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The Investigation of Behaviour of Soliton Transported Bio-energy along α -Helix Protein Molecules with three Channels

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Abstract: *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=300K 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 or T=0 and long time or T=300K and can go through each other without scattering in their collisions. In these cases its lifetime is, at least, 120PS at 300K, 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 300K. Then we can conclude that the new soliton in in the α-helix protein molecules with three channels is a possible carrier of bio-energy transport and the improved model is possibly a candidate for the mechanism.*

Keywords: *soliton, protein molecule, bio-energy transport, thermal stablization, Runge-Kutta method.*

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1. INTRODUCTION

A lot of biological processes in the living systems are associated with bio-energy transport through protein molecules, where energy is released by hydrolysis of adenosin triphosphate (ATP) molecules. This is a very important problem in biology. However, understanding the mechanism of the bio-energy transport in macrobiomolecular systems is a long-standing problem that remains of great interest up to now. One can assume that the energy is stored as vibrational energy in the C=O stretching mode (amide=I) of a polypeptide chains in protein molecules. Following Davydov's idea[1], one can take into account the coupling between the amide-I vibrational quantum (exciton) and the acoustic phonon (molecular displacements) in the protein molecules. Through the coupling, non linear interaction appears in the motion of the vibrational quanta, which could lead to a self-trapped state of the vibrational quantum and a soliton to occur[1],which can move over macroscopic distances along the molecular chains retaining the wave shape and energy and momentum and other properties of quasiparticle. Therefore the bio-energy is transported as a localized" wave packet" or soliton along protein chains. This is just the Davydov model for the bio-energy transport which is proposed first by Davydov in α -helix protein molecules with three channels as is shown in Fig.1 in the 1970s[1].

Davydov's idea yields a compelling picture for the mechanism of bio-energy transport in the protein molecules and consequently has been the subject of a large number of works[2-16]. Problems related to the Davydov model, including the foundation and the accuracy of the theory, the quantum and classical properties, and the thermal stability and lifetimes of the Davydov soliton, have been extensively studied by many scientists[2-16]. However, considerable controversy has been arisen in recent years over whether the Davydov soliton is sufficiently stable in the region of biological temperature to provide a viable explanation for bio-energy transport. Many numerical simula-

tions[7-9] have been based essentially on classical motion and are subject to the criticism that are likely to equations of Fig.1, Molecular structure of α -helix protein. yield unrelieable estimates for the stability of the soliton since the dynamics of the soliton is not being determined by the Schrödinger equation[6]. For the thermal equili- brium properties of the Davydov soliton there is quantum Monte Carlo simulation[12]. In the simulation correlations characteristic of soliton- like quasiparticles occur only at low tempera- tures about T<10K for widely accepted parame- ter values. This is consistent at a qualitative level with the result of Cottingham et al[13]. The latter is a straightforward quantum- mechanical perturbation calculation, in which the lifetime of the Davydov soliton obtained is too small (about 10^{-12}-10^{-13}Sec.) to be useful in the biological processes. This shows clearly that the Davydov soliton is not a true wave function of the systems. Therefore, it is necessary to reform Davydov's wave function. Scientists thought that the soliton with multiquantum state (n>2), for example, Brown et. al's coherent state[5], and Kerr et. al's[11] and Schweitzer et. al's[13] multiquantum state, and Cruzeiro–Hansson's[9] and Förner's[10] two quantum state, and so on, would be thermally stable in the region of biological temperature, and could provide a realistic mechanism for the bio-energy transport in the protein molecules. However, the assumption of the standard coherent state is unsuitable or impossible for the protein molecules because the numbers of particle in this state are unnumerable and one could not retain conservation of the number of particles of the system. The assumption of a multiquantum state(n>2) along with a coherent state also consist not with the fact that the energy released in ATP hydrolysis (about 0.43eV) can excite only two quanta of amide-I vibration. On the other hand, Cruzeiro-Hansson[9] had thought that Förner's two-quantum state in the semiclassical case was not exact. We proved[17] the Cruzeiro-Hansson's ansatz contains four excitons (quanta), instead of two excitons. Obviously, it is not possible at all to create the four excitons by the energy released in the ATP hydrolysis.

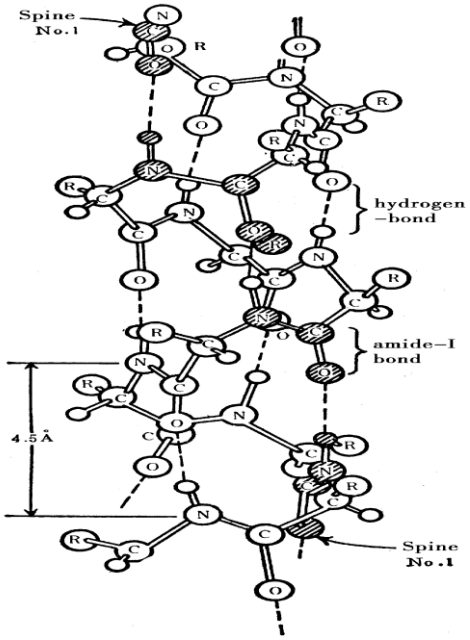

Fig1. *Molecular Structure of α -Helix Protein*

Based on the work of Cruzeiro-Hansson and Förner, and so on, we improve and develop the Davydov model by changing simultaneously the Hamiltonian and the wave function of the systems. We add new coupling interaction between the acoustic phonon and amide-I vibrational modes into original Davydov's Hamiltonian, and replace the one-quantum (exciton) state in the Davydov's wave function by a quasi-coherent two-quantum state. Thus, the equation of motion and the properties of the soliton excited in the improved model are completely different from that in the Davydov model. I suppose that this model could resolve the controversy on the thermal stability and lifetime of the soliton excited in protein molecules. In our theory the wave function and Hamiltonian of the protein molecules with one-channel was represented by[17]

