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The features of nonlinear excitation and energy transport in the protein molecules

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ABSTRACT

The features of nonlinear excitation (or soliton motion) and energy transport in the α–helical protein molecules arising from the energy released in the hydrolysis of adenosine triphosphate (ATP) molecules, which is a basic problem in life science and related to many biological processes, are studied and reviewed systematically. Based on different understanding of properties of structure of α–helical protein molecules some theoretical models of the nonlinear excitation and energy transport along the molecular chains have been proposed and established, A brief survey of past researches on different models and theories of energy, including Davydov's, Takeno's, Yomosa's, Brown et al's, Schweitzer's, Cruzeiro-Hansson's, Forner's and Pang's models were first stated and reviewed in this paper. Subsequently we studied and reviewed mainly and systematically the properties, thermal stability and lifetimes of the carriers (solitons) transporting the energy at physiological temperature 300K in Pang's and Davydov's theories. From these investigations we know that the carrier (soliton) of energy transport in the α–helical protein molecules in Pang's model has a higher binding energy, higher thermal stability and larger lifetime at 300K relative to those of Davydov's model, in which the lifetime of the new soliton at 300K is enough large and belongs to the order of 10^{-10} second or $\tau/\tau_0 \geq 700$. Thus we can conclude that the soliton in Pang's model is exactly the carrier of the energy transport, Pang's theory is appropriate to α–helical protein molecules.
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INTRODUCTION

What is life or life activity? In the light of biophysicist's view, the so-called life or life activity is just processes of mutual changes and coordination and unity for the bio-material, energy and bio-information in the live systems. Their synthetic movements and co-operative changes are just total life activity. Therefore we can say that the bio-material is the foundation if life, the energy is its center, the bio-information is the key of life activity, but the transformation and transfer of bio-information are always accompanied by the transport

of energy in living systems[1]. Thus, the energy and its transport are an fundamental and important process in life activity. The energies needed are mainly provided by that released in adenosine phosphate (ATP) hydrolysis in the living systems. Namely, an ATP molecule reacts with water, which results in the energy release of 0.43eV under normal physiological conditions. The reaction can be represented by

$$ATP^{4-} + H_2O \rightarrow ADP^{3-} + HPO_4^{2-} + H^+ + 0.43eV$$
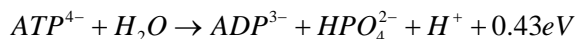
where ADP is the adenosine diphosphate. The bio-energies needed in biological processes in the bio-tissues come basically from this energy, namely, it is mainly used in these processes, for example, the muscle contraction, DNA duplication and the neuroelectric pulse transfer on the membranes of neurocytes as well as work of calcium pump and sodium pump. Therefore, there is always a process of energy transport from the producing place to required organisms in the living systems. However, understanding of mechanism of the energy transport in the living systems is a long standing problem which retains interesting up now. Plenty of the models of energy transport were proposed, but most of them are not successful[1-4]. In general, ATP molecules bind often to a specific site on the protein molecule, the energy supply for most protein activity and functions is provided by the ATP hydrolysis. Thus the transport of energy released by ATP hydrolysis is always related to the protein molecules and their changes of conformation and configuration.

As it is known, the protein molecules are composed of more than twenty different kinds of individual building blocks called amino acids. Each amino acid is again constructed by an amino group (NH_2), a carboxyl group (COOH), and a side group, or radical attached to an α carbon atom. The radical is what distinguishes one amino acid from another. Amino acids polymerize to form long chains of residues that constitute a protein molecule. When two amino acids join together, they release one water molecule and form a peptide bond. When the polypeptide chain has been formed, it can fold into a variety of complex three-dimensional conformations. Of particular are the three structural configurations that recur over and over in proteins: the α–helix, the ²-sheet and globular conformation. In the α-helix the polypeptide chain is tightly coiled about its longitudinal axis. In the ²sheet the chain can be visualized as pleated strands of protein. The globular conforma-

tion is most complex since the chains are folded irregularly into a compact near- spherical shape. Part of the chain can often be in the α-helix or the ²sheet configuration[1,4,5].

Generally speaking, the energy can be converted to a particular vibrational excitation within a protein molecule. A likely recipient exchange is the amide-I vibration. Their vibration is primarily a stretch and contraction of the C=O bond of the peptide groups. The amide-I vibration is also a prominent feature in infrared and Raman spectra of protein molecules. Experimental measurement shows that one of the fundamental frequencies of the amide-I vibration is about 0.205eV. This energy is about half the energy released during the ATP hydrolysis. Moreover, it remains nearly constant from protein to protein, indicating that it is rather weakly coupled to other degrees of freedom. All these factors can lead to the assumption that the energy released by ATP hydrolysis might stay localized and stored in the amide-I vibration excitation. A biological role for vibrational excited states was first proposed by McClare in connection with a possible crisis in bioenergetics[6] (for more information about McClare's work see the article by Luca Turin, in this issue[7]). Then, as an alternative to electronic mechanisms, one can assume that the energy is stored as vibrational energy in the C=O stretching model (amide-I)of polypeptide chains in the protein molecules. In view of the features of energy some theoretical models of the energy transport have been proposed subsequently. In this review paper we will survey these theoretical models as well as their properties and correctness.

THEORETICAL MODELS OF NONLINEAR EXCITATION AND ENERGY TRANSPORT IN PROTEIN MOLECULES

Davydov's theory

It is well known that an inspection of the α-helix structure reveals three channels of hydrogen-bonded peptide groups approximately in the longitudinal direction with the sequence:….H-N-C=O…H-N-C=O…H-N-C=O…H-N-C=O…., where the dotted lines indicate the hydrogen bond, Davydov worked out this idea in the α-helix protein molecules, which is shown in Figure 1, based on McClare's proposal for explaining the conformational changes responsible for muscle

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contraction[7,8], where the trigger is the energy donating reaction of ATP hydrolysis. His theory has shown how a soliton (nonlinear excitation) could travel along the hydrogen-bonded spines of the α-helix protein molecular chains. Davydov's assumption was that the first event after the ATP hydrolysis is the storing of the energy released by the chemical reaction in a vibrational mode of the peptide group. In 1973 Davydov suggested that the amide-I energy could stay localized through the nonlinear interactions of the vibrational excitation with the deformation in the protein structure caused by the presence of the excitation. The excitation and the deformation balance each other and form a soliton (nonlear excvitation).
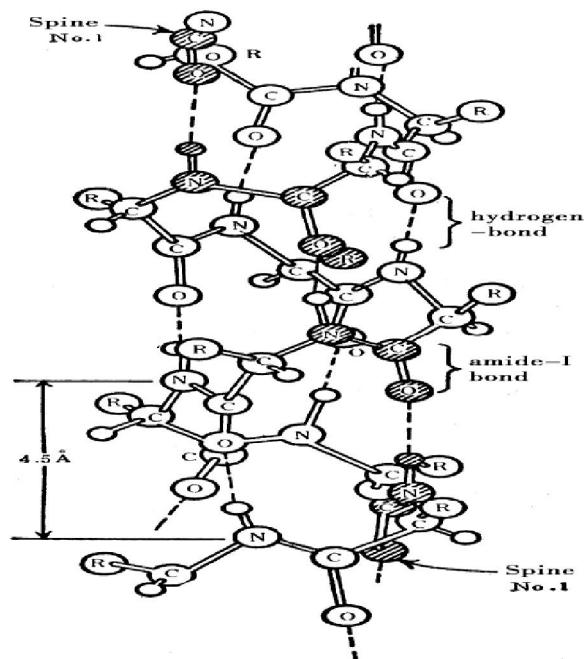

Figure 1 : Structure of α–helical protein

Thus the energy can transport along the protein molecules in virtue of the motion of the soliton. This mechanism can be described classically as follows. Vibrational energy of the C=0 stretching (or amide-I) oscillators that it localized on the helix chains acts, through a phonon coupling effect, to deform the structure of the amino acid residue, the deformation of amino acid residues reacts, again through phonon coupling, to trap the amide-I vibrational quanta and prevent its dispersion. Thus a soliton is formed in this process. This effect is called self-trapping of the amide-I vibrational quantum (or exciton). The soliton can moves over a macroscopic distances along the molecular chains keeping its shape and energy and momentum and other quasi-particle properties. This is

just Davydov theory of bioenergy transport in α-helical protein molecules, which was proposed by Davydov in1973[8-12]. The mathematical techniques that are used to analyze Davydov's soliton are analogous to some that have been developed for the 'polaron' effect suggested by Landau[13,14] and studied by Pekar[15], Frohlich[16,17], Holstein[18] and many others.

Therefore, Davydov's first main addition to McClare's proposal was to point out a specific vibrational band that is found in proteins and that is ideal for the storage and propagation of energy. His second main contribution to the field of bioenergetics was to realize that the amide-I energy depends on the strength of the hydrogen bond that may exist between the oxygen of one peptide group and the nitrogen of another, Thus Davydov took into account the coupling between the amide-I vibration (intramolecular excitation or exciton) and deformation of amino acid residues (or, acoustic phonon) in the α-helix proteins and gave further the Hamiltonian of the system[8-12], which is as follows

$$\mathbf{H} = \mathbf{H}_{ex} + \mathbf{H}_{ph} + \mathbf{H}_{int} \tag{1}$$

with

$$H_{ex} = \sum_{n}\left[\left(\varepsilon_0 - D\right)B_n^+ B_n - J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)\right] \tag{2}$$

$$H_{ph} = \sum_{n}\left[\frac{P_n^2}{2M} + \frac{1}{2}w(u_n - u_{n-1})\right] \text{ and}$$

$$H_{int} = \sum_{n}\chi(u_{n+1} - u_{n-1})B_n^+ B_n \tag{3}$$

which are the Hamiltonians of the excitons with energy ε_0, the vibration of amino acid residue and their interaction, respectively, where $B_n^+ (B_n)$ is the exciton creation (annihilation) operator at the nth site with an energy $\varepsilon_0 = 0.205$ eV. They satisfy the commutation relation:

$$\left[B_n, B_m^+\right] = \delta_{nm}, \left[B_n, B_m\right] = [B_n^+, B_m^+] = 0. \tag{4}$$

Also in Eq. (84), the $\varepsilon_0 B_n^+ B_n$ denotes the kinetic energy of the exciton, $J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)$ represents the resonant (or dipole-dipole) interaction between neighboring excitons, $J = 2\vec{d}^2/r_0^3$ is the resonance (or dipole-dipole) interaction that determines the transition of an exciton from one molecule to another. Then $DB_n^+ B_n$ denotes the interaction of the exciton with the lattice or peptide groups. D is the deformation excitation energy,

and is approximately a constant, u_n and P_n are the displacement of the peptide groups and its conjugate moment, M is the mass of the peptide group, w is the spring constant of the molecular chains and $\chi = \partial J/u_n$ is the coupling constant between the exciton and vibrational quantum of the peptide group (phonon). Obviously, the Hamiltonian in Eq.(1) represents the elementary motions of the exciton and phonon as well as their interactions in the systems.

Davydov used the following wave function to represent the collective states of excitation of the excitons and phonons arising from the energy released by ATP hydrolysis

$$|D_2(t)\rangle = |\varphi(t)\rangle |\beta(t)\rangle =$$

$$\sum_n \varphi_n(t) B_n^+ \exp\left(-\frac{i}{\hbar}\sum_n[\beta_n(t)P_n - \pi_n(t)u_n]\right)|0\rangle \quad (5a)$$

or

$$|D_1(t)\rangle = \sum_n \left\{ \varphi_n(t) B_n^+ \exp \right.$$

$$\left. \left(\sum_q \left[\alpha_{nq}(t)a_q^+ - \alpha_{nq}^*(t)a_n\right]\right)\right\}|0\rangle \quad (5b)$$

where

$$\langle D_2|P_n|D_2\rangle = \langle D_2|P_n|D_2\rangle = \sum_n |\varphi_n(t)|^2 = 1 \quad (6)$$

$|0\rangle = |0\rangle_{ex}|0\rangle_{ph}$ are the ground states of the exciton and phonon, respectively, $a_q (a_q^+)$ is annihilation (creation) operator of the phonon with ware vector q, $\varphi_n(t)$, $\beta_n(t)$ = $\langle \Phi|u_n|\Phi\rangle$, $\pi_n(t) = \langle \Phi|P_n|\Phi\rangle$ and $\alpha_{nq}(t) = \langle D_1(t)|a_q|D_1(t)\rangle$ are some undetermined functions of time. Evidently, equation (5) is an excited state of single particle for the excitons, but it is a coherent state for the phonons in Eq.(5). This is just basic features of Davydov's wave function.

