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The influence of the heat bath and structural disorder in protein molecules on soliton transported bio-energy in an improved model

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Abstract

Temperature and structural disorder can have a strong influence on the stability of solitons excited in protein molecules. This problem has been studied in depth with an improved model, using numerical simulation and the Runge–Kutta method, for biological temperatures. The results obtained show that the soliton is thermally stable in the region of biological temperatures, 300 K $<$ T $<$ 320 K, and is very robust against structural disorder, including substantial disorder in the sequence of masses of the amino acids and fluctuations of the spring constant, coupling constant, dipole–dipole interaction constant and ground state energy, due to its larger binding energy which can suppress the destructive effect of the above types of disorder and thermal perturbation. Therefore this soliton is a possible carrier for bio-energy transport in protein molecules. However, very strong structural disorder can also destroy the stability of this soliton.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

As is known, many biological processes or phenomena, for example, muscle contraction, DNA reduplication and neuroelectric pulse transfer on the neurolemma and work of the calcium pump and sodium pump, are associated with bio-energy transport through protein molecules, where the energy is released by hydrolysis of adenosine triphosphate (ATP). Thus, studying the mechanism and features of the bio-energy transport has important meaning in life sciences. However, understanding the mechanism of the bio-energy transport is a long-standing problem that remains of great interest. Davydov thinks that this transport in the protein molecules could

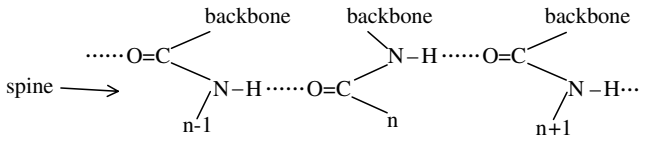

Figure 1. Schematic picture of a hydrogen bonded channel (spine) in a protein helix (indicated by a backbone, perpendicular to the spine).

be carried out by a soliton mechanism [1]. Following Davydov's idea [1], the energy can cause stretching vibration of the C=O mode (amide-I) in a polypeptide chains as shown in figure 1; thus coupling between the amide-I vibrational quantum (exciton) and acoustic phonon (molecular displacements) in the lattice occurs. Through the coupling, nonlinear interaction appearing in the motion of the excitons leads to self-trapping of the exciton; thus the exciton becomes like a soliton [1], which, plus the deformational lattice, can move over macroscopic distances along the molecular chains retaining the wave shape, energy and momentum and other properties of quasiparticles. This is just the Davydov model for the bio-energy transport which was proposed first by Davydov 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 accuracy of the theory, the quantum and classical properties, and the thermal stability and lifetimes of the Davydov soliton, have been extensively studied [2–16]. However, considerable controversy has arisen in recent years over whether the Davydov soliton is sufficiently stable in the region of biological temperature to provide a viable explanation for the bio-energy transport. Many numerical simulations [8–10] have been based essentially on classical equations of motion and are subject to the criticism that they are likely to yield unreliable 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 equilibrium properties of the Davydov soliton there is quantum Monte Carlo simulation [12]. In the simulation, correlations characteristic of solitonlike quasiparticles occur only at low temperatures, about $T < 10$ K, for widely accepted parameter values. This is consistent at a qualitative level with Cottingham *et al*'s result [13]. The latter is a straightforward quantum mechanical perturbation calculation, in which the lifetime of the Davydov soliton is too small (about 10^{-12}–10^{-13} s) to be useful in the biological processes. This shows clearly that the Davydov model is not a true wavefunction of the systems. Therefore, it is necessary to reform Davydov's wavefunction. Scientists had thought that the soliton with a multiquantum state ($n > 2$), for example, Brown *et al*'s coherent state [3], 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 particles in this state are innumerable and one could not retain conservation of the number of particles in the system. The assumption of a multiquantum state ($n > 2$) along with a coherent state is also inconsistent with the fact that the energy released in ATP hydrolysis (about 0.43 eV) can only excite two quanta of amide-I vibration.

On the basis of the work of Cruzeiro-Hansson and Förner, and so on, we improve and extend the Davydov model through simultaneous changes of the Hamiltonian and wavefunction of the systems. A new coupling interaction between the acoustic phonon and amide-I vibrational modes was added in the original Davydov Hamiltonian, and the one-quantum

(exciton) state in the Davydov wavefunction was replaced by a quasi-coherent two-quantum state. In the improved model the wavefunction and Hamiltonian of the protein molecules were, respectively, represented by [17]

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

and

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

where $B_n^\dagger$ and B_n are boson creation and annihilation operators for the exciton, $|0\rangle_{\rm ex}$ and $|0\rangle_{\rm ph}$ are the ground states of the exciton and phonon, respectively. u_n and P_n are the displacement and momentum operators of the lattice oscillator 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 sites of unknown functions, λ is a normalization constant and is chosen here as 1. $\varepsilon_0 = \hbar\omega_0 = 1665\ \mathrm{cm}^{-1} = 0.2035$ eV is the excitation energy of an isolated amide-I oscillator or energy of the exciton (the C=O stretching mode). The present nonlinear 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 molecular displacements, respectively. M is the mass of an amino acid molecule, W is the elasticity constant of the protein. J is the dipole–dipole interaction energy for neighbouring sites. Usually for all parameters in equations (1) and (2) site independent mean values are used. The average value of the dipole–dipole coupling between neighbouring amide-I oscillators is $\bar{J} = 0.967$ meV. The average spring constant of the hydrogen bonds is taken usually to be $\bar{W} = 13\ \mathrm{N\,m}^{-1}$. The average mass $\bar{M}$ is taken as that of myosine ($\bar{M} = 114\,m_{\rm p}$; $m_{\rm p}$ is a proton mass). For $\bar{\chi}_1$ the experimental value is 62 pN; $\bar{\chi}_2 = 10$–15 pN.