$$|\Phi(t)\rangle = |a(t)\rangle|\beta(t)\rangle = \frac{1}{\lambda}\left[1 + \sum_n a_n(t)B_n^+ + \frac{1}{2!}\left(\sum_n a_n(t)B_n^+\right)^2\right]|0\rangle_{ex} \cdot \exp\left\{-\frac{i}{\hbar}\sum_n\left[\beta_n(t)P_n - \pi_n(t)u_n\right]\right\}|0\rangle_{ph} \quad (1)$$

and

$$H = H_{ex} + H_{ph} + H_{\text{int}} = \sum_n \left[\varepsilon_0 B_n^+ B_n - J(B_n^+ B_{n+1} + B_n B_{n+1}^+)\right] + \sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2}W \cdot (u_n - u_{n-1})^2\right] + \sum_n [\chi_1 (u_{n+1} - u_{n-1}) B_n^+ B_n + \chi_2 (u_{n+1} - u_n)(B_{n+1}^+ B_n + B_n^+ B_{n+1})] \quad (2)$$

where B_n^+ and B_n are Boson creation and annihilation operators for the exciton, $|0\rangle_{ex}$ and $|0\rangle_{ph}$ are the ground states of the exciton and phonon, respectively. u_n and P_n are the displacement and momentum operators of amino acid residue in site n, respectively. the $a_n(t), \beta_n(t) = \langle \Phi(t)|u_n|\Phi(t)\rangle$ and $\pi_n(t) = \langle \Phi(t)|P_n|\Phi(t)\rangle$ are three setes of unknown functions, λ is a normalization constant. Where $\varepsilon_0 = \hbar\omega_0 = 1665\text{cm}^{-1} = 0.2035\text{eV}$ is excitation energy of an isolated amide-I oscillator or energy of the exciton (the C=0 stretching mode). Present non-linear coupling constants are χ_1 and χ_2, they represent the modulations of the one-site energy and resonant (or dipole-dipole) interaction energy for the excitons caused by the displacement of amino acid residue, respectively. M is the mass of an amino acid residue, and W is the elasticity constant of the protein, J is the dipole-dipole interaction energy between neighbouring amino acids, $|0\rangle_{ph}$ and $|0\rangle_{ex}$ are vacuum states of phonon and exciton, respectively. H_{ex} here describe Boson-type Frenkel excitons excited by the energy released in ATP hydrolysis in the protein molecules, H_{ph} describes a harmonic feature of amino acid residues, H_{int} represents the interaction between the two modes of motion. Usually for all parameters in Eqs. (1)-(2) site-independent mean values are used. The average value of the dipole-dipole coupling between neighboring amide-I oscillators is J =0.967 meV. The average spring constant of the hydrogen bonds is taken usually to be W =13 N/m. The average mass M is taken as that of myosine (M =114m_p, m_p is a proton mass). For $\overline{\chi}_1$ the experimental value is 62 pN, $\overline{\chi}_2$ =10-15 pN.

The Hamiltonian and wave function shown in Eqs. (1)- (2) are different from the Davydov's Haniltonian and wave function. We add a new interaction term, $\sum_n \chi_2 (u_{n+1} - u_n)(B_{n+1}^+ B_n + B_n^+ B_{n+1})$, into the originally Davydov's Hamiltonian. Thus the Hamiltonian now has better symmetry and can also represent the features of mutual correlations of the collective excitations and motions of quasi-particles in the protein molecules. The present wave function of the exciton in Eq. (1) is not an excitation state of single-particle, but a coherent state, accurately speaking, a quasi-coherent state. It retains only three terms of the expansion of a standard coherent state, which mathematically is justified in the case of small $a_n(t)$ *(i. e., $|a_n(t)| << 1$),* it can be viewed as an effective truncation of a standard coherent state. Therefore we call $|a(t)\rangle$ *a* quasi-coherent state. However, it is not an eigenstate of the number operator, $\hat{N} = \Sigma_n B_n^+ B_n$, it is a coherent superposition of the excitonic state with two quunta and the ground state of exciton. However, in this state the number of quantum is determinate, instead of unnumerable. To find out how many excitons this state contains, we have to compute the expectation value of the number operator $\hat{N}$ in this state and sum over the sites. The average number of excitons for this state is. $N = \langle a(t)|\hat{N}|a(t)\rangle = \sum_n \langle a(t)|B_n^+ B_n|a(t)\rangle = 2$. Therefore, it contains really two excitons. Thus, we see that the improved model is completely different from the Davydov model. Then, the results obtained from this model are fully different from that of the Davydov model. The distinctions between the two models are shown in Table 1[17]. From this table 1we know that the improved model repulse and refuse the shortcoming of the Davydov model[1], the new soliton in the model is thermal stable at biological temperature 300K, has so enough long lifetime, thus it can plays important role in biological processes, i. e., the new soliton is a very good carrier of bio-energy transport in the protein molecules in the living systems.