Using the functional $\langle \Phi(t)|H|\Phi(t)\rangle$ and the variational approach, Davydov et al got:

$$i\hbar\frac{\partial\varphi_n}{\partial t} = [\varepsilon_0 + W + \chi(\beta_{n+1} - \beta_{n-1})]\varphi_n - J(\varphi_{n+1} + \varphi_{n-1}) \quad (7)$$

and

$$\frac{\partial^2\beta^2}{\partial t^2} + \frac{w}{M}(2\beta_n - \beta_{n-1} - \beta_{n+1}) = \frac{\chi}{M}(|\varphi_{n+1}|^2 - |\varphi_{n-1}|^2) \quad (8)$$

where,

$$\beta_n(t) = \langle\Phi(t)|u_n|\Phi(t)\rangle, \pi_n = \langle\Phi(t)|P_n|\Phi(t)\rangle =$$

$$M\frac{\partial\beta_n}{\partial t}, W = \frac{1}{2}\sum_n\left[M(\frac{\partial\beta_n}{\partial t})^2 + w(\beta_n - \beta_{n-1})^2\right]$$

In the continuity approximation the equations (7) and (8) becomes:

$$\left[i\hbar\frac{\partial}{\partial t} - \Lambda + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - 2\chi\frac{\partial\beta(x,t)}{\partial x}\right]\phi(x,t) = 0, \quad (9)$$

and

$$\left[\frac{\partial^2}{\partial t^2} - v_0^2\frac{\partial^2}{\partial x^2}\right]\beta(x,t) - \frac{2\chi r_0}{M}\frac{\partial}{\partial x}|\phi(x,t)|^2 = 0 \quad (10)$$

where $\Lambda = \varepsilon_0 - 2J + W$, $v_0 = r_0\sqrt{w/M}$ is the sound speed of the molecular chain. Clearly, equation (9) is a nonlinear Schrödinger equation (NLSE) having a soliton solution as given by

$$\phi(x,t) = \sqrt{\frac{\mu_D}{2}}\sec h\left[\frac{\mu_D}{r_0}(x - x_0 - vt)\right]$$

$$\exp\left\{\frac{\hbar v}{2Jr_0^2}(x - x_0) - \frac{E_D t}{\hbar}\right\} \quad (11)$$

Thus from Eqs.(10)-(11) we can give the solution of Eq. (10) as follows:

$$\beta(x,t) = -\frac{\chi r_0^2}{w(1 - s^2)}\tanh\left[\frac{\mu_D}{r_0}(x - x_0 - vt)\right] \quad (12)$$

Equations (11)-(12) show clearly that the energy transports along the protein molecular chains in the form of bell-type of soliton in Eq.(11). The soliton is localized over a scale r_0/μ_D, where $\mu_D = -\chi_1^2/[(1 - s^2)Jw^2]$, $G_D = 4J\mu_D$, $s^2 = v^2/v_0^2$, $v_0 = r_0(w/M)^{1/2}$ is the sound speed in the protein molecular chains, v is the velocity of the soliton, r_0 is the lattice constant. From the above result we know that a positive χ means that when the hydrogen bond length decreases, the energy of the amide I vibration decreases, and vice versa. When $\chi = 0$, the amide I energy does not depend on the relative positions of the peptide groups and the amide I excitation propagates from one peptide group to the next because of the dipole–dipole interactions J. In this case, an amide I excitation that is initially located at one peptide group will spread to other peptide groups, and the state will quickly cease to be localized. On the other hand, when $\chi \neq 0$, an excitation initially located at one peptide group will induce a distortion of the associated hydrogen bond (a compression for positive χ and an expansion for nega-

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tive χ), which, in turn, will decrease the energy of the corresponding amide I state. When the (negative) interaction energy is greater, in absolute terms, than the distortion energy, which is always positive, the state of the amide- I excitation together with the distortion has an energy that is lower than the state of the amide-I excitation in the absence of the distortion.

Evidently, the Davydov soliton contains only one exciton, i.e., $N = \langle \varphi_D(t) | \hat{N} | \varphi_D(t) \rangle$, where the particle number operator $\hat{N} = \sum_n B_n^+ B_n$. This shows that the Davydov soliton is formed through self- trapping of one exciton with binding energy $E_{BD} = -\chi_1^4 / 3Jw^2$.

The Takeno soliton model

Takeno[19-22] proposed also an alternative model for the propagation of bio- energy in the α-helix protein. He regarded that the dispersion term in the Davydov model in Eq.(1), may not be appropriate for the migration of vibrational energy, the exchange interaction is more relevant for the excitons. Thus he generalized his theory to deal with more complex systems where the amide-I energy is coupled to both acoustic and optic phonons. Then he denoted the Hamiltonian of the system by

$$H_1 = \sum_n \left[\frac{p_n^2}{2m} + \frac{1}{2} m\omega_0^2 q_n^2 - 2L q_{n+1} q_n \right] +$$

$$\sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2} w(u_{n+1} - u_n)^2 \right] + \sum_n \frac{1}{2} A_a q_n^2 (u_{n+1} - u_{n-1})$$

$$= H_v + H_p + H' \qquad (13)$$

where q_n and p_n are the displacement and momentum coordinates for the high frequency intramolecular (amide-I) oscillator with mass m and frequency ω_0, L is the coupling strength between neighbouring oscillators, which we have restricted to nearest neighbours. Also, u_n and P_n are the displacement and momentum coordinates for the molecule at site n; M and w are the molecular mass and intramolecular force constant. The last term couples these two oscillating fields with coupling constant A_a.

In order to make a comparison with the Davydov model, we now view Eq.(13) as a quantum Hamiltonian, with the displacement and momentum coordinates replaced by operators. Thus we introduce creation and annihilation operators for the high-frequency oscillator at site n by the equations

$$q_n = \left(\frac{\hbar}{2\mu\omega_0} \right)^{1/2} (B_n^+ + B_n); p_n = i \left(\frac{\hbar\mu\omega_0}{2} \right)^{1/2} (B_n^+ - B_n); \quad (14)$$

thus the q_n-dependent part of Eq.(13) can be written

$$H_s = \sum_n \hbar\omega_0 \left(B_n^+ B_n + \frac{1}{2} \right) - \frac{\hbar L}{m\omega_0}$$

$$\sum_n (B_{n+1}^+ B_n^+ + B_n^+ B_{n+1} + B_{n+1}^+ B_n + B_{n+1} B_n) \qquad (15)$$

and

$$H' = \frac{\hbar A_a}{4m\omega_0} \sum_n (B_n^+ B_n^+ + 2B_n^+ B_n + B_n B_n)(u_{n+1} - u_{n-1}) \quad (16)$$

Comparing Eq.(16) with the Davydov Hamiltonian in Eq.(1) it is clear that there are additional $B_n^+ B_n^+$ and $B_n B_n$ terms both in the dispersive and interaction parts of the quantum version of the Takeno Hamiltonian. The equation of motion for the Heisenberg operator B_n obtained from Eq.(13) is

$$i\hbar \dot{B}_n = \hbar\omega_0 B_n - \frac{\hbar L}{m\omega_0} (B_{n+1}^+ + B_{n+1} + B_{n-1}^+ + B_{n-1})$$

$$+ \frac{\hbar A_a}{2m\omega_0} (B_n^+ + B_n)(u_{n+1} - u_{n-1}) \qquad (17)$$

This differs from corresponding equation in Davydov theory, which is

$$i'B_n = \varepsilon_0 B_n - J(B_{n+1} + B_{n-1}) + \chi B_n(u_{n+1} - u_{n-1}) \qquad (18)$$

The form of the equation in Eq.(18) is such that a phase transformation

$$B_n(t) = \tilde{B}_n(t) e^{-iE_0 t/\hbar} \qquad (19)$$

removes the energy of the amide-I quantum from the equation, that is the equation for $B_n(t)$ is Eq.(18) but without the term proportional to ε_0. Thus this simple transformation removes from the equations of motion any knowledge of the magnitude of ε_0 relative to other energies in the problem, for example, the Debye energy of the acoustic phonon spectrum associated with H_p.

However, the presence of those terms in Eq.(17) means that a phase transformation of the form in Eq.(19)) cannot remove the energy of the amide-I quantum $\hbar\omega_0 = \varepsilon_0$ from the equation (18). Carrying out that transformation on Eq.(17) produces factors osaillating at $2\omega_0$ in the creation operator terms. In this formulation the magnitude of E_0 relative to other energies in the problem remains important. The lack of $B_n^+ B_n^+$ and $B_n B_n$ terms in the Davydov Hamiltonian has also been questioned by Fedyanin *et al.*[23].

We note that if we drop the creation operators from Eq.(17), then we can relate the parameters of the two theories by $L = (\mu\omega_0 / h)J$, $Aa = (2\mu\omega_0 / h)\chi$.

The equations of motion derived from the classical Hamiltonian in Eq.(13) are

$$m\ddot{q}_n + m\omega_0^2 q_n - 2L(q_{n+1} + q_{n-1}) + A_a q_n(u_{n+1} - u_{n-1}) = 0 \tag{20a}$$

$$M\ddot{u}_n - w(u_{n+1} - 2u_n + u_{n-1}) - \frac{1}{2}A_a(q_{n+1}^2 - q_{n-1}^2) = 0 \tag{20b}$$

Takeno used a continuum approximation to Eq.(20) and obtained this way coupled nonlinear Klein-Gordon equations for the coordinates $q(x, t)$ and $u(x, t)$. A rotating-wave approximation then finally leads to an NLSEs (9)-(10), but now with a classical coordinate for the amplitude of the amide-I vibration compared to Davydov's NLSE for the probability amplitude.

If Eq.(13) is augmented with the additional optic mode and interaction term:

$$H_{op} = \sum_n \left[\frac{1}{2}M_0 y_n^2 + \frac{1}{2}K_0 y_n^2 \right] + \sum_n \frac{1}{2}A_0 q_n^2 y_n \tag{21}$$

the equation of motion become

$$m\ddot{q}_n + m\omega_0^2 q_n - 2L(q_{n+1} + q_{n-1}) + A_a q_n(u_{n+1} - u_{n-1}) + A_0 q_n y_n = 0 \tag{22a}$$

$$M\ddot{u}_n - w(u_{n+1} - 2u_n + u_{n-1}) - \frac{1}{2}A_a(q_{n+1}^2 - q_{n-1}^2) = 0 \tag{22b}$$

$$M_0 y_n + K_0 y_0 + \frac{1}{2}A_0 q_n^2 = 0 \tag{22c}$$

Takeno[19-22] has used these equations to describe self-trapped states in crystalline acetanilide, where the optic mode mass is $M_0 = 1.56 \times 10^{-27}$ kg (the reduced mass of the N-H unit), and $A_a = A_0$ since both acoustic and optic mode couplings include the hydrogen bond. The system is initially prepared in a state that had a large local displacement in the vibron (amide-I) field, no energy in the optic field, and kinetic energy and displacement of the acoustic field corresponding to 300K. Then the wave-form graphs obtained from Eq.(22) show essentially the kinetic energy in the vibron and optic fields and the discrete gradient $(u_{n+1} - u_{n-1})$ approximately 60ps into the simulation. The amide-I energy is clearly still localized and a significant correlation is seen to have developed in the acoustic and optic fields. Additional studies of the Takeno model are clearly needed, but it seems that the classical solitons described by

Eq.(22) are more stable at biologically relevant temperatures than the Davydov soliton described by Eqs.(9)-(10).

