DNA chain, the deformability of specific DNA sequences, as well as the threshold nature of the effects of DNA unzipping and overstretching. The presented results can also be useful for a deeper understanding of the mechanisms of DNA functioning in the cell, and for the development of modern technologies in the fields of molecular medicine, DNA engineering, smart materials and nanodevices.

The lecture is dedicated to the memory of A.S. Davydov - an outstanding scientist, academician of the National Academy of Sciences of Ukraine, Hero of Socialist Labor, and director of the Institute of Theoretical Physics of the National Academy of Sciences of Ukraine (1973-1988).

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Session Classification: Physics of Biological Macromolecules

Track Classification: Physics of Biological Macromolecules