

The Investigation of Behaviour of Soliton Transported Bio-Energy along the Protein Molecules

Pang Xiao-feng

University of Electronic Science and Technology of China, China

The propagated properties of soliton transported bio-energy excited in the α -helix protein molecules with three channels in the cases of short-time and the long-time motion and its features of collision at temperature $T=0$ and biological temperature $T=300$ K are studied numerically by the dynamic equations in the improved Davydov theory and fourth-order Runge-Kutta method, respectively. From these simulation experiments we see that the new solitons in the improved model can move without dispersion at a constant speed retaining its shape and energy in the cases of motion of both short-time and $T=0$ and long time or $T=300$ K and can go through each other without scattering in their collisions. In these cases its lifetime is, at least, 120 PS at 300 K, in which the soliton can travel over about 700 amino acid residues. These results obtained are consistent with analytic result obtained by quantum perturbed theory in this model. In the meanwhile, the influences of structure disorder of α -helix protein molecules, including the inhomogeneous distribution of amino acids with different masses and fluctuations of spring constant, dipole-dipole interaction, exciton-phonon coupling constant and diagonal disorder, on the solitons are also studied by the fourth-order Runge-Kutta method. Therefore, the soliton still is very robust against the structure disorders and thermal perturbation of proteins at biological temperature 300 K. From this investigations of the properties of soliton solutions of equations of motion in the cases of short-time and long-time motion and its features of collision in the α -helix protein molecules with three channels at the biological temperature 300 K in the improved model by the fourth-order Runge-Kutta method we finally obtain that this soliton in the improved model is very stable whether in the cases of long- and short-time motions and mutual collision at 300 K, it can move along the protein molecular chains without dispersion at a constant speed retaining its shape and energy in the cases of motion of both short-time and $T=0$ and long time and $T=300$ K and can go through each other without scattering in the collision. In this case its lifetime is at least, 120 PS at 300 K, in which the soliton can travel over about 700 amino acid residues.

This result is consistent with analytic result obtained by quantum perturbed theory in this model. In the meanwhile, the influences of structure disorder of protein molecules, including the inhomogeneous distribution of amino acids with different masses and fluctuations of spring constant, dipole-dipole interaction, exciton-phonon coupling constant and diagonal disorder, on the solitons are also studied. The results show that the soliton is easily undisturbed and very robust against the structure disorders and thermal perturbation. Therefore the new soliton in the improved model is a possible carrier of bio-energy transport and the model is possibly a candidate for the mechanism of this transport.