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How the multidimensional geometry helps to understand the physics of the formation of the spatial structure of biopolymers

The report deals with the dynamics of linear polymers in viscous media and the problems of the formation of unique spatial structures of biopolymers (proteins, etc.). The role of the viscosity of the medium is that in the equations of motion inertial terms can be neglected. Using the general symmetry properties for interatomic interactions, a conservation law is formulated for the sum of the vectors of rotations around bonds during conformational motions of the hinge chain in a viscous medium. The problem of the dynamics of conformational movements (due to rotations around bonds) of a linear polymer chain in a viscous medium is reduced to the problem of rotation of the center of a hypersphere, which describes the law of conservation of energy over the surface of another hypersphere, the radius of which is equal to half the radius of the hypersphere, which describes the rate of energy dissipation. The solution of the system of equations of mechanics for conformational motions in a viscous medium is specified by the point of contact between the energy dissipation hypersphere and the energy conservation law hypersphere. In the limit of large dimensions (the number of polymer chain nodes), the average rates of energy dissipation turn out to be practically the same for all chain nodes (except for the extreme ones). The main conclusion from the above consideration is that the movement of a representative point on a multidimensional surface of potential energy obeys (statistically) a certain rule — a representative point tends to avoid areas in which a sharp change in potential energy occurs over a relatively small number of degrees of freedom. This rule is of the same order as the well-known rule, for example, for a system of a large number of particles at a given temperature T — it is extremely unlikely that a significant fraction of particles, for example, have an energy that differs sharply from the average thermal energy. These considerations are used further when discussing the convergence paradox of the potential energy of a macromolecular system, which is represented as the sum of paired atom-atom interactions.

The second part of the report is devoted to the issues of topography of multidimensional energy surfaces of biopolymers, which form unique spatial structures. In contrast to the problem of the formation of crystal structures in the case of biopolymers, we cannot use considerations of dense packing of balls. The main idea of the proposed approach is to use the topology of the configuration space of the polymer (multidimensional torus) and represent the potential energy surface in the form of a multidimensional Fourier series. Using considerations of the symmetry of biopolymers with respect to rearrangements in the chain of identical monomer units, as well as a number of experimental facts, a Gaussian model is proposed for the dependence of the expansion coefficients on the vector of harmonic numbers. The consequences of this approximation for the structure and dynamics of biopolymers are discussed. The parameter of the characteristic temperature of denaturation (or destruction of the compact spatial structure) of the biopolymer naturally arises. An assessment is being made for the possible chemical composition of polymers that form unique spatial structures under different conditions (for example, on different planets). In particular, on our planet, the threshold for protein denaturation is about 60C (or 333K), which, according to the model presented, corresponds to the chemical composition of polymers in which hydrogen bonds are formed in an aqueous medium.

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