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Konstantin V. Shaitan

Mathematical problems of the formation of unique 3D-structures of linear biopolymers

The report examines the mathematical problems of the dynamics of folding or the dynamics of spontaneous folding of linear polymer chains into unique spatial structures. Until now, there is no clear understanding of the mechanics of the internal movements of long flexible chains, and the physical laws governing the formation of ultra-high-dimensional potential energy surfaces with a global minimum, which are necessary for 100% implementation of strictly defined configurations of a folded chain (without this, the phenomenon of life is impossible!).

In the first part of the lecture, the mechanics of movements of a long flexible chain in a viscous medium is considered. The folding processes of biopolymers take place in an aqueous solution. Water for molecular motion is a very highly viscous liquid. In the system of equations of motion of chain nodes in a highly viscous medium, inertial terms can be neglected. A multidimensional geometric approach is proposed for deriving the laws of motion of flexible chains in a viscous medium. The result is that the rate of energy dissipation of the chain nodes is almost uniformly spread throughout the chain. This leads to certain rules for the movement of a representative point on multidimensional energy surfaces, which are figuratively formulated as the principle of a "novice skier" — a representative point goes around sharp irregularities of a potential surface with a relatively low dimension. There are also extreme principles for the folding dynamics — the principle of the maximum rate of reduction of potential energy and, at the same time, the minimum rate of energy dissipation.

In the second part of the report (if we have time?), the principles of the formation of multidimensional energy surfaces for linear polymer (biopolymer) chains are considered. The main idea is that the configuration space of the polymer chain has the topology of a multidimensional torus and the potential energy function should be represented as a multidimensional Fourier series. In this case, certain conditions should be imposed on the expansion coefficients, the meaning of which becomes clear when comparing the experimentally observed effects for folding and the predictions of the theory. The main idea is that the expansion coefficients are functions of certain invariants of the algebraic vectors of the harmonic numbers of the members of the Fourier series. This consideration also gives rise to some ideas for the physicochemical evolution of linear polymers, from which protoforms of functional biopolymers could be obtained.

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