Table1. *Comparison of features of the solitons in the improved model and Davydov model*

model	The features of the solitons							
	nonlinear interaction G(10^{-21}J)	amplitude	width 10^{-10}m	binding energy (10^{-21}J)	lifetime at 300K (S)	thermal stability at 300K	critical temperature (K)	number of amino acid traveled by soliton in lifetime
our model	3.8	1.72	4.95	-7.8	10^{-9}-10^{-10}	stable	320	several hundreds
Davydov model	1.18	0.974	14.88	-0.188	10^{-12}-10^{-13}	unstable	<200	Less than 10

However, this analytic results are only related to the periodic protein molecules with one-channel, some approximate ways containing long-wave approximation, continuum approximation and long-

time approximation, and so on, were used in the calculation. As a matter of fact, any single channel of biological protein molecules consists of 20 different amino acid residues with molecular weights between $75m_p$(glycine) and $204m_p$(tryptophane), which correspond to the variation of mass between $o.67M$ <M <$1.8M$, here M =$114m_p$ is an average mass of amino acid residue, m_p is proton mass, Therefore the protein molecules are not periodic, but or aperiodic or nonuniform of structure. This structure aperiodicity results necessarily in the fluctuations of spring constant, dipole-dipole interaction, exciton-phonon coupling constant, diagonal disorder and chain-chain interaction in the proteins, Thus the states of new solitons will be changed. In such a case, it is very necessary to study the properties of the soliton in the bio-energy transport process in aperiodic protein molecules. In this paper we will study the influences of structure aperiodicities on the features of soliton excited in the α -helix protein molecules with three channels as shown in Fig.1 by numerical simulation and Runge-Kutta way[18]. We could see that the soliton is still very robust against these structure aperiodicites of the protein molecules. In Sec. Ⅱ we introduce the calculated method; the results and discussion are described in Sec.Ⅲ. In Sec.Ⅳ we state the conclusions of this paper.

2. NUMERICAL SIMULATION METHOD

For the α -helix protein molecules with three channels the Hamiltonian and the wave function in Eqs.(1) and (2) are , respectively, replaced by[17]

$$H = H_{ex} + H_{ph} + H_{inx} = \sum_n [\varepsilon_0 B^+_{n\alpha} B_{n+1\alpha} - J(B^+_{n\alpha} B_{n+1\alpha} + B_{n\alpha} B^+_{n+1\alpha})] + \sum_n [\frac{P^2_{n\alpha}}{2M} + \frac{1}{2}W(q_{n\alpha} - q_{n-1\alpha})^2]$$
$$+ \sum_n [\chi_1(q_{n+1\alpha} - q_{n-1\alpha}) B^+_{n\alpha} B_{n\alpha} + \chi_2(q_{n+1\alpha} - q_{n-1\alpha})(B^+_{n+1\alpha} B_{n\alpha} + B^+_{n\alpha} B_{n+1\alpha}) + L(B^+_{n\alpha} B_{n+1\alpha} + B^+_{n\alpha} B_{n-1\alpha})] \quad (3)$$

$$|\Phi(t)\rangle = |\Phi(t)\rangle |\beta(t)\rangle$$
$$= \frac{1}{\lambda}[1 + \sum_{n\alpha} a_{n\alpha}(t) B^+_{n\alpha} + \frac{1}{2!}(\sum_{n\alpha} a_{n\alpha}(t) B^+_{n\alpha})^2] |0\rangle_{ex} \times \exp\{-\frac{i}{\hbar}\sum_n [q_{n\alpha}(t) P_{n\alpha} - \pi_{n\alpha}(t) u_{n\alpha}]\} |0\rangle_{ph} \quad (4)$$

where subscript α =1,2,3 denote the number of three channels, L is the coefficient of chain-chain interaction among the three channels in the protein molecules. From time-dependent SchrÖdinger equation

$$H |\Phi> = i\hbar \frac{\partial}{\partial t} |\Phi> \quad (5)$$

with the Hamiltonian Eq.(3) and above time-dependent wave function Eq.(4) and

$$i\hbar \frac{\partial}{\partial t} < \Phi(t) | u_n | \Phi(t) > = < \Phi(t) | [u_n, H] | \Phi(t) > \quad (6)$$

$$i\hbar \frac{\partial}{\partial t} < \Phi(t) | P_n | \Phi(t) = < \Phi(t) | [P_n, H] | \Phi(t) > \quad (7)$$

and considering further the neighboring interactions among the three channels we can find out

$$i\hbar \dot{a}_{n\alpha}(t) = \varepsilon_0 a_{n\alpha}(t) - J[a_{n+1\alpha}(t) + a_{n-1\alpha}(t)] + \chi_1[q_{n+1\alpha}(t) - q_{n-1\alpha}(t)] a_{n\alpha}(t)$$
$$+ \chi_2[q_{n+1\alpha}(t) - q_{n-1\alpha}(t)][a_{n+1\alpha}(t) + a_{n-1\alpha}(t)]$$
$$+ \frac{5}{2}\{w(t) - \frac{1}{2}\sum_m [q_{m\alpha}(t)\pi_{m\alpha}(t) - \dot{\pi}_{m\alpha}(t)\dot{q}_{m\alpha}(t)]\} a_{n\alpha}(t) + L[a_{n\alpha+1}(t) + a_{n\alpha-1}(t)] \quad (8)$$

$$M\ddot{q}_{n\alpha} = W[q_{n+1\alpha}(t) - 2q_{n\alpha}(t) + q_{n-1\alpha}(t)] + 2\chi_1[|a_{n+1\alpha}(t)|^2 - |a_{n-1\alpha}(t)|^2]$$
$$+ 2\chi_2\{a^*_{n\alpha}(t)[a_{n+1\alpha}(t) - a_{n-1\alpha}(t)] + a_{n\alpha}(t)[a^*_{n+1\alpha}(t) - a^*_{n-1\alpha}(t)]\} \quad (9)$$