The Hamiltonian and wavefunction in equations (1) and (2) in the improved model are different from Davydov's. There is new interaction term, $\sum_n \chi_2(u_{n+1}-u_n)(B_{n+1}^\dagger B_n + B_n^\dagger B_{n+1})$, in the improved Hamiltonian. Thus the Hamiltonian now has better symmetry and can better represent the features of mutual correlations of the collective excitations in the protein molecules. The present wavefunction of the exciton in equation (1) is not an excitation state of a 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. Thus it can approximately represent a standard coherent state, if the $a_n(t)$ is small, for example, $|a_n(t)| \ll 1$, which is also justified mathematically, i.e., it can be viewed as an effective truncation of a standard coherent state. Therefore we can refer to the $|a(t)\rangle$ as a quasi-coherent state. However, it is not an eigenstate of the number operator, $\hat{N} = \sum_n B_n^\dagger B_n$, but a coherent superposition of the exciton state with two quanta and the ground state of the exciton. In this state the number of quanta is not indeterminate. We can find out through the expectation value of the number operator $\hat{N}$ in this state that the number of excitons is $N = \langle a(t)|\hat{N}|a(t)\rangle = \sum_n\langle a(t)|B_n^\dagger B_n|a(t)\rangle = 2$. Therefore, it contains really two excitons. (We point out that it is very erroneous that equation (2) contains three quanta [9], which was obtained from adding three eigenvalues, zero, one and two, for $\hat{N}$ corresponding to each term in equation (2). This calculation violates basic principles of quantum mechanics and is completely mistaken. We can only use the

Table 1. Comparison of features of the solitons, between our model and the Davydov model.

Model	Nonlinear interaction, G (10^{-21} J)	Amplitude	Width (10^{-10} m)	Binding energy (10^{-21} J)	Lifetime at 300 K (s)	Critical temperature (K)	Number of amino acid travelled by soliton in lifetime
Our model	3.8	1.72	4.95	−7.8	10^{-9}–10^{-10}	320	Several hundred
Davydov model	1.18	0.974	14.88	−0.188	10^{-12}–10^{-13}	<200	Less than 10

above way to get the number of particles contained in equation (2) because this state is not the eigenstate of the number operator $\hat{N}$.) Hence, we can say that the improved model is completely different from the Davydov model. Thus, the equation of motion of the soliton and its properties in the improved model are also different from those in the Davydov model. The distinction of their features is shown in table 1 [16]. From table 1 we know that our new model can deal with the shortcomings of the Davydov model [1]; the 'new' soliton in the improved model is thermal stable, and has long enough lifetime at biological temperature 300 K; thus it can play an important role in biological processes. We can suppose that this model could resolve the controversy on the thermal stability and lifetime of the soliton in the protein molecules; thus the new soliton is possibly an exact carrier of bio-energy transport for the protein molecules.

However, the above results were obtained in an analytic way where the protein molecules were thought to be periodic systems, all physical parameters of the protein molecules were used at their average values and some approximations, including long wave approximation and continuum approximation, were used in the calculation. In practice, the biological proteins consist of 20 different amino acid residues with molecular weights between $75m_{\mathrm{p}}$ (glycine) and $204m_{\mathrm{p}}$ (tryptophan) which correspond to variation between $0.67\bar{M}$ and $1.80\bar{M}$; thus they are not periodic, but aperiodic and nonuniform systems, in which there is structural disorder. Careri *et al*'s experiments [19] appear to indicate that even relatively small amounts of disorder in amorphous film of acetanilide (ACN), a protein-like crystal (i.e., the molecular structure of acetanilide crystal is quite analogous to that of alpha-helix protein), is enough to destroy the spectral signature of a 'soliton'. In such a case it is very much necessary to study influences of the structural disorders on the solitons at the biological temperature. In this paper we will study the states and features of the new soliton in nonuniform and aperiodic proteins using numerical simulation and the Runge–Kutta method [18]. We will see that the soliton is still stable at the biological temperature 300 K and robust against these structural disorders of the protein molecules. In this paper we state the calculated method in section 2; the results and discussion are given in section 3. In section 4 we give the conclusions of this investigation.

2. Calculation method

Utilizing equations (1) and (2) and the equations

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle = H|\Phi|(t)\rangle$$

and

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\langle|\Phi(t)|u_n|\Phi(t)\rangle = \langle\Phi(t)|[u_n, H]|\Phi(t)\rangle$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\langle\Phi(t)|P_n|\Phi(t) = \langle\Phi(t)|[P_n, H]|\Phi(t)\rangle$$

we can obtain

$$\begin{aligned} \mathrm{i}\hbar\dot{a}_n(t) &= \varepsilon_0 a_n(t) - J[a_{n+1}(t) + a_{n-1}(t)] + \chi_1[q_{n+1}(t) - q_{n-1}(t)]a_n(t) \\ &\quad + \chi_2[q_{n+1}(t) - q_n(t)][a_{n+1}(t) + a_{n-1}(t)] \\ &\quad + \tfrac{5}{2}\left\{w(t) - \tfrac{1}{2}\sum_m q_m(t)\pi_m(t) - \dot{\pi}_m(t)\dot{q}_m(t)]\right\}a_n(t) \end{aligned} \tag{3}$$

$$\begin{aligned} M\ddot{q}_n(t) &= W[q_{n+1}(t) - 2q_n(t) + q_{n-1}(t)] + 2\chi_1[|a_{n+1}|^2 - |a_{n-1}|^2] \\ &\quad + 2\chi_2\{a_n^*(t)[a_{n+1}(t) - a_{n-1}(t)] + a_n(t)[a_{n+1}^*(t) - a_{n-1}^*(t)]\} \end{aligned} \tag{4}$$

and using the transformation $a_n(t) \to a_n \exp[\mathrm{i}\varepsilon_0 t/h]$ we can eliminate the term of $\varepsilon_0 a_n(t)$ in equation (3).