Yomosa's model

Yomosa[24,25] proposed also another classical soliton model for energy transport in the α helix proteins, in which he thought solely the α-helix structure is stabilized through the nonlinearity and asymmetry of the hydrogen bonds. Then the potential of the nth hydrogen bond in the polypeptide chain can be approximately represented by

$$V_n(r_n) = A r_n^2 - B r_n^3, \quad r_n = u_{n+1} - u_n \tag{23}$$

where u_n is the displacement of the nth peptide group, r_n is the elongation of the nth peptide bond. The lattice constant is denoted by r_0. The values of the constants A and B can be determined from self-consistent-field molecular orbital calculations[25]. Yomosa here choose a cubic potential for reflecting the nonlinearity and asymmetry of the hydrogen bond in Eq.(23). Then the Hamiltonian of the system is

$$H = \frac{1}{2}M\sum_n u_n^2 + \sum_n \left[A(u_n - u_{n-1})^2 - B(u_n - u_{n-1})^3 \right] \tag{24}$$

where M is the mass of the peptide group. The equations of motion in terms of r_n are:

$$M r_n = 2A(r_{n+1} + r_{n-1} - 2r_n) - 3B(r_{n+1}^2 + r_{n-1}^2 - 2r_n^2) \tag{25}$$

Yomosa introduces the continuum limit of (25) $(nr_0 \rightarrow x, r_n \rightarrow r(x,t))$ and looking only at right-going waves he obtains a Korteweg-de Vries (KdV) equation[24-26]:

$$\phi_\tau - 12\phi\phi_\xi + \phi_{\xi\xi\xi} = 0 \tag{26}$$

where

$$\phi = x / r_0 - (2A / M)^{1/2} t, \tau = (t / 24)(2A / m)^{1/2},$$
$$\phi = 3Br / A \tag{27}$$

In terms of the original elongation $r(x,t)$ the one-soliton solution is given as

$$r(x,t) = -\frac{A}{12B}k^2 \operatorname{sech}^2\left(\frac{k}{2r_0}(x - vt) - \delta \right) \tag{28}$$

with $v = v_0\left(1 + \frac{k^2}{24} \right)$.

Here $v_0 = (2A / m)^{1/2} r_0$ is the sound velocity. This velocity indicates that Yomosa's solitons are supersonic. The parameter k to be in the range 2-3 by equating the energy released during ATP hydrolysis (0.43eV) to the energy of the KdV one-soliton in Eq. (28). This gives

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an effective soliton width of about $4\,{}^{0}_{A}$, that is, approximately on the validity of the continuum approximation.

The exact form of the potential in Eq.(23) is probably not very important; Yomosa[24] has also studied the properties of a Toda-type potential, with a Lenard-Jones potential[27], which shows effectively the same phenomena as predicted by Yomosa's continuum KdV theory, that is, the formation and propagation of supersonic solitons. These molecular dynamics simulations were also extended to biologically relevant temperatures by addition of noise and damping force terms to the equations of motion. When 0.43eV of energy was initiated on one bond, coherent pulses of energy were observed above the thermal noise for at least 25ps at T=310K. A window of most efficient energy transport was found around 40-60°C; at lower temperatures the viscosity of the solvent (modeled throughΓ) inhibited transport, while at high temperatures the thermal noise is the limiting factor.

It seems that the supersonic lattice solitons proposed by Yomosa present a reasonable alternative to the Davydov and Takeno models of transport of biological energy. These lattice solitons may also be more efficient in doing mechanical work since they have no rest energy associated with them. However, more theoretical and numerical work are still needed in this area.

The improved models of Davydov's theory

Davydov's idea yields a compelling picture for the mechanism of bioenergy transport in protein molecules and consequently has been the subject of a large number of works[28-95]. A lot of issues 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 and critically examined by many scientists[28-95] and the following questions have been of particular concern. (1) What is the correct quantum mechanical description of Davydov's soliton at low twmperature? (2) How does the soliton get started on an alpha-helix proteins''? (3) Is Davydov's soliton stable at the biological temperature 300K? If not, how long will it last? (4) How may Davydov's theory be generalized to include charge transfer and more general protein structures? Therefore, considerable controversy has arisen in recent years concerning whether the Davydov soliton can provide a viable explanation for energy trans-

port. It is out of question that the quantum fluctuations and thermal perturbations are expected to cause the Davydov soliton to decay into a delocalized state. Some numerical simulations indicated that the Davydov soliton is not stable at the biological temperature 300K[48-66,73-78]. Other simulations showed that the Davydov soliton is stable at 300K[28-35], but they were based on classical equations of motion which are likely to yield unreliable estimates for the stability of the Davydov's soliton[9-12]. The simulations based on the $ID_2 >$ state in Eq.(5a) generally show that the stability of the soliton decreases with increasing temperatures and that the soliton is not sufficiently stable in the region of biological temperature. Since the dynamical equations used in the simulations are not equivalent to the Schrödinger equation, the stability of the soliton obtained by these numerical simulations is unavailable or unreliable. The simulation[9] based on the $ID_1 >$ state in Eq.(5b) with the thermal treatment of Davydov[9,48], where the equations of motion are derived from a thermally averaged Hamiltonian, yields the wondering result that the stability of the soliton is enhanced with increasing temperature, predicting that $ID_1 >$-type soliton is stable in the region of biological temperature. Evidently, the conclusion is doubtful because the Davydov procedure in which one constructs an equation of motion for an average dynamical state from an average Hamiltonian, corresponding to the Hamiltonian averaged over a thermal distribution of phonons, is inconsistent with standard concepts of quantum-statistical mechanics in which a density matrix must be used to describe the system. Therefore, there exists not an exact fully quantum-mechanical treatment for the numerical simulation of the Davydov soliton. However, for the thermal equilibrium properties of the Davydov soliton, there is a quantum Monte Carlo simulation[63,64]. In the simulation, correlation characteristic of solitonlike quasiparticles occur only at low temperatures, about T<10K, for widely accepted parameter values. This is consistent at a qualitative level with the result of Cottingham et al.[65,66]. The latter is a straightforward quantum-mechanical perturbation calculation. The lifetime of the Davydov soliton obtained by using this method is too small (about $10^{-12}-10^{-13}$ sec) to be useful in biological processes. This shows clearly that the Davydov solution is not a true wave function of the systems. A through study in terms of parameter values, different types of disorder, different

thermalization schemes, different wave functions, and different associated dynamics leads to a very complicated picture for the Davydov model[50-62]. These results do not completely rule out the Davydov theory, however they do not eliminate the possibility of another wave function and a more sophisticated Hamiltonian of the system having a soliton with longer lifetimes and good thermal stability.

Indeed, the question of the lifetime of the soliton in protein molecules is twofold. In Langevin dynamics, the problem consists of uncontrolled effects arising from the semiclassical approxima- tion. In quantum treatments, the problem has been the lack of an exact wave function for the soliton. The exact wave function of the fully quantum Davydov model has not been known up to now. Different wave functions have been used to describe the states of the fully quantum- mechanical systems[33-43]. Although some of these wave functions lead to exact quantum states and exact quantum dynamics in the J=0 state, they also share a problem with the original Davydov wave function, namely that the degree of approximation included when $J \neq 0$ is not known. Therefore, it is necessary to reform Davydov's wave function.

Scientists had though that the soliton with a multiquantum ($n \geq 2$), for example, the coherent state of Brown et al.[33], the multiquantum state of Kerr et al.[62] and Schweitzer[66], the two-quantum state of Cruzeiro -Hansson[52] and Forner[57], and so on, would be thermally stable in the region of biological temperature and could provide a realistic mechanism for bioenergy transport in protein molecules. In the Brown et al's model[33], the state of the excitons was denoted by a coherent state vector $|A(t)\rangle$, which is defined by
$$|A(t)\rangle = |a_1(t)\rangle \otimes |a_2(t)\rangle \otimes \ldots |a_N(t)\rangle$$
wherein $|a_n(t)\rangle$ is a pure coherent state defined by

$$\left|a_n(t)\right\rangle = \exp[-\frac{1}{2}\left|\alpha_n\right|^2]\exp[\alpha_n(t)a_n^+]\left|0\right\rangle_{ex}$$

where the complex scalar $a_n(t)$ is the coherent-state amplitude, which may take on all values in the complex plane, The product state $|A(t)\rangle$ may be defined by the property that $a_n|A(t)\rangle = a_n(t)|A(t)\rangle$ for all of the a_n. The expectation value of a Hamiltonian operator of the system $H[a, a^+]$ in the state $|A(t)\rangle$ is therefore a real scalar function $H[a(t), a^*(t)]$ for all the $a_n(t)$ and their complex conjugates. Thus we can presume that the starting Hamiltonian operator is in normal ordered form so that there

is no ambiguity in the relationship between $H[a, a^+]$ and $H[a(t), a^*(t)]$. Then we can obtain the properties of the exciton-soliton in the system by general method. However, the assumption of the standard coherent state is unsuitable or impossible for biological protein molecules because there are innumerable particles in this state and one could not retain conservation of the number of particles of the system and is also inconsistent with the fact that the energy released in ATP hydrolysis can excite only two quanta of amide-I vibration.

In the Schweitzer's model[66] of the multiquantum state the state of the excitons was denoted by

$$\left|\varphi(t)\right\rangle = \sum_m \alpha(m,t)\left|0\right\rangle_{ex} = \frac{1}{\sqrt{m!}}\sum_{nm} \varphi_{nm}(t)(B_n^+)^m\left|0\right\rangle_{ex}$$

However, the assumption of a multiquantum state (m>2) along with a coherent state is also inconsistent with the fact that the bioenergy released in ATP hydrolysis can excite only two quanta of amide-I vibration.

In Forner's model of two-quanta[57], he represented the state of the exciton by

$$\left|\varphi(t)\right\rangle == \frac{1}{\sqrt{2!}}(\sum_n \varphi_n(t)B_n^+)^2\left|0\right\rangle_{ex}$$

Forner's numerical results[54-60] shows that the soliton of two-quantum state is more stable than that with a one-quantum state.

Cruzeiro-Hansson[52] had thought that Forner's two-quantum state in the semiclassical case was not exact. Therefore, he constructed again a so-called exactly two-quantum state for the semiclassical Davydov system as follows[52]:

$$\left|\phi(t)\right\rangle = \sum_{n,m=l}^{N} \varphi_{nm}\left(\{u_l\},\{P_l\},t\right)B_n^+B_m^+\left|0\right>_{ex}, \qquad (29)$$

where $B_n\left(B_n^+\right)$ is the annihilation (creation) operator for an amide-I vibration quantum (exciton), u_l is the displacement of the lattice molecules, P_l is its conjugate momentum, and $|0>_{ex}$ is the ground state of the exciton. He calculate the average probability distribution of the exciton per site, and average displacement difference per site, and the thermodynamics average of the variable, $P = B_1^+B_1 - B_2^+B_2$, as a measure of localization of the exciton, versus quantity $\nu = JW/\chi_1^2$ and $\text{Ln}\beta(\beta = 1/K_BT)$ in the so-called two-quantum state, Eq.(29), where χ_1 is a nonlinear coupling parameter related to the interaction of the exciton-phonon in the Davydov model. Their energies and stability are com-

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pared with that of the one-quantum state. From the results of above thermal averages, he drew the conclusion that the wave function with a two-quantum state can lead to more stable soliton solutions than the wave function with a one-quantum state, and that the usual Langevin dynamics, whereby the thermal lifetime of the Davydov soliton is estimated, must be viewed as underestimating the soliton lifetime.