We can eliminate the term containingε_0 in Eq.(8) by the following transformation:

$$\varphi_{n\alpha}(t) = a_{n\alpha}(t)\exp[-i\varepsilon_0 t/\hbar] \tag{10}$$

Because $a_n(t)$ in Eqs.(8)-(9) is a complex function, thus we can make transformation

$$a_{n\alpha}(t) = ar_{n\alpha}(t) + iai_{n\alpha}(t) \qquad \text{with} \qquad |a_n|^2 = |ar_n|^2 + |ai_n|^2, \tag{11}$$

Thus Eqs.(8)-(9) change as

$$\hbar\dot{a}r_{n\alpha} = -J(ai_{n+1\alpha} + ai_{n-1\alpha}) + \chi_1(q_{n+1\alpha} - q_{n-1\alpha})ai_{n\alpha} + \chi_2(q_{n+1} - q_{n-1\alpha})(ai_{n+1\alpha} + ai_{n-1\alpha}) + L[ai_{n\alpha+1}(t) + ai_{n\alpha-1}(t)] \tag{12}$$

$$-\hbar\dot{a}i_{n\alpha} = -J(ar_{n+1\alpha} + ar_{n-1\alpha}) + \chi_1(q_{n+1\alpha} - q_{n-1\alpha})ar_{n\alpha} + \chi_2(q_{n+1\alpha} - q_{n-1\alpha})(ar_{n+1\alpha} + ar_{n-1\alpha}) + L[ai_{n\alpha+1}(t) + ai_{n\alpha-1}(t)] \tag{13}$$

$$\dot{q}_{n\alpha} = \frac{y_{n\alpha}}{M} \tag{14}$$

$$\dot{y}_{n\alpha} = W[q_{n+1\alpha} - 2q_{n\alpha} + q_{n-1\alpha}] + 2\chi_1[ar^2_{n+1\alpha} + ai^2_{n+1\alpha} - ai^2_{n-1\alpha} - ai^2_{n-1\alpha}] + 4\chi_2[ar_{n\alpha}(ar_{n+1\alpha} - ar_{n-1\alpha}) + ai_{n\alpha}(ai_{n+1\alpha} - ai_{n-1\alpha})], \tag{15}$$

where $ar_{n\alpha}$ and $ai_{n\alpha}$ are real and imaginary part of $a_{n\alpha}$ (t). Eqs.(12)-(15) are equations we use in simulation calculations. The dynamic properties of a peptide group or amino acid molecules is described by the above four-equations[18]. Thus the protein molecules consisted of *N* amino acid molecules should associatively solve 4*N* equations .From these equations we can find out their solutions, $ar_{n\alpha}$ and $ai_{n\alpha}$, by numerical simulation of fourth-order Runge-Kutta method and by using the following initial condition at a point $n_{0\alpha}$: $a_{n\alpha}(t=0) = A\sec h[(n-n_{0\alpha})(\chi_1+\chi_2)^2/4JW]$ for the α -helix protein molecules with three channels, where α =1,2,3, A is normalization factor. Thus we can determine the solutions of Eqs.(8)-(9). However, in the simulation calculation the following boundary conditions must be satisfied: (1) the energy of the soliton must retain constant up to 0.0012%, i.e., the energy must be conservative at any position and time; (2) in motion of soliton, the probability of the soliton must be in normalized at any time, or speaking ,numbers of particle for the system must be conservative; (3) the energy of the soliton is real, its imaginary part must be approach to zero up to an accuracy of 0.001fev. In accordance with The three criterions and utilizing above equations and above initial conditions we can calculate the evolution of time and space for the probability by MATLAB language and data-parallel programming, where the time step size is chosen as 0.01ps. In this calculation the values of the physical parameters we used are as follow. The mass M =5.73×10^{-25}kg=114×3 amu (atomic mass units) , 114amu is a mass of myosine, W =39N/m, ε_0 =0.2035*eV*, J =9.68×10^{-4}*eV*, χ_1 = 6.2×10^{-11}N, χ_2 =(10-18)×10^{-12}N and L =1.5meV for the α -helix protein molecules with three channels [1-17]. Applying the above descrete equations and data we can calculate numerically their solutions related the time, where $|a_{n\alpha}(t)|^2$ is probability of the soliton occurred at nth amino acid molecule. Thus we can plot the state of the soliton in three dimensional time-place in the case of structure disorder for the protein molecules as follows.