The above equations can determine states and behaviours of the new soliton [18]. We simulate numerically the solutions of the above equations by the fourth-order Runge–Kutta method. In the calculation, the system of units eV for energy, Å for length and ps for time proved to be suitable for the numerical solutions of equations (3) and (4). In the numerical simulation by the fourth-order Runge–Kutta method [18], we require that the following conditions must be satisfied:

(1) the energy of the soliton, $E = \langle\Phi(t)|H|\Phi(t)\rangle$, must remain constant up to (0.0012%), i.e., the energy must be conservative at any position and time;
(2) in motion of the soliton, the probability of the soliton must be normalized at any time or, so to speak, the number of particles in the system must be conservative, i.e., $\sum_n |a_n(0)|^2 = \sum_n |a_n(t)|^2 = 1$;
(3) the energy of the soliton is real—its imaginary part must be approach zero to an accuracy of 0.001 feV, and the norm is conserved to 0.3 ppm (parts per million).

An initial excitation is required in this calculation; it is chosen as $a_n(0) = A\ \mathrm{sech}[(n - n_0)(\chi_1 + \chi_2)^2/4JW]$ (where A is the normalization constant) at the size n; for the lattice, $q_n(0) = \pi_n(0) = 0$ are applied. The molecular chain is fixed, N is chosen to be $N = 50$ and a time step size of 0.0195 is used in the simulations. The total numerical simulation is performed by a data parallel algorithm using MATLAB language.

3. Calculation results and discussion

3.1. Influence of structural disorder on the new soliton

Applying the above equations of motion and the fourth-order Runge–Kutta method [18] we can numerically calculate their solutions related the time and $|a_n|^2$, where $|a_n|^2$ is the probability that the soliton occurred at the jth amino acid molecule. Thus we can plot the state of the soliton in the time and place in nonuniform and aperiodic protein molecules with different structural disorders. If the above average values of all physical parameters are used, the numerical result for the uniform protein molecular chain is as first shown in figure 2. From this figure we see that the amplitude of the solution of the above equations is constant; therefore it is a real soliton. Thus we can confirm that the above equations have exactly the soliton solution.

When the effects of the 'structural disorder' of the protein molecules are taken into account the states and features of the new soliton will be changed. In such a case we should use a random number generator to produce or represent the random sequences of the different parameters in the protein molecules. We first study influences of disorder of mass sequences on the state of the now soliton. In this case we consider the disorder of mass sequences in which the mass of the amino acid molecule at a certain site is varied relative to the average mass of

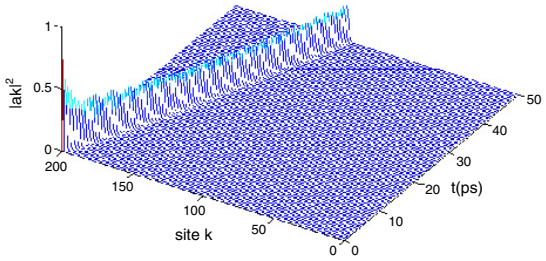

Figure 2. The state of the new soliton in the free case.

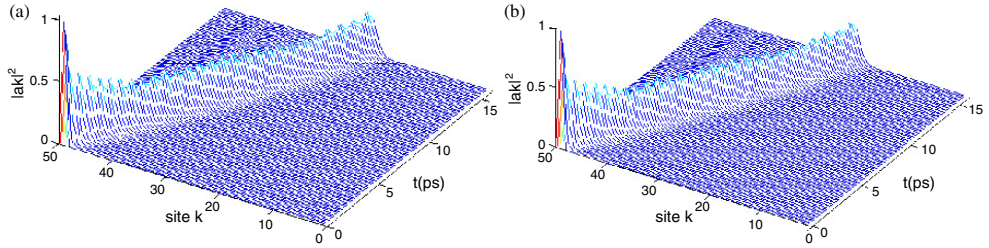

Figure 3. The state of the new soliton at $M_{49} = 100\bar{M}$ (a) and $M_{49} = 100\,000\bar{M}$ (b).

$\bar{M} = 114m_{\mathrm{p}} = (1.17\text{–}1.91) \times 10^{-25}$ kg, but other masses remain equal to $\bar{M}$. In figure 3 we show the features of the new solitons, when the mass of the amino acid residues at site 49 increases to $M_{49} = 100\bar{M}$ and $100\,000\bar{M}$, respectively. Surprisingly, up to quite large masses of $100\bar{M}$ no obvious perturbations and decays appear in the motion of the new soliton; the motion of the new soliton does not change, a quite small fraction of the sound energy is trapped at the impurity and the major fraction is scattered back, and these fractions do not increases up to $M_{49} = 100\,000\bar{M}$. From these results one can conclude that an impurity at one site, which may also be some other molecule bound to the protein at this site (like reactive centres, e.g. haeme groups), does not disturb the soliton at all.