However, by checking carefully Eq.(29)[52], we can find that the Cruzeiro-Hansson wave function does not represent exactly the two-quantum state. To find out how many quanta the state Eq.(29) indeed contains, we have to compute the expectation value of the exciton number operator. $N = \sum_n B_n^+ B_n$, in this state, Eq.(29), and sum over the sites, i.e., the exciton numbers N are

$$
\begin{aligned}
N &= <\varphi \left| \sum_n B_n^+ B_n \right| \varphi > = \sum_{ijlmn} \varphi_{im}^* \varphi_{jlex} \\
&\quad < 0 \left| B_i B_m B_n^+ B_n B_j^+ B_l^+ \right| 0 >_{ex} \\
&= \sum_{nj} \left(\varphi_{nj}^* \varphi_{jn} + \varphi_{jn}^* \varphi_{jn} \right) + \\
&\quad \sum_{nl} \left(\varphi_{nl}^* \varphi_{nl} + \varphi_{ln}^* \varphi_{nl} \right) = 4
\end{aligned}
\tag{30}
$$

where we use the relations

$$
[B_n, B_j^+] = \sigma_{nj}, \sum_{nl} |\varphi_{nl}|^2 = 1
$$

$$
_{ex}<0|B_n^+|0>_{ex} =_{ex}<0|B_n^+ B_n|0>_{ex} =_{ex}<0|B_n^+ B_m B_1|0>_{ex} = ... = 0
$$

Therefore, the state, Eq.(29), as it is put forward[10] in Eq.(29) deals, in contradiction to the author's statements, with four excitons (quanta), instead of two excitons. Obviously it is not possible to create the four excitons by the energy released in the ATP hydrolysis (about 0.43 eV). Thus the author's wave function is still not relevant for protein molecules, and his discussion and conclusion are all unreliable and implausible in that paper[52].

We think that the physical significance of the wave function, Eq.(29), is also unclear, or at least is very difficult to understand. As far as the physical meaning of Eq.(29) is concerned, it represents only a combinational state of single-particle excitation with two quanta created at sites n and m; $\varphi_{nm}(\{u_1\}, \{P_1\}, t)$ is the probability amplitude of particles occurring at the sites n and m simultaneously. In general, $n=m$ and $\varphi_{nm} \neq \varphi_n \varphi_m$ in

accordance with the author's idea. In such a case it is very difficult to imagine the form of the soliton formed by the mechanism of self-trapping of the two quanta under the action of the nonlinear exciton-phonon interaction, especially when the difference between n and m is very large. Hansson has also not explained the physical and biological reasons and the meaning for the proposed trial state. Therefore, we think that the Cruzeiro-Hansson representation is still not an exact wave function suitable for protein molecules. Thus, the wave function of the systems is still an open problem today.

Recently, Cruzeiro L.et al[96-99] and Pouthier et al[100,101] proposed a dynamical model of nonconserving Davydov monomer involving a nonconserving Davydov Hamiltonian for the energy transport, in which they thought that the Davydov's model cannot describe the conversion of that energy into work, because it conserves the number of excitations. With the aim of describing conformational changes, they considered a nonconserving generalization of the model, which is found to describe essentially a contraction of the hydrogen bond adjacent to the site where an excitation is present. Unlike the one-site Davydov model, that contraction is time dependent because the number of excitations is not conserved. However, considering the time average of the dynamical variables, the results reported here tend to the known results of the Davydov model.

Meanwhile, K.Moritsugu et.al[102] and H.Fujisaki et al[103] considered the anharmonic coupling between the amide-I mode and intramolecular normal modes. These models are helpful for solving the problem of energy transport in protein molecules.

In one words, the above soliton theories of energy transport in protein molecules attract the careful attention of the bioenergetics community. Obviously, they cannot explain every aspect of energy transport and protein dynamics, but they are motivating exciting question and new experiments. There are clearly still many open problems and no single theory presently has answers to all questions. However, most of these models stay only in the designs of mechanism of energy transport, a deepened and complete investigation lacks now. Therefore it now is quite required to continue work on the extension and improvement of these theories for forming a complete and correct theory of energy transport in protein molecules.

Pang's model

The results obtained by many scientists over the years show that the Davydov model, whether it be the wave function or the Hamiltonian, is indeed too simple, i.e.., it does not denoted elementary properties of the collective excitations occurring in protein molecules, and many improvements to it have been unsuccessful, as mentioned above. What is the source of this problem? It is well known that the Davydov theory on bioenergy transport was introduced into protein molecules from an exciton-soliton model in generally one-dimensional molecular chains[104-106]. Although the molecular structure of the alpha-helix protein is analogous to some molecular crystals, for example acetanilide (ACN) (in fact, both are polypeptides; the alpha-helix protein molecule is the structure of three peptide channels, ACN is the structure of two peptide channels. If comparing the structure of alpha helix protein with ACN, we find that the hydrogen-boned peptide channels with the atomic structure along the longitudinal direction are the same except for the side group), a lot of properties and functions of the protein molecules are completely different from that of the latter. The protein molecules are both a kinds of soft condensed matter and bio-self -organization with action functions, for instance, self-assembling and self-renovating. The physical concepts of coherence, order, collective effects, and mutual correlation are very important in bio-self-organization, including the protein molecules, when compared with generally molecular systems[107-111]. Therefore, it is worth studying how we can physically describe these properties. We note that Davydov operation also is not strictly correct. Therefore, we think that a basic reason for the failure of the Davydov model is just that it ignores completely the above important properties of the protein molecules.

Let us consider the Davydov model with the present viewpoint. First, as far as the Davydov wave functions, both $|D_1\rangle$ and $|D_2\rangle$, are concerned, they are not true solutions of the protein molecules. On the one hand, there is obviously asymmetry in the Davydov wave function since the phononic parts is a coherent state, while the excitonic part is only an excitation state of a single particle. It is not reasonable that the same nonlinear interaction generated by the coupling between the excitons and phonons produces different states for the phonon and exciton. Thus, Davydov's wave function should be modified, i.e., the excitonic part in it should

also be coherent or quasicoherent to represent the coherent feature of collective excitation in protein molecules. However, the standard coherent[33] and large-n excitation states[66] are not appropriate for the protein molecules due to the above reasons. Similarly, Forner's[57] and Cruzeiro-Hansson's[52] two- quantum states do not fulfill the above request. In view of the above discussion, we proposed the following wave function of two-quanta quasi-coherent state for the protein molecular systems[112-148]

$$|\Phi(t)\rangle = |\varphi(t)\rangle|\beta(t)\rangle =$$

$$\frac{1}{\lambda}\left[I + \sum_n \varphi_n(t)B_n^+ + \frac{1}{2!}\left(\sum_n \varphi_n(t)B_n^+\right)^2\right]|0\rangle_{ex}$$

$$\times \exp\left\{-\frac{i}{h}\sum_n\left[\beta_n(t)P_n - \pi_n(t)u_n\right]\right\}|0\rangle_{ph} \quad (31)$$

where B_n^+ (B_n) is boson creation (annihilation) operator 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 the lattice oscillator at site n, respectively. λ is a normalization constant, we assume hereafter that $\lambda = 1$ for convenience of calculation, except when explicitly mentioned. The $\varphi_n(t)$, $\beta_n(t) = \langle\Phi(t)|u_n|\Phi(t)\rangle$ and $\pi_n(t) = \langle\Phi(t)|P_n|\Phi(t)\rangle$ are there sets of unknown functions.

A second problem arises for the Davydov Hamiltonian[8-12]. The Davydov Hamiltonian takes into account the resonant or dipole-dipole interaction of the neighboring amide-I vibrational quanta in neighboring peptide groups with an electrical moment of about 3.5D, but why do we not consider the changes of relative displacement of the neighboring peptide groups arising from this interaction? Thus, it is reasonable to add the

new interaction term, $\chi_2\left(u_{n+1} - u_n\right)\left(B_{n+1}^+ B_n + B_m^+ B_{n+1}\right)$, into the Davydov Hamiltonian to represent correlations of the collective excitations and collective motions in the protein molecules, as mentioned above[8-12]. Although the dipole-dipole interac- tion is small as compared with the energy of the amide-I vibrational quantum, the change of relati- ve displacement of neighboring peptide groups resulting from this interaction cannot be ignored due to the sensitive dependence of dipole-dipole interaction on the distance between amino acids in the protein molecules, which is a kind of soft condensed

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matter and bio-self- organization. Thus, we replace Davydov's Hamiltonian[112-148] by

$$H = H_{ex} + H_{ph} + H_{int} =$$

$$\sum_n \left[\varepsilon_0 B_n^+ B_n - J\left(B_n^+ B_{n+1} + B_n B_{n+1}^+ \right) \right] +$$

$$\sum_n \left(\frac{P_n^2}{2M} + \frac{1}{2} w\left(u_n - u_{n-1} \right)^2 \right)$$

$$+ \sum_n [\chi_1 \left(u_{n+1} - u_{n-1} \right) B_n^+ B_n +$$

$$\chi_2 \left(u_{n+1} - u_n \right)\left(B_{n+1}^+ B_n + B_n^+ B_{n+1} \right)] \qquad (32)$$

where $\varepsilon_0 = 0.205$ ev is the energy of the exciton (C=0 stretching mode). The present nonlinear coupling constants are χ_1 and χ_2. They represent the modulations of the on-site energy and resonant (or dipole-dipole) interaction energy of excitons caused by the molecules displacements, respectively. M is the mass of a amino acid molecule and w is the elasticity constant of the protein molecular chains. J is the dipole-dipole interaction energy between neighboring sites. The physical meaning of the other quantities in Eq.(32) are the same as those in the above explanations.

The Hamiltonian and wave function shown in Eqs.(31)-(32) are different from Davydov's. We added a new interaction term, $\sum_n \chi_2 \left(u_{n+1} - u_n \right)\left(B_{n+1}^+ B_n + B_n^+ B_{n+1} \right)$, into the original Davydov Hamiltonian. Thus the Hamiltonian now has an one-by-one correspondence on the interactions and can represent the features of mutual correlations of the collective excitations and of collective motions in the protein molecules. We should point out here that the different coupling between the relevant modes was also considered by Takeno et al.[53-58] and Pang[73-95] in the Hamiltonian of the vibron-soliton model for one-dimensional oscillator-lattice and protein systems, respectively, but the wave functions of the systems they used are different from Eqs.(31)-(32).