3. RESULTS OF NUMERICAL SIMULATION AND DISCUSSION

3.1. The Motion of Solitons in the Protein Molecules

When the above initial condition is imported from the end of the molecular chain, the numerical solution of Eqs.(12)-(15) obtained by using the fourth order Runge-Kutta method[18] and the above average values of parameters for the α -helix protein molecules with three channels in the improved model is shown in Fig.2. In Fig.2a we show the behaviors of motion of the solution, when the initial condition of $a_{n\alpha}(t=0) = A\sec h[(n-n_{0\alpha})(\chi_1+\chi_2)^2/4JW]$,where α =1,2,3, are simultaneously motivated on the first ends of the three channels. From this figure we see that this solution can retain the clock shape to move over a long distances in the range of spacings of 400 amino acid residues and the time of 40ps without dispersion along the molecular chains, i.e., this solution is a soliton. Therefore Eqs.(8)-(9) have exactly soliton solution with a clock shape. This is

same with the analytic results obtained for the protein with single channel in continuum approximation in this model in which the dynamical equation is a standard nonlinear Schrodinger equation[17]. In Fig.2b and 2c we plot also the feature of motion of the solutions, where the initial conditions of $a_{n\alpha}$ (t=0) =0, where α =1,2, $a_{n3}(t=0) = A\sec h[(n-n_{03})(\chi_1+\chi_2)^2/4JW]$, and $a_{n\alpha}(t=0) = A\sec h[(n-n_{0\alpha})(\chi_1+\chi_2)^2/4JW]$ where α =1,2, a_{n3}(t=0)=0 are used, respectively. These initial conditions denote that the first ends of one channel and two channels are motivated, but other two channels and one channel are not linked, respectively. We see from Fig.2b that the new two waves with small amplitudes are generated, except for one soliton occurred on the channel linked by above initial condition. Obviously, the new two waves are still excited by the above initial condition through the interactions among the three channels. Although the two excitations are small, they can move over long distances along the two chains keeping their amplitudes. Therefore, they are still some solitons with a small amplitude and clock shape. However, we see a strange phenomenon from Fig.2c that the amplitudes of solitons generated in the two motivated chains are small, in an unmotivated chain the soliton formed from the superposition of waves induced by other two chains is greater. From this study we know that the solitons formed have same and higher energy, when the initial conditions are simultaneously motivated on the first ends of the three channels, which corresponds to practical case, but the soliton feature of solutions is substandard in other two cases which occur not in practical case.

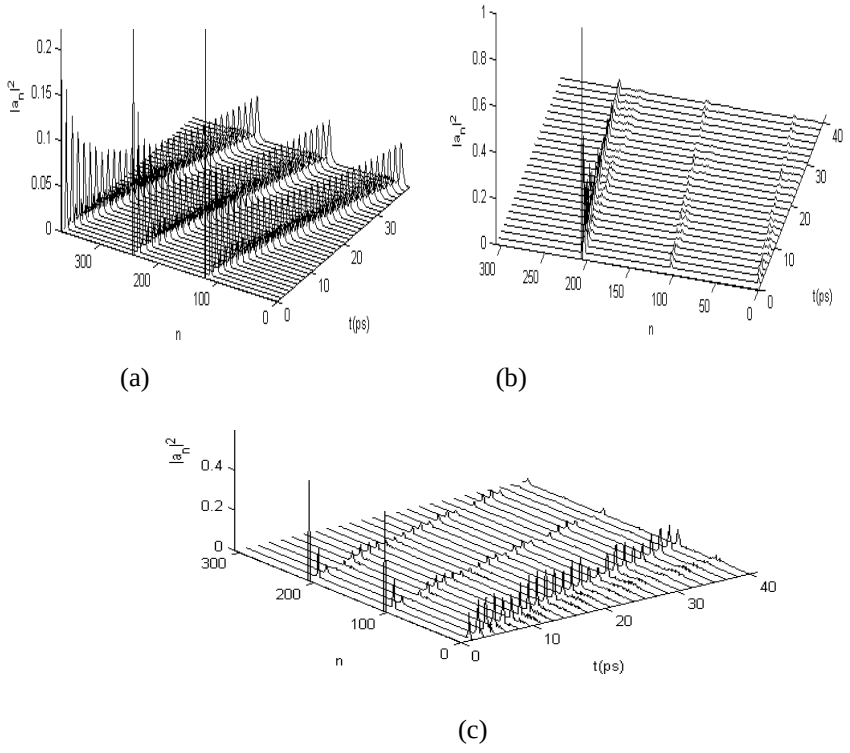

Fig2. *Features of soliton solution of Eqs.(10)-(13) for α -helix protein with three channels*

In order to confirm farther the soliton feature of the solutions of Eqs.(8)- (9), we study farther the collision property of the solitons with a clock shape, set up from opposite ends of the channels for the α -helix protein molecules with three channels, the result is shown in Fig3a, when the above initial conditions motivate simultaneously the opposite ends of the three channels as mentioned above. From this figure we see clearly that initial two solitons with clock shapes separating 100 amino acid spacings in each channel collide with each other at about 17ps. After this collision, two solitons in each channel go through each other without scattering and retain still their shapes of clock to propagate toward and separately along the three chains, which satisfy the rule of collision of macroscopic particles. Thus we can also judge from this result that the solution of Eqs.(8)-(9) in the α -helix protein is an exact soliton. In Fig.3b and 3c we plot also the feature of collision of the two solitons generated from opposite ends of the channels, when the above initial conditions motivate the opposite ends of one channel and two channels, but are not linked with the opposite ends of other two channels and one channel, respectively. In the two cases the soliton feature of solutions after the collision is substandard, especially for the initial condition to motivate only the opposite ends of single channel shown in Fig.3b. Thus the solutions of Eqs.(8)-(9) have better soliton feature, when the opposite ends of the three channels are motivated simultaneously by the

above initial conditions in the α -helix protein molecules. Hence we conclude from Figs.2-3 that the soliton excited in the α -helix protein molecules has higher stability in the case of simultaneous motivation of initial condition to the three channels, then we only work in the case in following study.