On the other hand, if the random series of masses are distributed over the whole molecular chain, then the variations of the new soliton will differ from the above case. In such a case we should introduce a small parameter α_k to denote the mass at each point in the molecular chain, i.e., $M_k = \alpha_k\bar{M}$; here the α_k were determined by a random number generator with equal probability within a prescribed interval. The result shows that the aperiodicity due to the smaller intervals for α_k, for example, $0.67 \leqslant \alpha_k \leqslant 400$, does not significantly affect the stability of the new soliton, but in the case of large intervals such as $0.67 \leqslant \alpha_k \leqslant 700$, the vibrational energy is dispersed. These results are shown in figure 4. As is known, the variation of masses of the natural amino acids in the protein molecules is $0.67 \leqslant \alpha_k \leqslant 1.80$. Obviously, the interval, $0.67 \leqslant \alpha_k \leqslant 400$, over which motion of the new soliton is unperturbed is evidently larger than $0.67 \leqslant \alpha_k \leqslant 1.80$. Otherwise, there are also some small elongations perpendicular to the protein molecular backbone in the case forming the soliton, but the influence of mass disorder is very small. Therefore we can conclude that the disorder determined by the different masses of the amino acid molecules in the biological proteins cannot destroy the stability of the new soliton, which is quite robust against the mass disorder effects in the improved model.

We also simulate numerically the influence of change of force constant W, arising from the structural disorder, on the stability of the new soliton. Up to a random variation of $\pm 45\%\bar{W}$

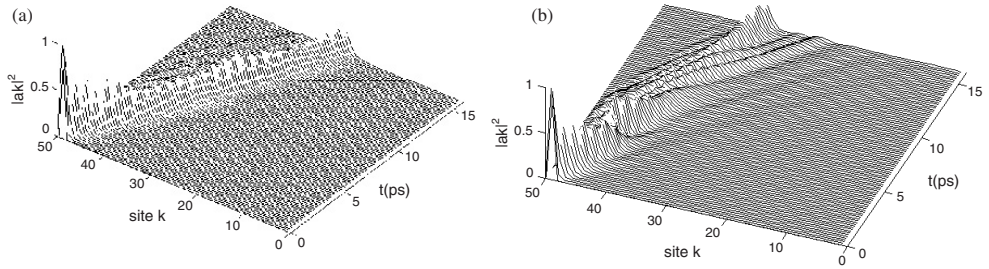

Figure 4. The state of the new soliton at $0.67 < \alpha_K < 400$ (a) and $0.67 < \alpha_K < 700$ (b).

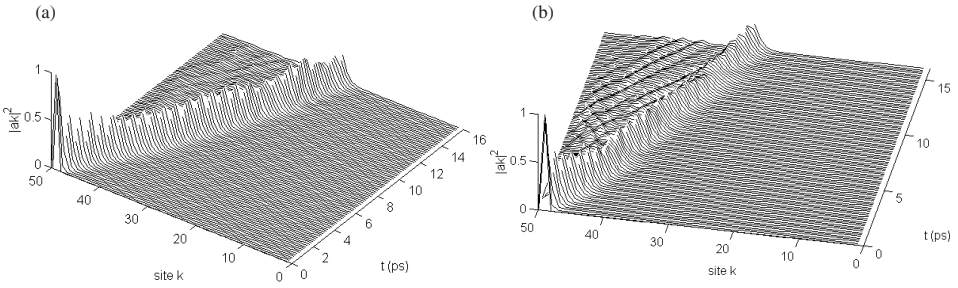

Figure 5. The state of the new soliton at the changes $\Delta W = \pm 45\% \bar{W}$ (a) and $\Delta W = \pm 55\% \bar{W}$ (b).

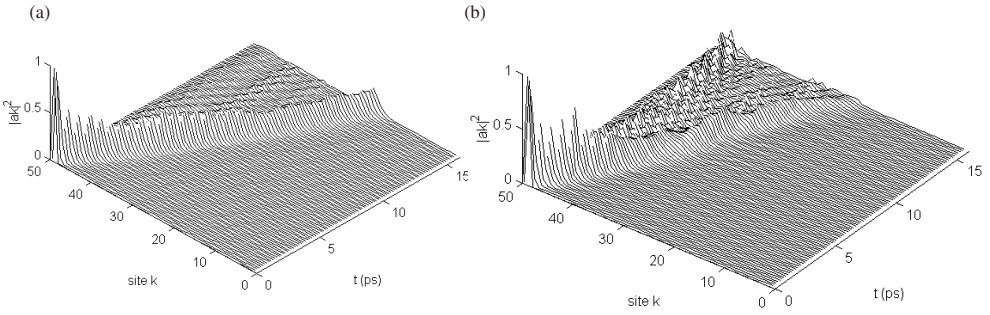

Figure 6. The state of the new soliton at change $\Delta J = \pm 9\% \bar{J}$ (a) and $\Delta J = \pm 15\% \bar{J}$ (b).

we find no change in the dynamics of the new soliton. For $\pm 55\% \bar{W}$, the soliton velocity is only somewhat diminished, when compared with the case of $\bar{W}$. The results are as shown in figure 5. Finally, for $\pm 70\% \bar{W}$, the new soliton disperses slowly and propagation is irregular.

If in addition W is aperiodic, the new soliton is stable up to $\pm 35\% \bar{W}$, while at $45\% \bar{W}$ a slowly dispersive phenomenon for the soliton occurs.

Studies show that the new soliton is more sensitive to the variation in J caused by the disorder of structure, when compared with the other parameters. In fact, for variation in J alone the soliton is stable up to $9\% \bar{J}$, but it disperses at $\Delta J = \pm 15\% \bar{J}$, as shown in figure 6.