Obviously, the new wave function of the exciton in Eq.(31) is not an excitation state of a single particle, but rather a coherent state, or more accurately, a quasicoherent state because it is just an effective truncation of a standard coherent state, retains only fore three terms of expansion of a standard coherent state, at the same time, when the $\varphi_n(t)$ is small, for example, $|\varphi_n(t)| \ll 1$, it also can approximately represent math-

ematically as a standard coherent state:

$$| \varphi(t) > \sim \exp\left[-\frac{1}{2}\sum_n | \varphi_n(t) |^2 \exp\left\{ \sum_n \varphi_n(t) B_n^+ \right\} \right] | 0 >_{ex}$$

$$\exp\left\{ \sum_n \left[\varphi_n(t) B_n^+ - \varphi_n^* B_n \right] \right\} | 0 > \qquad (33)$$

where $\sum_n |\varphi_n(t)|^2 = 1$, n denotes the sites of amino acids. Therefore we refer to it as quasi- coherent state due to these characteristics. Thus Eq.(31) can represent simultaneously the coherent features of collective excitations, phonons and excitons, in the proteins. The condition of $|\varphi_n(t)| \ll 1$ is also quite correct and resonable for the proteins consisting of amino acids of several hundreds or thousands because of $\sum_n |\varphi_n(t)|^2 = 1$. Therefore, Eq.(33) is justified and a correct representation. It is well known that the coherent state is certainly normalized, then it is natural that the $|\varphi_n(t)\rangle$ in Eq.(31) or $|\Phi(t)>$ in Eq.(31) should be also normalized. Thus we should choose $\lambda = 1$ in Eq.(31). This means that we cannot choose other values of $\lambda \neq 1$ in Eq. (31), or else, $|\varphi_n(t)\rangle$ cannot represent as a standard coherent state in Eq.(33). With that, in this case of $\lambda \neq 1$, $|\varphi_n(t)\rangle$ is neither a quasi-coherent state nor a excited state of single particle, that is, has not any biological and physical meanings. This shows clearly that choice of »=1 in Eq.(31) is correct and reasonable. In such a case it is not an eigenstate of number operator because of

$$\hat{N}|\varphi(t) >= \sum_n B_n^t B_n \left| \varphi(t) >= \left\{ \sum_n \varphi_n(t) B_n^t + \right. \right.$$

$$\left. \left(\sum_n \varphi_n \varphi_n(t) B_n^t \right)^2 \right\} | 0 >_{ex} = 2|\varphi(t) - \left(2 + \sum_n \varphi_n(t) B_n^t \right)| 0 >_{ex} \qquad (34)$$

Therefore, the $|\varphi(t)>$ represents indeed a superposition of multiquantum states. Concretely speaking, it is a coherent superposition of the excitonic state with two quanta and the ground state of the exciton. However, in this state the numbers of quanta are determinate instead of innumerable. To find out how many excitons this state contains, we have to compute the expectation value of the number operator N in this state and sum over the states. The average number of excitons for this state is

$$N =< \varphi(t)|\hat{N}|\varphi(t) >= \sum_n < \varphi(t)|B_n^t B_n | \varphi(t)$$

$$= \left\{ \sum_n |\varphi_n(t)|^2 + \left(\sum_n |\varphi_n(t)|^2 \right)\left(\sum_m |\varphi_m(t)|^2 \right) \right\}$$

$$= \left(\sum_n |\varphi_n(t)|^2 \right)\left(1 + \sum_m |\varphi_m(t)|^2 \right) = 2 \qquad (35)$$

where we utilize Eq.(8) and the following relations[24]:

$$\sum_n |\varphi_n(t)|^2 = 1, \sum_m |\varphi_m(t)|^2 = 1, [B_n . B_m^t] = \delta_{nm} \quad (36)$$

$$_{ex}<0|B_n^+|0>_{ex} =_{ex}<0|B_n^+B_n|0>_{ex} =_{ex}<0|B_n^+B_m|0>_{ex}$$
$$=_{ex}<0|B_n^+B_mB_1|0>_{ex} =_{ex}<0|B_n^+B_mB_i^+B_n|0>_{ex}$$
$$=_{ex}<0|B_n^+B_mB_i^+B_lB_j|0>_{ex} =_{ex}<0|B_n^+B_mB_i^+B_lB_jB_n|0>_{ex} .... = 0$$

Therefore, the new wave function in Eq.(31) is a quasi-coherent state containing only two quanta, thus completely different from Davydov's. The latter is an excitation state of a single particle with one quantum and an eigenstate of the number operator. In the meanwhile, as far as the form of new wave function in Eq.(31) is concerned, it is either two- quanta states proposed by Forner[54-60] and Cruzeiro-Hansson[50-53] or a standard coherent state proposed by Brown et al.[33-41] and Kerr et al's[61,62] and Schweitzer *et al's* multiquanta states[65,66]. Therefore, the wave function, Eq.(31), is new for the protein molecular systems. It not only exhibits the basic features of collective excitation of the excitons and phonons caused by the nonlinear interaction generated in the system but also agrees with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) may only create two amide-I vibrational quanta, thus, it can also make the numbers of excitons maintain conservation in the Hamiltonian, Eq.(32). Meanwhile, the new wave function has another advantage, i.e., the equation of motion of the soliton can also be obtained from the Heisenberg equations of the creation and annihilation operators in quantum mechanics by using Eqs.(31) and (32), but cannot be obtained by the wave function of state of the system in other models, including the one-quanta state[8-12] and the two-quanta state[50-60]. Therefore, the above Hamiltonian and wave function, Eqs.(31) and (32), are reasonable and appropriate to the protein molecules.

We now derive the equations of motion in Pang's model. First of all, we give the interpretation of $\beta_n(t)$ and $\pi_n(t)$ in Eq.(31). We know that the phonon part of the new wave function in Eq.(31) depending on the displacement and momentum operators is a coherent state of the normal model of creation and annihilation operators. Utilizing again the above results and the formulas of the expectation values of the Heisenberg equations of operators, u_n and P_n, in the state $|\Phi(t)\rangle$,

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

$$i\hbar \frac{\partial}{\partial t} \langle \Phi(t)|P_n|\Phi(t) \rangle = \langle \Phi(t)|[u_n, H]\Phi(t) \rangle \quad (37)$$

we can obtain the equation of motion for the $\beta_n(t)$ as

$$M\ddot{\beta}_n(t) = w[\beta_{n+1}(t) - 2\beta_n(t) + \beta_{n-1}(t)]$$
$$+ 2\chi_1 \left[|\varphi_{n+1}(t)|^2 - |\varphi_{n-1}(t)|^2 \right] + 2$$
$$\chi_2 \left\{ \varphi_n^*(t)[\varphi_{n+1}(t) - \varphi_{n-1}(t)] + \varphi_n(t)[\varphi_{n+1}^*(t) - \varphi_{n-1}^*(t)] \right\} \quad (38)$$

From Eq.(38) we see that the presence of two quanta for the oscillators increases the driving force on the phonon field by that factor when compared with the Davydov theory.

A basic assumption in the derivation is that $|\Phi(t)\rangle$ in Eq.(31) is a solution of the time- dependent Shrödinger equation[26,149]: $i\hbar \frac{\partial}{\partial t}|\Phi(t)\rangle = H|\Phi(t)\rangle$ we can obtain

$$i\hbar \frac{\partial}{\partial t}\varphi_n(t) = \varepsilon_0\varphi_n(t) - J[\varphi_{n+1}(t) + \varphi_{n-1}(t)] +$$
$$\chi_1[\beta_{n+1}(t) + \beta_{n-1}(t)]\varphi_n(t)$$
$$- \chi_2[\beta_{n+1}(t) + \beta_n(t)] \times [\varphi_{n+1}(t) + \varphi_{n-1}(t)]$$
$$+ \frac{5}{2}\left(W(t) - \frac{1}{2}\sum_m [\dot{\beta}_m(t)\pi_m(t) - \dot{\pi}_m(t)\beta(t)]\right)\varphi_n(t) \quad (39)$$

In the continuum approximation we get from Eqs.(38) and (39)

$$i\hbar \frac{\partial}{\partial t}\varphi(x,t) = R(t)\varphi(x,t) -$$
$$Jr_0^2 \frac{\partial^2}{\partial x^2}\varphi(x,t) - G_p|\varphi(x,t)|^2\varphi(x,t) \quad (40)$$

and

$$\frac{\partial\beta(x,t)}{\partial\xi} = \frac{\partial\beta(x,t)}{\partial x} = -\frac{4(\chi_1 + \chi_1)}{w(1-s^2)r_0}|\phi(x,t)|^2 \quad (41)$$

where $\xi = x - x_0 - vt$

$$R(t) = \varepsilon_0 - 2J + \frac{5}{2}\left\{W(t) - \frac{1}{2}\sum_m [\dot{\beta}_m(t)\pi_m(t) - \dot{\pi}_m(t)\beta(t)]\right\}$$

and $s = v/v_0$. The soliton solution of Eq.(40) is thus

$$\phi(x,t) = \left(\frac{\mu_p}{2}\right)^{1/2} \sec h\left[(\mu_p/r_0)(x-x_0-vt)\right] \times$$
$$\exp\left\{i\left[\frac{\hbar v}{2Jr_0^2}(x-x_0) - E_v\frac{t}{\hbar}\right]\right\} \quad (42)$$

with

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$$\mu_P = \frac{2(\chi_1 + \chi_2)^2}{w(1-s^2)J}, \quad G_P = \frac{8(\chi_1 + \chi_2)^2}{w(1-s^2)} \tag{43}$$

These are just the form and representation of carrier (soliton) of energy transport in Pang's model.

THE PROPERTIES OF CARRIER (SOLITON) OF ENERGY TRANSPORT AND ITS LIFETIMES AT BIOLOGICAL TEMPERATURE 300K

The properties of carrier (soliton) of energy transport in protein molecules

Although forms of the above equations of motion and corresponding solutions, Eqs.(40-43), are quite similar to those of the Davydov soliton, the properties of the new soliton have very large differences from the latter because the parameter values in the equation of motion and its solutions Eqs. (40) and (42), including $R(t)$, G_P and μ_P, have obvious distinctions from that those of Davydov model. A straightforward result in Pang's model is to increase the nonlinear interaction energy, $G_P(G_P = 2G_D[1 + 2(\chi_2/\chi_1) + (\chi_2/\chi_1)^2])$ and amplitude of the new soliton and decrease its width due to an increase of $\mu_P(\mu_P = 2\mu_D[1 + 2(x_2/x_1) + (x_2/x_1)^2])$ when compared with those of Davydov soliton, where $\mu_D = x_1^2/w(1-s^2)J$ and $G_D = 4x_1^2/w(1-s^2)$ are the corresponding values in the Davydov model. Thus the localized feature of the new soliton is enhanced. Then we can predict that its features and stability against the quantum fluctuation and thermal perturbations increased considerably as compared with the Davydov's soliton.

As a matter of fact, the energy of soliton in Pang's model[112-148] becomes

$$E = < \Phi(t) | H | \Phi(t) = \frac{1}{r_0} \int_{-\infty}^{\infty} 2\left[Jr_0^2\right.$$

$$\left(\frac{\partial\varphi}{\partial x}\right)^2 + R|\varphi(x,t)|^2 - G_p|\varphi(x,t)|^4 dx +$$

$$\frac{1}{r_0}\int_{-\infty}^{\infty}\frac{1}{2}\left[M\left(\frac{\partial\beta(x,t)}{\partial t}\right)^2 + wr_0\left(\frac{\partial\beta(x,t)}{\partial x}\right)^2\right]dx$$

$$= E_0 + \frac{1}{2}M_{sol}v^2 \tag{44}$$

The rest energy of the new soliton is

$$E_0 = 2(\varepsilon_0 - 2J) - \frac{8(x_1 + x_2)^4}{3w^2J} \tag{45}$$

The effective mass of the new soliton is

$$M_{sol} = 2m_{ex} + \frac{8(x_1 + x_2)^4(9s^2 + 2 - 3s^4)}{3w^2J(1-s^2)^3 v_0^2} \tag{46}$$

The binding energy of the new soliton is

$$E_{BP} = \frac{-8(x_1 + x_2)^4}{3Jw^2} \tag{47}$$

The new soliton shown in Eq.(42) yields a localized coherent structure with size of order $2\pi r_0/\mu_p$ that propagates with velocity v and can transfer energy E_{S01} $2\varepsilon_0$. Unlike bare excitons that are scattered by the interactions with the phonons, but this soliton state describes a quasi-particle consisting of the two excitons plus a lattice deformation and hence a priori includes interaction with the acoustic phonons. So the soliton is not scattered and spread by this interaction of lattice vibration, and can maintain its form, energy, momentum and other quasiparticle properties moving over a macroscopic distance. The bell-shaped form of the new soliton in Eq. (42) does not depend on the excitation method. It is self-consistent. Since the soliton always move with velocity less than that of longitudinal sound in the chain, then they do not emit phonons, i.e., their kinetic energy is not transformed into thermal energy. This is an important reason for the high stability of the new soliton. In addition the energy of the new soliton state is below the bottom of the bare exciton bands, the energy gap being $4\mu_p^2 J/3$ for small velocity of propagation. Hence there is an energy penalty associated with the destruction with transformation from the new soliton state to a bare exciton state, i.e, the destruction of the new soliton state requires simultaneous removal of the lattice distortion. We know in general that the transition probability to a lattice state without distortion is very small, in general, being negligible for a long chain. Considering this it is reasonable to assume that the new soliton is stable enough to propagate through the length of a typical protein structure.

