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GMPC as 1d Potts-like model and the helix-coil transition in biopolymers

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We summarize the results of our investigations of helix-coil transition both in single-strand (polypeptides) and two-strand (polynucleotides) macromolecules. The Hamiltonian of the Generalized Model of Polypeptide Chain (GMPC) is introduced to describe the system in which the conformations are correlated over some dimensional range . The Hamiltonian does not contain any parameter designed especially for helix-coil transition and uses pure molecular microscopic parameters (the energy of hydrogen bond formation, reduced partition function of repeated unit, the number of repeated units fixed by one hydrogen bond, the flexibility of chain, the energies of interaction between the repeated units and the solvent molecules). We evaluate the partition function using transfer-matrix approach. An important problem of relation between GMPC and many particle one-dimensional Potts model is solved. We describe the influence of solvent interaction with biopolymer, both with competing and non-competing for hydrogen bond formation ways, considered stacking and hydrogen bonding simultaneously, the influence of side-by-side interaction and took into account structural heterogeneity of biopolymers. System cooperativity we describe in terms of two-particle correlation function and correlation length. Handling of the problem of solvent influence on helix-coil transition we obtained, depending on energy of solvent-macromolecule interaction, how solvents change transition temperature and interval. We obtained, that two type interaction of solvent brings to appear low temperature coil-helix transition, which we connect with cold denaturation. We considered joint stacking and hydrogen bonding interactions, using two-scale GMPC. Here we solved two problems- generalized stacking and restriction of helix regular sequence. Stacking on the background of H-bonding increases stability and decreases cooperativity of melting, restriction of helix regular sequence brings to appear new correlation peak, which nature is anticooperativity in long helical sequences. We also took into account two biopolymers side-by-side interactions, which brings to different effects. In case of effective attraction, the cooperativity rises sharply, in case of effective repulsion; the shape of melting curve is two-phase with high and wide correlation length in a plateau on denaturation curve.

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