If $(\chi_1 + \chi_2)$ alone or together are aperiodic with the natural mass variation, arising from the disorder of the structure, then the states of the new soliton will be changed. When the $(\chi_1 + \chi_2)$ can be varied up to $\pm 25\%$ $(\bar{\chi}_1 + \bar{\chi}_2)$ and in the cases of $0.67\bar{M} \leqslant M < 2\bar{M}$ and $\Delta(\chi_1 + \chi_2) = 25\%(\bar{\chi}_1 + \bar{\chi}_2)$, the new solitons are stable; the results are shown in figure 7. If the fluctuation increases further, the soliton disperses.

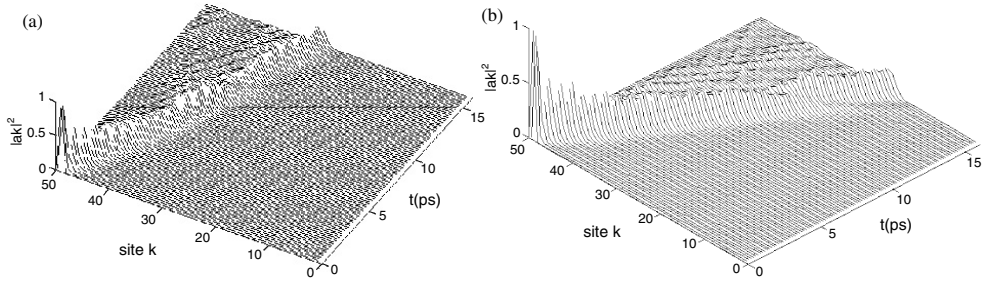

Figure 7. The state of the new soliton at change of $\Delta(\chi_1 + \chi_2) = \pm 25\%(\bar{\chi}_1 + \bar{\chi}_2)$ (a), and $0.67\bar{M} < M < 2\bar{M}$ and $\Delta(\chi_1 + \chi_2) = \pm 25\%(\bar{\chi}_1 + \bar{\chi}_2)$ (b).

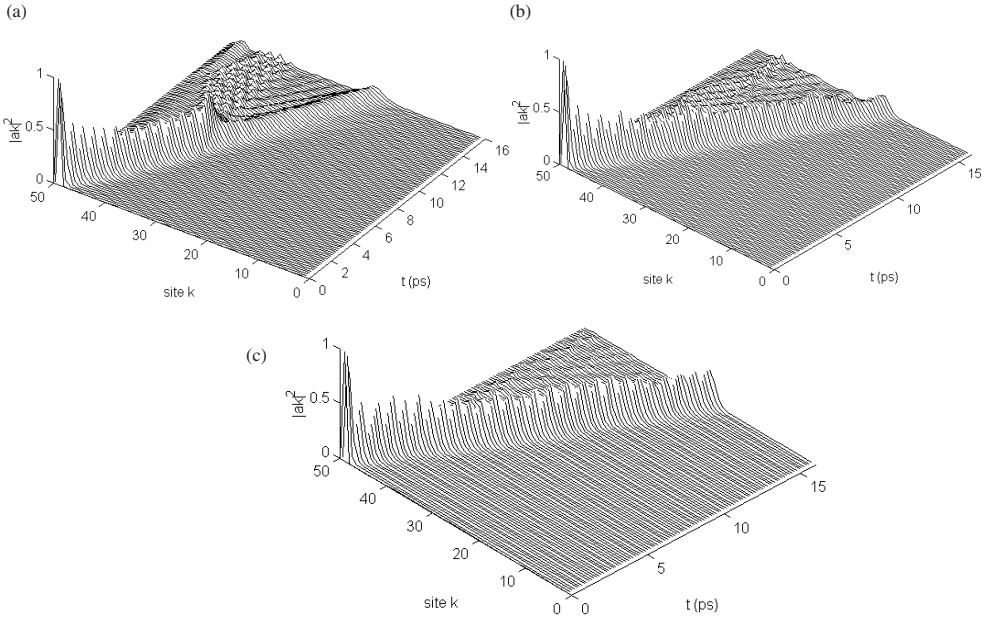

Figure 8. The state of the new soliton at $\Delta\varepsilon_0 = \varepsilon\delta$, $\varepsilon = 0.5$ meV (a), $\Delta\varepsilon_0 = \varepsilon|\beta_n|$, $\varepsilon = 1$ meV, $|\beta_n| \leqslant 0.5$ (b) and $\Delta W = \pm 10\%\bar{W}$, $\Delta J = \pm 5\%\bar{J}$, $\Delta(\chi_1 + \chi_2) = \pm 5\%(\bar{\chi}_1 + \bar{\chi}_2)$, $0.67\bar{M} < M < 2\bar{M}$, $\Delta\varepsilon_0 = \varepsilon|\beta_n|$, $\varepsilon = 0.4$ meV $|\beta_n| \leqslant 0.5$ (c).

In the case of change of the ground state energy $\Delta\varepsilon_0$, caused by different amino acid side groups and corresponding local geometric distortions due to the impurities imported, we found that for an isolated impurity in the middle of the chain, for which the change of the energy caused is denoted by $\Delta\varepsilon_0 = \varepsilon\delta_n$, the new soliton can pass the impurity only if $\varepsilon < 1$ meV. In other cases it is reflected or dispersed. In the case of a random sequence, which is denoted by $\Delta\varepsilon_0 = \varepsilon|\beta_n|$, where $|\beta_n|$ is a random number generator, only for $\varepsilon < 1$ meV and $|\beta_n| \leqslant 0.5$ can the new soliton pass the chain. These results are shown in figures 8(a) and (b). For higher values of ε the new soliton disperses. Finally, if the five parameters in this model are all randomly varied the maximal possible disorders that would still occur in the soliton motion are $\Delta W = \pm 10\%\bar{W}$, $\Delta J = \pm 5\%\bar{J}$, $\Delta(\chi_1 + \chi_2) = \pm 5\%(\bar{\chi}_1 + \bar{\chi}_2)$, $0.67\bar{M} < M < 2\bar{M}$,

$\varepsilon = 0.4$ meV ($\Delta\varepsilon_0 = \varepsilon|\beta_n|$) as shown in figure 8(c). This shows that the new soliton is also very robust against these structural disorders.