Obviously, E_{BP} in Eq.(47) is larger than that of the Davydov soliton. The latter is $E_{BD} = -x_1^4/3Jw^2$. They have the following relation:

$$E_{BP} = 8E_{BD}\left[1 + 4\left(\frac{x_2}{x_1}\right) + 6\left(\frac{x_2}{x_1}\right)^2 + 4\left(\frac{x_2}{x_1}\right)^3 + \left(\frac{x_2}{x_1}\right)^4\right] \quad (48)$$

We can estimate that the binding energy of the new soliton is about several decades larger than that of the Davydov soliton. This is a very interesting result. It is helpful to enhance thermal stability of the new soliton. Obviously, the increase of the binding energy of the new soliton comes from its two-quanta nature and the added interaction. $\sum_i \chi_2 (u_{n+1} - u_n)(B_{n+1}^+ B_n + B_n^+ B_{n+1})$, in the Hamiltonian of the systems, Eq.(32). However, we see from Eq.(48) that the former plays the main role in the increase of the binding energy and the enhancement of thermal stability for the new soliton relative to the latter due to $\chi_2 < \chi_1$. The increase of the binding energy results in significant changes of properties of the new soliton, which are discussed as follows.

In comparing various correlations to this model, it is helpful to consider them as a function of a composite coupling parameter like that of Young *et al*.[150] and Scott[28-32] that can be written as

$$4\pi\alpha_P = (\chi_1 + \chi_2)^2 / 2w\hbar\omega_D \quad (49)$$

where $\omega_D = (w / M)^{1/2}$ is the band edge for acoustic phonons (Debye frequency). If $4\pi\alpha_P << 1$, it is said to be weak. Using widely accepted values for the physical parameters for the alpha helix protein molecule[8-32,112-120],

J = 1.55 × 10⁻²² J.   w = (13 – 19.5) N/m.

M = (1.17 – 1.91) × 10⁻²⁵ kg χ_1 = 62 × 10⁻¹² N.

χ_2 = (10 – 18) × 10⁻¹² N. r_0 = 4.5 × 10⁻¹⁰ m.   (50)

we can estimate that the coupled constant lies in the region of $4\pi\alpha_P$ = 0.11 – 0.273, but $4\pi\alpha_P$ = 0.036 – 0.045 for the Davydov model, which is a weakly coupled theory, but we can say that Pang's model is not a weakly coupled theory. Using again the notation of Venzel and Fischer[151], Nagle[152], and Wagner and Kongeter[153], it is convenient to define another composite parameter[8-12]

$$\gamma = J / 2\hbar w_D \quad (51)$$

In terms of the two composite parameters, $4\pi\alpha_P$ and γ, the binding energy of the new soliton in Pang's model can be written by

$E_{BP} / J = 8(4\pi\alpha_P / \gamma)^2 / 3$, $M_{sol} = 2m_{ex}[1 + 32(4\pi\alpha_P)^2 /3]$

From the above parameter values in Eq.(50), we find $\gamma = 0.08$. Utilizing this value, the E_{BP} / J versus $4\pi\alpha$

relations in Eq.(51) are plotted in Figure 2. However, $E_{BD} / J = (4\pi\alpha_P / \gamma)^2 / 3$ for the Davydov model (here $M_{sol}' = m_{ex}\left[1 + 2(4\pi\alpha_P / \gamma)^2 /3\right]$, $4\pi\alpha_D = \chi_1^2 / 2w\hbar\omega_D$, then the E_{BD} / J versus $4\pi\alpha_D$ relation is also plotted in Figure 2. From this figure we see that the difference of soliton binding energies between two models becomes larger with increasing $4\pi\alpha$.
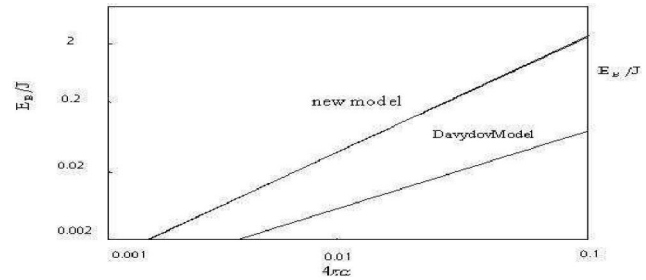

Figure 2 : Comparison of E_{BD} / J versus $4\pi\alpha_D$ relation between Pang's model and Davydov's model.

On the other hand, the nonlinear interaction energy forming the new siliton in Pang's model is $G_P = 8(\chi_1 + \chi_2)^2 / (1 - s^2)w = 3.8 \times 10^{-32}$ J, and it is larger than the dispersion energy, $J = 1.55 \times 10^{-32}$ J, i.e., the nonlinear interaction is so large than the latter in Pang's model, thus it can actually cancel or suppress the dispersion effect in the dynamic equation,thus the new soliton is stable in this case according the soliton theory[10,26,149]. However,the nonlinear interaction energy in the Davydov model is only $G_D = 4\chi_1^2 / (1 - s^2)w = 1.8 \times 10^{-21}$ J, and it is about three to four times smaller than G_P. Therefore, the stability of the Davydov soliton is weaker than that of the new soliton.

Moreover, the binding energy of the new soliton in Pang's model is $E_{BP} = (4.16 - 4.3) \times 10^{-21}$ J in Eq.(47), which is somewhat larger than the thermal perturbation energy, $k_B T = 4.13 \times 10^{-21}$ J, at 300K and about four times larger than the Debye energy, $k\Theta = \hbar\omega_D = 1.2 \times 10^{-21}$ J (there ω_D is the Debye frequency). This shows that transition of the new soliton to a delocalized state can be suppressed by the large energy difference between the initial (solitonic) state and final (delocalized) state, which is very difficult to compensate for the exciton with the energy of the absorbed phonon. Thus, the new soliton is robust against quantum fluctuations and thermal perturbation,therefore it has a large lifetime and good thermal stability in the region of biological temperature. In practice, according to Schweitzer *et al*.'s studies, i.e., the lifetime of the soliton increases as μ_P

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and $T_0 = \hbar \nu_0 \mu_p / K_B \pi$ increase at a given temperature[65], then we could roughly draw an inference that the lifetime of the new soliton will increase considerably as compared with that of the Davydov soliton due to the increase of μ_p and T_0 because the latter are about three times larger than those of the Davydov model. However, the binding energy of the Davydov soliton

$E_{BD} = \chi_1^4 / 3w^2 J = 0.188 \times 10^{-21} J$, and it is about 23 times smaller than that of the new soliton, about 22 times smaller than $K_B T$, and about 6 times smaller than $K_B \Theta$, respectively. Therefore, the Davydov soliton is easily destructed by the thermal perturbation energy and quantum transition effects. Thus we can naturally obtain that the Davdov soliton has only a small lifetime,and it is unstable at the biological temperature 300 K. This conclusion is consistent at a qualitative level with the results of Wang *et al.*[63,64] and Cottingham *et al.*[65].

One can sum up the differences between Pang's model and the Davydov's model, Eqs.(1)-(4), as follows. Firstly the parameter μ_p is increased ($\mu_p = 2\mu_{D} \times$

$\left[1 + 2(\frac{\chi_2}{\chi_1}) + (\frac{\chi_2}{\chi_1})^2 \right]$). Secondly the nonlinear coupling energy becomes $G_p = 2G_D > G_D$ resulting from the two-quanta nature and the enhancement of the coupling the coefficient ($\chi_1 + \chi_2$). In fact, the nonlinear interaction, G_p, is increased by about a factor of 3 over that of the Davydov soliton and is larger than the dispersion energy J in the equation of motion. A straightforward consequence of these effects is that the binding energy of new soltion or, in other words, the energy gap between the solitonic and excitonic states are greatly increased or $E_{BP} = -4\mu_p^2 J / 3 = -G_p^2 / 12J = 8E_{BD}$. For α-helical protein molecules we can calculate the values of the main parameters in this model by above parameter values listed in Eq.(50). These values and the corresponding values in the Davydov model are simultaneously listed in TABLE 1. From TABLE 1 we can see clearly that Pang's model produces considerable changes in the properties of the new soliton, for example, large increase of the nonlinear interaction, binding energy and amplitude of the soliton, and decrease of its width as compared to those of the Davydov soliton. This shows that the new soliton in Pang's model is more localized and more robust against quantum and thermal fluctuations and has enhanced stability[8-12,112-120] which implies

an increase in lifetime for the new soliton. From Eq.(38) we also find that the effect of the two-quanta nature is larger than that of the added interaction. We can therefore refer to the new soliton as quasi-coherent.

TABLE 1 : Comparison of parameters used in the Davydov model and Pang's model

Parameters→ Models↓	μ	G ($\times 10^{-21}$J)	Amplitude of soliton A'	Width of soliton ΔX ($\times 10^{-10}$m)	Binding energy of soliton E_B ($\times 10^{-21}$J)
Pang's Model	5.94	3.8	1.72	4.95	-7.8
Davydov model	1.90	1.18	0.974	14.88	-0.188

This feature of the Davydov soliton can be justified by experiments. Lomdahl et al[61] gave the results of computer simulation for Eqs.(7)-(8), which are shown in Figure 3, which was obtained by soliton detector[61]. The results are presented with certain diagnostics: One is of "waveform" graphs: that is, plots of $|\varphi_n|^2$ and the discrete gradient $\beta_{n+1} - \beta_{n-1}$ as a function of *n* at a given time *t*. Also used are 'soliton detector' plots: on the (*t, n*)-plane, a mark was put at those times and positions where both $|\varphi_n|^2$ exceeded a certain level and $\beta_{n+1} - \beta_{n-1}$ is negative. The temporal extent of such a marked region shows the trajectory of a solution. In Figure 3 we see how several solitons are nucleated from random initial conditions and how they move along the chain. A correlation of the maximum in $|\varphi_n|^2$ and the minimum in $\beta_{n+1} - \beta_{n-1}$ is simultanously occurred, in accordance with the characteristics of a solution, namely Eqs. (11) and (12).
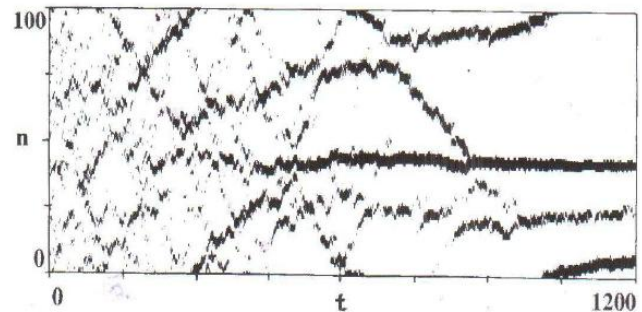
Figure 3 : The formation of Davydov soliton from initial conditions consisting of one quantum of amide-I energy distributed randomly along the molecular chains.

Davydov[8-12] also treated this situation. His analysis was based on the Hamiltonian in Eq.(1) with wave function in Eq.(2). After a number of approximations he obtained an NLSE, but now with a temperature-dependent coefficient for the nonlinear term. This coef-

ficient goes to zero with increasing temperature and vanishes at $TH \approx 400K$ indicating that soliton solutions should be stable for lower temperatures. This result is in direct contradiction with Lomdahl et al's computer simulations of Eq.(13) at finite temperatures[61]. The result of these simulations is as follows.

To describe the interaction of the system with a thermal reservoir at temperature T, Lomdahl and Kerr[61] added a damping force and noise force.

$$F_n = -m\Gamma\beta_n + \eta_n(t) \qquad (52a)$$

to Eq,(8) for the molecular displacements. The correlation function for the random noise was $\langle \eta_n(t)\eta_{n'}(t') \rangle = 2m\Gamma k_B T\delta(t - t')$ (k_B is Boltzmann's constant and Γ is a phenomenological damping constant). This extension converts Eq.(8) to Langevin equations. The effect of the above two terms is to bring the system to thermal equilibrium; it was verified numerically that over sufficiently long time intervals the mean kinetic energy satisfied

$$\left\langle \sum_n \frac{1}{2}m\beta_n^2(t) \right\rangle = \frac{1}{2}Nk_B T \qquad (52b)$$

where $\langle \ldots \rangle$ denotes time average. Equations (7) – (8)with the damping force and noise force included still imply the conservation of the norm in Eq.(6).