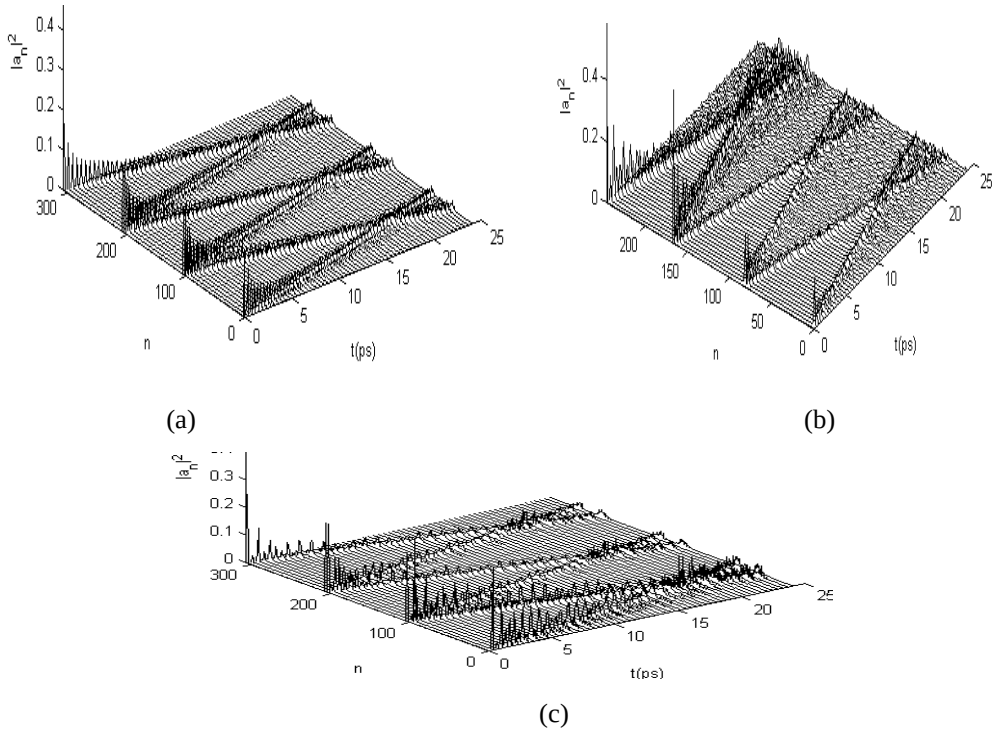

Fig3. *The collision features of the solitons in different conditions*

In the above simulation we study only the behavior of the soliton in the cases of short time of 40ps which exhibits clearly transport feature of this soliton. However, what does its behavior be in the cases of the longer-time and larger spacings? Thus we study further the behaviors of long-time for the solution of Eqs.(12)-(15) in the α -helix proteins with three channels. In Fig.4 we show the result of soliton solutions of Eqs.(12)-(15) obtained at 120ps times and 300 amino acid spacings, when above initial conditions are simultaneously linked on the first ends of the three channels. We can see clearly from Fig.4 that the soliton retain still its amplitude and shape of clock to move in such a case. This result shows that the lifetime of the soliton is, at least, 120Ps. What means the lifetime of 120Ps? We know that the characteristic unit of time for the model is $\tau_0 = r_0 / v_0 = (M / W)^{1/2} \approx 0.98 \times 10^{-13}\ s$, which is the time to move over one lattice space moving at the sound speed, v_o, in the molecular chain. Since one assumes that $v < v_0$, the soliton will not travel the length of the chain unless τ / τ_0 is large compared with L / r_0 where L is the typical length of the protein chain and τ is lifetime of the soliton. Hence for $L / r_0 = 100$, $\tau / \tau_0 > 500$ is a reasonable criterion for the soliton to be a possible mechanism for energy transfer in the proteins. Therefore the lifetime of the soliton, $\tau = 120\ ps$, corresponds to $\tau / \tau_0 > 700$ >500. This means that the soliton in the improved model is a possible carrier of bio-energy transport in the proteins. This conclusion agree also with analytic results in table 1 [16]. This shows that the our analytic results and the improved model are correct[17].