The actual degree of disorder in protein molecules remains unknown up to now. However, it is well known that the protein molecules show bio-self-organization with high order. The order distribution of the amino acid molecules in the proteins is a necessary condition for performing the biological functions of the proteins. Any large disorder means degeneration of structure and disappearance of the functions of the protein molecules, and disease of the living bodies will occur—not problems that this paper discusses. Meanwhile, the natural amino acids are not free particles, but are covalently bound in the main polypeptide chains of the proteins. Therefore, discussions of the influences of large disorder of all parameters on the stability of the soliton are not realistic and correct at all for normally biological protein molecules. A more realistic and correct problem for the disorder is studying the influences of the disorder in effective mass and small natural disorders of all parameters, arising from some changes of geometry of the main chain due to the side groups, on the stability of the soliton in the biological proteins. However, the above results obtained show clearly that the larger disorders of effective masses and other physical parameters cannot destroy the stability of the new soliton. Hence, it is not possible at all for it to occur in the protein molecules the case Careri *et al* spoke of, in which the small amounts of disorder can destroy the spectral signature of a 'soliton' in amorphous films of acetanilide [19]. Thus, we can conclude that the influence of the natural structural disorders on the new soliton is very small; the new soliton is very robust against normal or general structural disorders that appeared in the protein molecules.

3.2. Influence of the heat bath on the new soliton

Since the bio-protein molecules in the living systems work always at the biological temperature 300 K, the influences of the temperature on the new solitons at 300 K should be considered and studied in a realistic model of the bio-energy transport in the protein molecules. Thus we now turn to studying the influence of temperature of the heat bath on properties of the new soliton in the proteins by numerical simulation and the fourth-order Runge–Kutta method. In such a case we assume that the proteins are contacted with a heat bath with temperature of 300 K. As is known, the temperature effect on the soliton was previously studied in many models in the protein molecules [1, 4, 8–14, 20, 21]. Lomdahl and Kerr's model [11] exhibits the first instability of the Davydov soliton at 300 K, which results in questioning the validity and applicability of the Davydov model. Hence we here adopt Lomdahl and Kerr's way of calculating the temperature effect on the new soliton. In accordance with their approach [11], the decay term $M\Gamma\dot{q}_n$ and random thermal noise term, $F_n(t)$, resulting from the temperature and damping of the medium, were added in the displacement equation of the amino acids, equation (4); thus it now becomes

$$M\ddot{q}_n(t) = W[q_{nt1}(t) - 2q_n(t) + q_{n-1}(t)] + 2\chi_1[|a_{n+1}|^2 - |a_{n-1}|^2] + 2\chi_2\{a_n^*(t)[a_{n+1}(t) - a_{n-1}(t)] + a_n(t)[a_{n+1}^*(t) - a_{n-1}^*(t)]\} - M\Gamma\dot{q}_n + F_n(t) \tag{5}$$

where Γ is the dissipation or damping coefficient of vibration of amino acids; the correlation function of the random thermal noise force can be, in general, represented by

$$\langle F(x,t)F(0,0)\rangle = 2MK_{\mathrm{B}}J\delta(x)\delta(t)/r_0$$

where r_0 is the lattice constant. Γ should be now represented by an inverse number from the time constant of the heat bath; we here choose $\Gamma = 0.3 \times 10^8\ \mathrm{s}^{-1}$. Since time discretization affects the properties of the Langevin forces in the numerical simulations, we here use an ensemble of Gaussian forces F_n with variance equal to $\sigma = 2MK_{\mathrm{B}}T\Gamma/\tau_1$, where τ_1 is the

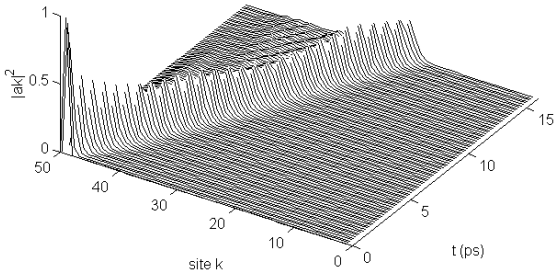

Figure 9. The state of the new soliton at 300 K through the time of 300 ps.

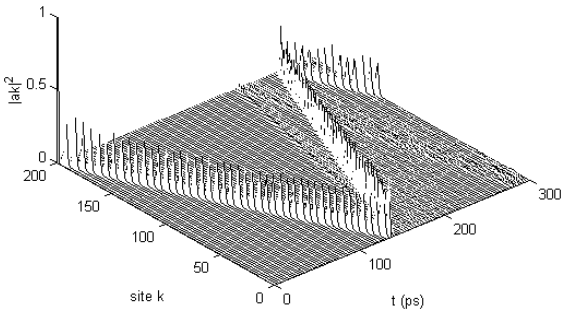

Figure 10. The state of the new soliton at 310 K.

time constant. This means that deviation of the random thermal noise satisfies the normal distribution with criterion of deviation

$$N(F_n) = \frac{1}{\sqrt{2\pi\sigma}} \exp[-F_n^2/2\sigma],$$

where

$$F_n(t) = \sqrt{\sigma} \sum_{r=1}^{L} [X_{\mathrm{nr}}(t) - \tfrac{1}{2}],$$

and has zero expectation value. We here assume $L = 12$; the random number $X_{\mathrm{nr}}(t)$ is in the region of $(0 \leqslant X_{\mathrm{nr}} \leqslant 1)$. Therefore the deviation of $[X_{\mathrm{nr}}(t) - \frac{1}{2}]$ is $1/12$; then the criterion of deviation of $F_n(t)$ is $\sqrt{\sigma}$. Thus the domain of random thermal noise force is $|F_n(t)| \leqslant 6\sqrt{\sigma}$. This choice of Gaussian width is compatible with the fluctuation dissipation theorem and time discretization [22].