With the same diagnostics as in Figure 3, we show the result of a simulation at $T=300K$ in Figure 4, which was obtained by soliton detector[61]. The initial conditions were constructed to mimic what might happen during ATP hydrolysis, A Davydov soliton (cf. Eqs.(11) and (12)) has somehow been nucleated and now evolves under the influence of the random forces. The soliton is seen to disintegrate in a time corresponding to about 3 picoseconds. The filamentary black regions in this picture are seen to have a certain slope, which corresponds to the sound velocity in the units used in the calculation.
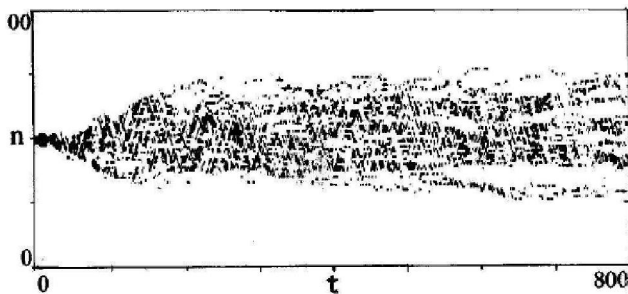
Figure 4 : The simulation of motion of Davydov soliton at T=300K, the soliton disappears in a few picoseconds after its formation.

The calculation with Eqs.(7)-(8) and (52a) is a combination of the above classical fluctuation -dissipation relation in Eq.(52b) with quantum-mechanical equations (7)-(8). The justification for this is that for the parameters relevant for α-helix, the highest acoustic frequency $\hbar\omega_{max}$ is about 100K. Since the equations are solved near 300K, the occupation numbers of all phonon modes are rather accurately given by the classical Boltzmann distribution and under those circumstances in Eq. (52b) is valid. At lower temperatures than say $TH \approx 200K$, the above approach would not be valid. The calculation with Eqs.(7)-(8) and Eq.(52a) is within the canonical ensemble, where the temperature is constant, but the energy allowed to vary. To check the consistency of the result, calculations were also done in the conventional microcanonical ensemble. The system was prepared with the use of Eq.(52a) at $T=300K$, it was then allowed to evolve only under the influence of the deterministic equations (7)-(8). The result of these simulations are essentially the same as presented above. The soliton seems to disappear in a few picoseconds. Similar results were also obtained by Lawrence *et al*.[68].

These result can be interpreted as shoeing that the wave function used by Davydov in Eq.(5), is not a good approximation for description of soliton-like objects at biological temperatures. The assumption that the state vector is decomposable into a pure phonon part and pure exciton part seems broken. The wave function that the two components remain distinct at all times neglects the phase- mixing characteristic of the evolution of the coupled quantum-mechanical system. This deficiency was also criticized on more general grounds by Brown *et al*.[33-41]. Since these results are somewhat negative, it is in order to state what cannot be concluded from this. The ability of the Hamiltonian in Eq. (1) to support soliton-like objects at finite temperatures is still open. It is also not possible based on the simulations to say what the lower temperature for soliton formation would be.

On the other hand, in order to investigate the influences of quantum and thermal effects on soliton state, which are expected to cause the soliton to decay into delocalized states, we postulate that the model Hamiltonian and the wavefunction in Pang's model together give a complete and realistic picture of the interaction properties and allowed states of the protein molecules. The additional interaction term in the Hamiltonian gives better symmetry of interactions. The new wavefunction is a reasonable choice

for the protein molecules because it not only can exhibit the coherent features of collective excitations arising from the nonlinear interaction between the excitons and phonons, but also retain the conservation of number of particles and fulfill the fact that the energy released by the ATP hydrolysis can only excite two quanta. In such a case, using a standard calculating method[65,66,112-115] and widely accepted parameters we can calculate the region encompassed of the excitation or the linear extent of the new soliton, $\Delta X = 2\pi r_0 / \mu_p$, to be greater than the lattice constant r_0 i.e., $\Delta X > r_0$ as shown in TABLE 1. Conversely we can explicitly calculate the amplitude squared of the new soliton using Eq.(42) in

its rest frame as $|\phi(X)|^2 = \dfrac{\mu_p}{2} \sec h^2(\dfrac{\mu_p X}{r_0})$. Thus the

probability to find the new soliton outside a range of width r_0 is about 0.10. This number can be compatible with the continuous approximation since the quasi-coherent soliton can spread over more than one lattice spacing in the system in such a case. This proves that assuming of the continuous approximation used in the calculation is still qualitatively valid because the soliton widths is large than the order of the lattice spacing, then the soliton stability is improved. Therefore we should believe that the above calculated results obtained from Pang's model is correct.

The lifetime of carrier (soliton) at physilogical temperature 300K

5.1, Partially diagonalized form of the model Hamiltonian

The thermal stability and lifetime of the soliton at 300K in the protein molecules is an centre and crucial problem in the process of bioenergy transport because the soliton possess certain biological meanings and can play an important role in the biological process, only if it has enough long lifetimes. In other word, the size of lifetime of the soliton is often used to judge directly the success and validity of the above theories of energy transport containing Pang theory. Therefore, it is very necessary to calculate carefully the lifetime of the solitons in different models.

I now calculate first the lifetime of the new soliton transporting the energy in Pang's model. Thus we introduce the following standard transformation[112-120]:

$$u_n = \sum_q \left[\frac{\hbar}{2NM\omega_q} \right]^{1/2} e^{iqnr_0} \left(a^+_{-q} + a_q \right),$$

$$P_n = i \sum_q \left[\frac{M\hbar\omega_q}{2N} \right]^{1/2} e^{iqnr_0} \left(a^+_{-q} - a_q \right) \tag{53}$$

Where $i = \sqrt{-1}$, $\omega_q = 2(w/M)^{1/2} \sin(\frac{r_0 q}{2})$, thus Eq.(32) becomes

$$
\begin{aligned}
\mathbf{H} = &\sum_n \left[\varepsilon_0 \mathbf{B}_n^+ \mathbf{B}_n - \mathbf{J}(\mathbf{B}_n^+ \mathbf{B}_{n+1} + \mathbf{B}_{n+1}^+ \mathbf{B}_n) \right] + \\
&\sum_q \hbar\omega_q (a_q^+ a_q + \frac{1}{2}) + \frac{1}{\sqrt{N}} \sum_{q,n} [\mathbf{g}_1(\mathbf{q})\mathbf{B}_n^+ \mathbf{B}_n + \\
&\mathbf{g}_2(\mathbf{q})(\mathbf{B}_n^+ \mathbf{B}_{n+1} + \mathbf{B}_n^+ \mathbf{B}_{n+1})](a_q + a_{-q}^+)e^{inr_0 q}
\end{aligned}
\tag{54}
$$

where

$$
\begin{aligned}
\mathbf{g_1(q)} &= 2\chi_1 i \left[\frac{\hbar}{2M\omega_q} \right]^{1/2} \sin r_0 q; \\
\mathbf{g_2(q)} &= \chi_2 \left[\frac{\hbar}{2M\omega_q} \right]^{1/2} (e^{ir_0 q} - 1)
\end{aligned}
\tag{55}
$$

We now diagonalize partially the model Hamiltonian in order to calculate the lifetime of the soliton in Eq.(43) using the quantum perturbation method[65,66]. Since one is interested in investigating the case where there is initially a soliton moving with a velocity v on the chains, it is convenient to do the analysis in a frame of reference where the soliton is at rest. We should then consider the Hamiltonian in this rest frame of the soliton, which is $\tilde{\mathbf{H}} = \mathbf{H} - v\mathbf{P}$, where P is the total momentum,

and $\mathbf{P} = \sum_q \hbar q(a_q^+ a_q - \mathbf{B}_q^+ \mathbf{B}_q)$, where $\mathbf{B}_q^+ = \dfrac{1}{\sqrt{N}} \sum_n e^{iqnr_0} \mathbf{B}_n^+$.

Also, in order to have simple analytical expressions we make the usual continuum approximation. This gives

$$
\begin{aligned}
\tilde{\mathbf{H}} = &\int_0^L \mathbf{dx} 2 \left[(\varepsilon_0 - 2\mathbf{J})\varphi^+(\mathbf{x})\varphi(\mathbf{x}) + \mathbf{J}r_0^2 \frac{\partial\varphi^+}{\partial\mathbf{x}}\frac{\partial\varphi}{\partial\mathbf{x}} - \right. \\
&\left. \frac{i\hbar\mathbf{v}}{2} \left(\frac{\partial\varphi^+}{\partial\mathbf{x}}\varphi(\mathbf{x}) - \varphi^+(\mathbf{x})\frac{\partial\varphi}{\partial\mathbf{x}} \right) \right] + \sum_q \hbar(\omega_q - q\mathbf{v})a_q^+ a_q + \\
&\frac{1}{\sqrt{N}} \sum_q 2[\mathbf{g}_1(\mathbf{q}) + 2\mathbf{g}_2(\mathbf{q})](a_{-q}^+ + a_q)\int_0^L \mathbf{dx} e^{ikx}\varphi^+(\mathbf{x})\varphi(\mathbf{x})
\end{aligned}
\tag{56}
$$

where $\varphi(x)$ represents now the field operator corresponding to B_n in the continuum limit (whereas before it only indicated a numerical value). Here $L=Nr_0$, $-\pi < kr_0 < \pi$, and $\omega_q H \approx (w/M)^{1/2} r_0.|q|$, $x = nr_0$. Since the soliton excitation is connected with the deformation of intermolecular spacing, it is necessary to pass in Eq.(56) to new phonons taking this deformation into account.

Such a transformation can be realized by means of the following transformation of phonon operators[154,113-116]:

$$b_q = a_p - \frac{1}{\sqrt{N}}\alpha_q, \; b_q^+ = a_q^+ - \frac{1}{\sqrt{N}}\alpha_q^*, \qquad (57)$$

which describe phonons relative to a chain with a particular deformation, where $b_q|\tilde{0}\rangle_{ph} = 0$, $b_q (b_q^+)$ is the annihilation (creation) operator of new phonon.. Then the Hamiltonian $\tilde{H}$ is now

$$\tilde{H} = \int_0^L 2dx\varphi(x)[\varepsilon_0 - 2J + V(x) - Jr_0^2\frac{\partial^2}{\partial x^2} + i\hbar\frac{\partial}{\partial x}]\varphi(x) +$$
$$\sum_q \hbar(\omega_q - qv)[b_q^+ b_q + \frac{1}{\sqrt{N}}(\alpha_q b_q^+ + \alpha_q^* b_q^+)] + W +$$
$$\frac{1}{\sqrt{N}}\sum 2[g_1(q) + 2g_2(q)](b_{-q}^+ + b_q)\int_0^L dxe^{iqx}\varphi^+(x)\varphi(x) \qquad (58)$$

where

$$W = \frac{1}{N}\sum_q \hbar(\omega_q - qv) \, | \, \alpha_q \, |^2,$$

$$V(x) = \frac{1}{N}\sum_q [g_1(q) + 2g_2(q)](\alpha_{-q}^* + \alpha_{-q})e^{iqx} \qquad (59)$$

To describe the deformation corresponding to a soliton in the subspace where there is $\int_0^L dx\varphi^+(x)\varphi(x) = 1$. **From the above formulae we can obtain**

$V(x) = -2J\mu_p^2 \sec h^2(\mu_p x / r_0)$ (60)