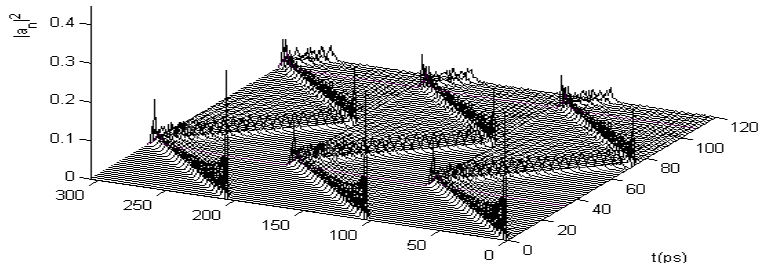

Fig4. *The behaviour of long-time motion for the solitons*

However, the 20 different amino acid residues with molecular weights between 75m_p (glycine) and 204m_p(tryptophane), which correspond to the variation of mass between o.67M <M <1.8M **,** are nonuniformly distributed in the protein molecules. This will result in changes or fluctuations of spring constant, dipole-dipole interaction, exciton-phonon coupling constant and diagonal disorder for the proteins, Thus the states of new solitons will change in such a case. Then in the nonuniform protein molecules we should introduce the random number generators, α_k and $|\beta_n|$, to designate the random features of the mass sequences and ground state energy, at the same time, represent the fluctuations of spring constant, dipole-dipole interaction, exciton-phonon coupling constant and diagonal disorder by $\Delta W = W - W$, $\Delta J = J - J$, $\Delta(\chi_1 + \chi_2) = (\chi_1 + \chi_2) - (\chi_1 + \chi_2)$, $\Delta\varepsilon_0 = \varepsilon - \varepsilon_0 = \varepsilon|\beta_n|$ in the non uniform proteins[10,17], respectively. When the disorder of mass sequence is in the region of $0.67\,M < M_k < 2M$,or 0.67 < α_k <2, where $M_k = \alpha_k M$, and fluctuations of $(\chi_1 + \chi_2)$, J, W and ground state energy ε_0 are about $\Delta(\chi_1 + \chi_2) = \pm 4\%(\chi_1 + \chi_2)$, $\Delta J = \pm 2\% J$, $\Delta W = \pm 8\% W$, $\Delta\varepsilon_0 = \varepsilon|\beta_n|$,ε=0.11meV, $|\beta_n| \le 1$, respectively, the states of the new soliton obtained by the above equations and fourth-order Runge-Kutta method[18] at T=300K are shown in Fig.5. From

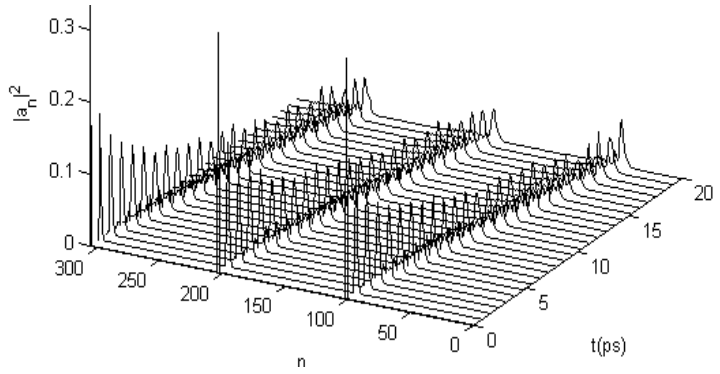

Fig5. *The state of soliton under influences of structure disorders of* $0.67\bar{M} < M_k < 2\bar{M}$ **,** $\Delta(\chi_1 + \chi_2) = \pm 4\%(\chi_1 + \chi_2)$, $\Delta J = \pm 2\% J$, $\Delta W = \pm 8\% W$, $\Delta\varepsilon_0 = \varepsilon|\beta_n|$,ε=0.11meV,$|\beta_n| \le 1$,

these figures we see clearly that the new soliton is still stable at 300K, when the structure nonuniformity occurs in the proteins. Therefore we can conclude that the new soliton is robust against the thermal perturbation and structure nonuniformity of protein molecules. Thus the new soliton in the improved model is a real carrier of the bio-energy transport in the protein molecules.

3.2. The States of Solitons in Proteins in Proteins at Biological Temperature

However, the α -helix protein molecules in the living systems work always at biological temperature of 300K, therefore, we must study the transported ehavior of the soliton at 300K and should add the effect of temperature on the soliton into the above equations. How do we consider this effect? As a matter of fact, this effect was studied in many models in the protein molecules[1,3-4,9-15]. We here adopt Lomdahl and Kerr's method[11] in the calculation because the Lomdahl and Kerr's numerical result exhibits just the thermal instability of the Davydov soliton. In the Lamdahl and Kerr's method[11] the decay term $M\Gamma q_n$ and random noise term, $F_n(t)$, resulting from the temperature, were added in displacement equation of the amino acid molecules Eq.(9). Thus The latter can now be represented by

$$M\ddot{q}_n(t) = W[q_{n+1}(t) - 2q_n(t) + q_{n-1}(t)] + 2\chi_1[|a_{n+1}|^2 - |a_{n-1}|^2] + 2\chi_2\{a_n^*(t)[a_{n+1}(t) - a_{n-1}(t)] + a_n(t)[a_{n+1}^*(t) - a_{n-1}^*(t)\} - M\Gamma\dot{q}_n + F_n(t) \quad (16)$$

where Γ is dissipation coefficient of vibration of amino acids. The correlation function of the random noise force is determined by

$$< F(x,t)F(0,0) >= 2MK_B J\delta(x)\delta(t)/r_0$$

Here r_0 is a lattice constant ,Assuming again that random noise force obeys the normal distribution with criterion deviation $\sqrt{\sigma}$ and zero expected value. Thus this distribution can be represented by

$$N(F_n) = \frac{1}{\sqrt{2\pi\sigma}}\exp[-F_n^2/2\sigma] \quad \text{where } \sigma = 2MK_B T\Gamma/\tau$$