According to the above explicit representation of the random thermal noise term, $F_n(t)$, we can find the numerical solution of equations (3) and (5) with the above decay effect and random noise force by the fourth-order Runge–Kutta method [18] at the biological temperatures. We first give the state of the new soliton in the cases of long times of 300 ps at 300 K in the uniform protein molecules, which is shown in figure 9. From this figure we see that there is still soliton motion, which is also very stable, in this case. This shows that the nonlinear coupling between the lattice and oscillators is still able to stabilize the soliton, despite there being large lattice energy fluctuations in such a case due to the heat bath. The result agrees with the analytic considerations in our previous studies [17]. The above behaviour of the soliton can still occur at higher temperature of 310 K as shown in figure 10. However, at the higher temperature of 320 K, the new soliton starts to disperse which is shown in figure 11.

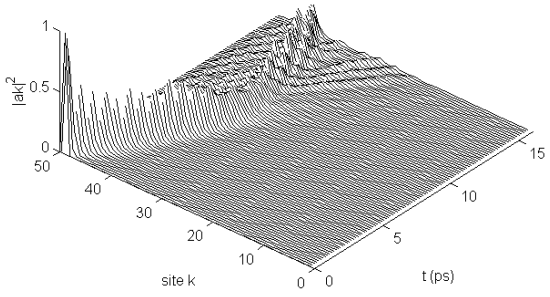

Figure 11. The state of the new soliton at 320 K.

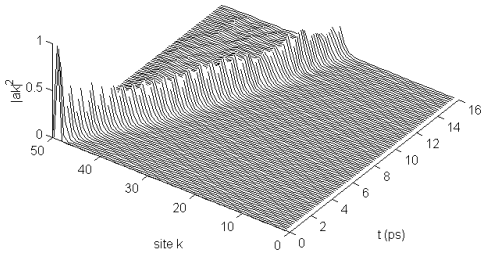

Figure 12. The state of the new soliton under influences of disorder at $0.67\bar{M} < M_{25} < 2\bar{M}$, $\Delta J = \pm 5\%\bar{J}$, $\Delta W = \pm 10\%\bar{W}$, $\Delta(\chi_1 + \chi_2) = \pm 5\%\overline{(\chi_1 + \chi_2)}$, $\Delta\varepsilon_0 = \varepsilon|\beta_n|$, $\varepsilon = 0.41$ meV, $|\beta_n| < 1$, for $T = 300$ K.

We see from figure 9 that the soliton remains invariable in amplitude and shape in the moving case of the long time of 300 ps. This shows that the lifetime of the new soliton is, at least, 300 ps. What does the lifetime of $\tau = 300$ ps mean? As is mentioned above, the characteristic unit of time, τ_0, in this model denotes the time for moving over one lattice space at the sound speed, v_0, 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. Because $L/r_0 = 100$, $\tau/\tau_0 = 500$ is a common and reasonable criterion for the soliton to be a possible mechanism of bio-energy transport in the proteins. Then the lifetime of $\tau = 300$ ps corresponds to $\tau/\tau_0 > 1000 > 500$. Thus this means that the new soliton is very stable in long time transport at 300 K.

From the above results we see clearly that the new soliton in the improved model is thermally stable at 300 K; the lifetime of the new soliton is, at least, about 300 ps. The critical temperature of the new soliton is about 320 K. These conclusions agree with that of analytic results as stable 1 for the improved model [16].

However, the structural nonuniformities of the protein molecules are not considered in the above calculation. Thus we should study further the influences of the structural nonuniformity on the new soliton at the biological temperatures of 300–310 K. According to above we introduce random number generators, α_k and $|\beta_n|$, to designate the random features of the mass sequences and ground state energy in the nonuniformity proteins [10, 17], respectively. When the disorder of the mass sequence is in the region of $0.67\bar{M} < M_k < 2\bar{M}$, or $0.67 < \alpha_k < 2$, where $M_k = \alpha_k\bar{M}$, and fluctuations of $(\chi_1 + \chi_2)$, J, W and ground state energy ε_0 are about $\Delta(\chi_1 + \chi_2) = \pm 5\%\overline{(\chi_1 + \chi_2)}$, $\Delta J = \pm 5\%\bar{J}$, $\Delta W = \pm 10\%\bar{W}$, $\Delta\varepsilon_0 = \varepsilon|\beta_n|$, $\varepsilon = 0.4$ meV, $|\beta_n| \leqslant 0.5$, respectively, the states of the new soliton obtained at $T = 300$ K are as shown

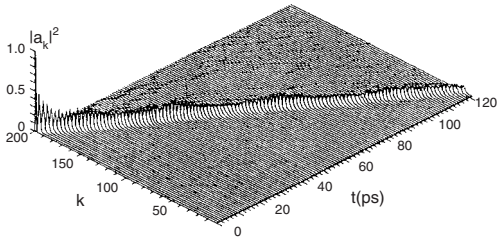

Figure 13. The state of the Davydov soliton at 30 K.

