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Influences of Temperature and Solvent Ions in Solution on States and Properties of Deoxyribonucleic Acid (DNA)

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Abstract: We here study the influences of the temperature and solvent ions in solution on the states and properties of DNA by a new dynamical model. This model admits three degrees of freedom per base-pair: two displacement variables related to the vibrations of the hydrogen atom in the hydrogen bonds and base (nucleotide), respectively, and an angular variable related to the rotation of each base, which delineate different forms of motion of the hydrogen atom and bases and the relations among them. In this model we stress specially the important role of the hydrogen atom in the hydrogen bonds of the bases in the dynamics of DNA. According to their properties of motion we give the Hamiltonian of the system and the corresponding equations of motion, and find out their soliton solutions. The solitons formed by the displacements of the hydrogen atoms and bases and their rotations are the excitation states arising from the energy absorbed by the DNA working at the biological temperature. We give further the free energy of the thermal excitation state in DNA system by transfer integral way and find out the corresponding specific heat. The specific heat increases with the increasing of the temperature and concentration of the solvent ions in the solution, but is not linear changes in the region of high temperature. If compared with experimental data, they are approximately consistent. Meanwhile we find that the solvent ion concentration influences seriously on the stability, states, and configurations of DNA.

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Key words: dynamical property, DNA, nonlinearity, soliton, solvent ion, specific heat

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