Where τ is a time constant, the quantity Γ is an inverse number of the time constant of the heat bath. Vice Versa. In practical calculation, the random noise force $F_n(t)$ is computed by the random number, which can be presented by $F_n(t) = \sqrt{\sigma}\sum_{r=1}^{L}[X_{nr}(t) - \frac{1}{2}]$. We have assumed L=12, the random number $X_{nr}(t)$ is in the region of $(0 \le X_{nr} \le 1)$ at each time step. Therefore the error where deviation difference of $[X_n(t)-1/2]$is about 1/12, then criterion deviation of $F_n(t)$ is $\sqrt{\sigma}$, its expected value is zero. Then, the size of random noise force is in the range of $|F_n(t)| \le 6\sqrt{\sigma}$. Hence, $F_n(t)$ is Gaussian distribution at $L \to \infty$. Thus we now can find out the soliton solution of the equations of motion, Eqs.(8) and (16) with decay effect and random noise force by the above method and fourth-order Runge-Kutta method[18]. This result at 300K are shown in Fig.6 for the α -helix protein molecules with three channels, when above initial conditions are simultaneously linked on the first ends of the three channels. From this figure we see that the new soliton in the improved model can move along the three channels at the constant speed and amplitude without dispersion in such a case. So, the soliton is still thermally stable at the biological temperature 300K. In Fig.7 we report also the result of motion of the soliton in the case of long time of 120Ps and large spacings of 1000 sites at 300K for the α -helix protein molecules, when above initial conditions are simultaneously linked on the first ends of the three channels. We see from this figure that the solitons are undisturbed in such a case, and move really over a long time and large spacing along the protein molecular chains to retain its amplitude and velocity at the bio-temperatures. In Fig.8 we plot the collision behaviors of the solitons with clock shape, set up from opposite ends of the channels in the α -helix protein molecules, when above initial conditions are simultaneously linked on the opposite ends of the three channels. From this figure we see **c**learly that initial two solitons with clock shapes separating 100 amino acid spacings in each channel collide with each other at about 16ps. After the collision, two solitons in each channel go through each other to retain still their shapes of clock and to propagate toward and separately along the three chains. These results show clearly that although there is the large lattice fluctuations in the protein molecules due to the influence of temperature, the nonlinear coupling interaction between the amino acids and excitons is still able to stabilize the soliton, therefore this soliton is very robust against the thermal perturbation of environment. In this case the lifetime of the new soliton is also, at least, 120Ps. This means that the new soliton could play an important role in the biological processes.

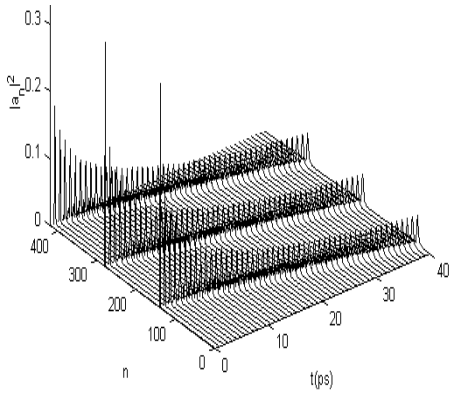

Fig6. *The behaviors of the new soliton at biological temperature 300K*

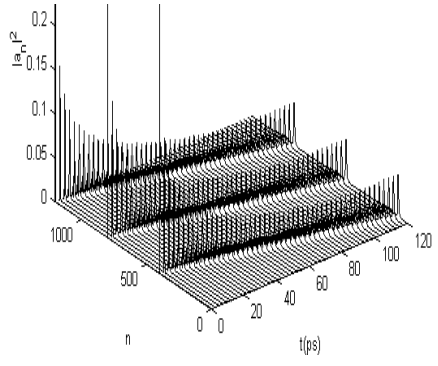

Fig7. *The state of the soliton in long-time motion at 300K*

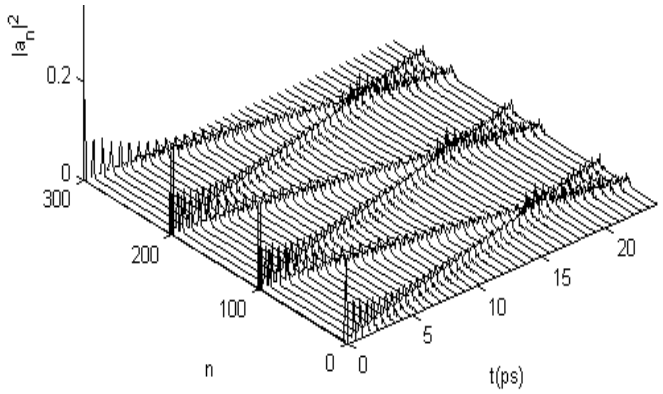

Fig8. *The properties of collision for the solitons at 300K*

4. CONCLUSION

In one word, we study numerically 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 300K in the improved model by the fourth-order Runge-Kutta method. We see clearly from these results that this soliton in the improved model is very stable whether in the cases of long- and short-time motions and mutual collision at 300K, 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=300K and can go through each other without scattering in the collision. In these case its lifetime is, at least, 120PS at 300K, 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.

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