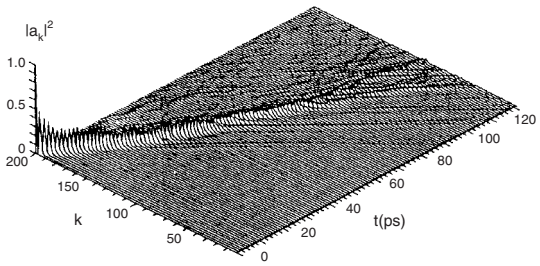

Figure 14. The state of the Davydov soliton at 40 K.

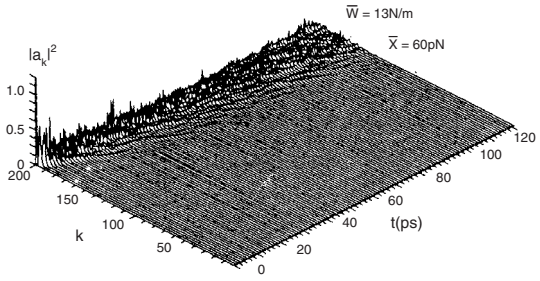

Figure 15. The state of the Davydov soliton at 300 K.

in figure 12. From these figures we see clearly that the new soliton is still thermally stable at 300 K, when the structural nonuniformity occurs in the proteins. Therefore we can conclude that the new soliton is robust against the thermal perturbation and structural nonuniformity of the protein molecules at the biological temperatures. Thus the new soliton in the improved model is a real carrier for the bio-energy transport in the protein molecules.

However, the Davydov soliton does not have the above behaviours. For comparison we listed the results for the Davydov soliton in the cases of same values of physical parameters obtained by Förner [23] which are shown in figures 13–15 for $T = 30$, 40 and 300 K, respectively. From these results we see clearly that the Davydov soliton is not thermally stable at 300 K; its critical temperature is only about 40 K. Therefore our new model has considerable differences from the Davydov model.

Why is this? Or, so to speak, why is this new soliton in the improved model more thermally stable than Davydov's? The reasons are as follows.

Although equations (3) and (4) can become dynamic equations in the Davydov model, when $\chi_2 = 0$ and $\sqrt{2}a_n$ is replaced by A_n (in such a case, the normalization condition

of the Davydov wavefunction becomes $\sum_n |A_n(t)|^2 = 2\sum_n |a_n(t)|^2 = 2$, at present; this again shows clearly that the new wavefunction in the improved model contains exactly two quanta, instead of three quanta [9], as compared with the Davydov wavefunction containing one quantum), the nonlinear coupling energy, $G_{\rm p}$, and binding energy, $E_{\rm BP}$, determining the features of the new soliton are greatly increased due to simultaneous changes of the Hamiltonian; a new interaction between the acoustic vibration of the amino acid and amide-I was added, and the wavefunction, the quasi-coherent two-quantum state, was used, for the system in the improved model; these are, respectively, larger by about three and twenty times than the Davydov soliton's, as shown by

$$G_{\rm p} = 2G_{\rm D}\left[1 + 2\left(\frac{\chi_2}{\chi_1}\right) + \left(\frac{\chi_2}{\chi_1}\right)^2\right] \qquad \text{and}$$

$$E_{\rm BP} = 16E_{\rm BD}\left[1 + 4\left(\frac{\chi_2}{\chi_1}\right) + 6\left(\frac{\chi_2}{\chi_1}\right)^2 + 4\left(\frac{\chi_2}{\chi_1}\right)^3 + \left(\frac{\chi_2}{\chi_1}\right)^4\right],$$

where $G_{\rm D} = 4\chi_1^2/(1-s^2)W$ and $E_{\rm BD} = -\chi_1^4/3JW$ are the corresponding values for the Davydov soliton. Thus the stability of the new soliton is greatly enhanced in the improved model. We concretely calculated these values by using the above parameters for the α-helix protein molecules [1–17]; the binding energy of the new soliton $E_{\rm BP} = 7.8 \times 10^{-21}$ J is also greater by about two times than the thermal energy $K_{\rm B}T = 4.14 \times 10^{-21}$ J at 300 K. Then, the binding energy can completely suppress the destructive effect of the thermal perturbation on the new soliton. This shows that the new soliton with quasi-coherent two-quantum states is very robust against the thermal fluctuation. Therefore, the new soliton is thermally stable. However, the binding energy of the Davydov soliton is $E_{\rm BD} = 0.188 \times 10^{-21}$ J with the same parameter values, which is smaller by about forty times than the above $E_{\rm BP}$ and the thermal energy $K_{\rm B}T$ at 300 K. Thus it is easily destroyed by the thermal perturbation. Therefore, the Davydov soliton is not thermally stable at 300 K which was verified by Forner's and Lomdahl *et al*'s numerical simulation [10, 11] and Cottingham *et al*'s [13] analytic calculation.

4. Conclusion

We study here the influences of structural disorder and temperature or a heat bath on the states of a new soliton in an improved model proposed by us [17]. The results obtained show that the new soliton is very stable against the structural disorder, for example, the random distribution of the sequence of masses of amino acids and fluctuations of the force constant, dipole–dipole interaction constant, coupling constant and ground state energy. Meanwhile, the new soliton is also thermally stable at 300–320 K, its lifetime may reach 300 ps and its critical temperature is about 320 K. Therefore the new soliton may be a real carrier for bio-energy transport in protein molecules.

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