In order to partially diagonalize the Hamiltonian in Eq.(58) we introduce the following canonical transformation[65,66,112-115]

$$\varphi(x) = \sum_j A_j C_j(x), \; \varphi^+(x) = \sum_j C_j^*(x)A_j^+ \qquad (61)$$

where

$$\int C_1^*(x)C_j(x)dx = \delta_{1j}, \sum_j C_j^*(x')C_j(x) = \delta(x - x'),$$
$$\int dx \, | \, C_j(x) \, |^2 = 1 \qquad (62)$$

The operators A_s^+ and A_k^+ are the creation operators for the bound states $C_s(x)$ and delocalized state $C_k(x)$, respectively. Thus the obtained partially diagonalized Hamiltonian is as follows

$$\tilde{H} = W + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - qv)b_q^+ b_q +$$
$$\frac{1}{\sqrt{N}}\sum_q \hbar(\omega_q - qv)(b_q^+\alpha_q + \alpha_q^* b_q)(1 - A_s^+ A_s) +$$
$$\frac{1}{\sqrt{N}}\sum_{kk'q} F(k,k',q)(b_{-q}^+ + b_q)A_{k'}^+ A_k -$$
$$\frac{1}{\sqrt{N}}\sum_{kq} \tilde{F}(k,q)(b_{-q}^+ + b_q)(A_s^+ A_{-k} - A_k^+ A_s) \qquad (63)$$

and

$$C_s(x) = (\frac{\mu_p}{2r_0})^{1/2} \sec h(\mu_p x / r_0)\exp[i\hbar xv / 2Jr_0^2],$$

with $E_s = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - \mu_p J\right]$ (64a)

$$C_k(x) = \frac{\mu_p \tanh(\mu_p x / r_0) - ikr_0}{\sqrt{Nr_0}[\mu_p - ikr_0]}\exp[ikx + \frac{i\hbar vx}{2Jr_0^2}],$$

$$E_k = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - J(kr_0)^2\right] \qquad (64b)$$

where

$$F(k,k',q) = 2[g_1(q) + 2g_2(q)]\int_0^L dxe^{iqx}C_{k'}^*(x)C_k(x)$$

$$\approx 2[g_1(q) + 2g_2(q)]\left\{1 - \frac{i\mu_p qr_0}{[\mu_p + i(k + q)r_0][\mu_p - ikr_0]}\right\} \qquad (65)$$
$$\approx F[k,(k + q),q]\delta_{k'k+q}$$

$$\tilde{F}(k,q) = 2[g_1(q) + 2g_2(q)]\int_0^L dxe^{iqx}C_{k'}^*(x)C_s(x)$$

$$= \frac{2\pi}{\sqrt{2\mu_p}}[g_1(q) + 2g_2(q)]\left\{\frac{iqr_0}{[\mu_p + ikr_0]}\right\}$$
$$\sec h[\pi(k - q)r_0 / 2\mu_p] \qquad (66)$$

where α_q is determined by V(x) and the condition, $(\omega_q - vq)\alpha_q = (\omega_q + qv)\alpha_q^*$, which is required to get the factor, $(1 - A_s^+ A_s)$, in the $\tilde{H}$ in Eq.(63). Thus we find

$$\alpha_q = \frac{i\pi(\chi_1 + \chi_2)}{w\mu_p(1 - s^2)}\left[\frac{M}{2\hbar\omega_q}\right]^{1/2}(\omega_q + qv)\csc h(\pi qr_0/2\mu_p) \text{ and}$$

$$W = \frac{2}{3}\mu_p^2 J.$$

We now calculate the transition probability and decay rate of the quasi-coherent soliton arising from the perturbed potential by using the first-order quantum perturbation theory developed by Cottingham, et al[65,66], in which the influences of the thermal and quantum effects on the properties of the soliton can be taken into account simultaneously.

For the discussion of the decay rate and lifetime of the new soliton state it is very convenient to divide $\tilde{H}$ in Eq.(63) into $H_0 + V_1 + V_2$, where

$$H_0 = W + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_K + \sum_q \hbar(\omega_q - vq)b_q^+ b_q +$$
$$\frac{1}{\sqrt{N}}\sum_q \hbar(\omega_q - vq)(\alpha_q b_q^+ + \alpha_q^* b_q)(1 - A_s^+ A_s) \qquad (67)$$

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and

$$V_1 = \frac{1}{\sqrt{N}} \sum_{kk'q} F(k, k+q, q)(b^+_{-q} + b_q) A^+_{k'} A_k$$

$$V_2 = \frac{1}{N} \sum_{kq} \tilde{F}(k, q)(b^+_{-q} + b_q)(A^+_s A_k - A^+_s A_{-k}) \tag{68}$$

where H_0 describes the relevant quasi-particle excitations in the protein. This is a soliton together with phonons relative to the distorted lattice. The resulting delocalized excitations belongs to an exciton-like band with phonons relative to a uniform lattice. The bottom of the band of the latter is at the energy $4J\mu_p^2 / 3$ relative to the soliton, in which the topological stability associated with removing the lattice distortion is included.

We now calculate the decay rate of the new soliton along the following lines by using Eq.(67) and V_2 in Eq.(68) and quantum perturbation theory. Firstly, we compute a more general formula for the decay rate of the soliton containing n quanta in the system in which the three terms contained in Eq.(31) is replaced by (n+1) terms of the expression of a coherent state $\frac{1}{\lambda} exp[\sum_n \varphi_n(t) B^+_n] 10 >_{ex}$. Finally we find out the decay rate of the new soliton with two-quanta. In such a case H_0 is chosen such the ground state, |n> has energy $W + n E'_s$ in the subspace of excitation number equal to n, i.e., $< n | \sum_i B^+_i B_i | n > = < n | (A^+_s A_s + \sum_k A^+_k A_k) | n > = n$. In this subspace the eigenstates have the simple form $|n-m, k_1 k_2 \ldots k_m, \{n_q\} >$

$$= \frac{1}{\sqrt{(n-m)!}} (A^+_s)^{n-m} A^+_{k_1} A^+_{k_2} \cdots A^+_{k_m} | 0 >_{ex} \prod_q \frac{(d^+_q)^{n_q}}{\sqrt{n_q!}} 1\tilde{0} >^{n-m}_{ph} \tag{69}$$

where

$$d_q = b_q + \frac{m}{n} \frac{1}{\sqrt{N}} \alpha_q = a_q - \frac{n-m}{n} \frac{1}{\sqrt{N}} \alpha_q$$

$$(m \leq n, \ n \ and \ m \ are \ all \ intgers) \tag{70}$$

with $d_q | \tilde{0} >^{n-m}_{ph} = 0$. The corresponding energy of the systems is

$$E^{(0)}_{n-m;k_1 \ldots k_{m_1};\{n_q\}} = (1-(m/n)^2)W + (n-m)E'_s +$$

$$\sum_{j=1}^m E'_{k_1} + \sum_q \hbar(\omega_q - vq) n_q \tag{71}$$

E'_s is the energy of a bound state with one soliton, E'_k is the energy of the unbound (delocalized) state with

one exciton. When m=0 the excitation state is a n-type soliton plus phonons relative to the chain with the deformation corresponding to the n-type soliton. For m=n the excited states are delocalized and the phonons are relative to a chain without any deformation. Furthermore except for small k, the delocalized states approximate ordinary excitons. Thus the decay of the soliton is just a transition from the initial state with the n-type soliton plus the new phonons:

$$| n > = \frac{1}{\sqrt{n!}} \prod_q \frac{(b^+_q)^{n_q}}{(n_q!)^{1/2}} (A^+_s)^n | 0 >_{ex} | \tilde{0} >_{ph} \tag{72}$$

with corresponding energy $E_s\{n_q\} = W + n E'_s + \sum_q \hbar(\omega_q - vq) n_q$ to the final state with delocalized excitons and the original phonons:

$$| \alpha k > = \prod_q \frac{(a^+_q)^{n_q}}{\sqrt{n_q!}} | 0 >_{ph} (A^+_k)^n | 0 >_{ex} \tag{73}$$

with corresponding energy $E_k\{n_q\} = n E'_k + \sum_q \hbar(\omega_q - vq) n_q$ caused by the part, V_2, in the perturbation interaction V. In this case, the initial phonon distribution will be taken to be at thermal equilibrium. The probability of the above transitions in lowest order perturbation theory is given by

$$\overline{W} = \frac{1}{\hbar^2} \int_0^t dt' \int_0^t dt'' \left\{ \sum_{\alpha k'} \sum_l P_l^{(ph)} < n | \right.$$
$$exp\left(\frac{iH_0 t''}{\hbar}\right) V_2 exp\left(\frac{-iH_0 t''}{\hbar}\right) | \alpha k' > .$$
$$\left. < \alpha k' | exp\left(\frac{iH_0 t'}{\hbar}\right) V_2 exp\left(\frac{-iH_0 t'}{h}\right) | n > \right\} \tag{74}$$

We should calculate the transition probability of the soliton resulting from the perturbed potential,$(V_1 + V_2)$, at first-order perturbation theory. Following Cottingham and Schweitzer[65,66], we estimate only the transition from the soliton state to delocalized exciton states caused by the potential V_2, which can satisfactorily be treated by means of perturbation theory since the coefficient $\tilde{F}(k,q)$ defined by Eq.(66) is proportional to an integral over the product of the localized state and a delocalized state, and therefore is of order $1/\sqrt{N}$. The V_1 term in the Hamiltonian is an interaction between the delocalized excitons and the phonons. The main effect of V_1 is to modify the spectrum of the delocalized excitatons

in the weak coupling limit ($J\mu_p / K_B T_0 << 1$, the definition of T_0 is given below). As a result the delocalized excitons and phonons will have their energies shifted and also have finite lifetimes. These effects are ignored in our calculation since they are only of second order in V_1.

Through tedious calculation we can finally obtain the decay rate, which is as follows[112-120]

$$\Gamma_n = \lim_{t\to\infty} \frac{d\overline{W}}{dt} = \frac{2}{n\mu_1 \hbar^2} \frac{\pi^2}{N^2} \sum_{kk'} \left[|\,\mathbf{g}_1(\mathbf{k}) + 2\mathbf{g}_2(\mathbf{k})\,|^2 \right.$$

$$\frac{(\mathbf{r}_0 \mathbf{k})^2 \operatorname{sech}^2[\pi(\mathbf{k}-\mathbf{k}')\mathbf{r}_0/2n\mu_1]}{(n\mu_1)^2 + (\mathbf{k}'\mathbf{r}_0)^2} \operatorname{Re} \int_0^\infty dt \cdot$$

$$\left\{ \exp[-i(n\mathbf{J}(\mathbf{k}'\mathbf{r}_0)^2 + n(n^2 - \frac{2}{3}n)\mu_1^2 \mathbf{J}\, t/\hbar + \right. \tag{75}$$

$$\left.\left. \mathbf{R}_n(\mathbf{t}) + \xi_n(\mathbf{t})] \frac{\exp[i(\omega_k - \mathbf{kv})t]}{\exp[\beta\hbar(\omega_k - \mathbf{kv})] - 1} \right\} \right]$$

where

$$\mathbf{R}_n(\mathbf{t}) = -\frac{1}{n^2 N} \sum_k |\alpha_k|^2 \{i - \exp[-i(\omega_k - \mathbf{kv})t]\},$$

$$\xi_n(\mathbf{t}) = -\frac{4}{n^2 N} \sum_k \frac{|\alpha_k|^2 \sin^2[\frac{1}{2}(\omega_k - \mathbf{kv})t]}{\exp[\beta\hbar(\omega_k - \mathbf{kv})] - 1} \tag{76}$$

This is just a generally analytical expression for the decay rate of the soliton containing n quanta at any temperature within lowest order perturbation theory. Note that in the case where a phonon with wavevector k in Eq.(76) is absorbed, the delocalized excitation produced does not need to have wavevector equal to k. The wavevector here is only approximately conserved by the sech²[π(k-k')r₀ / 2nμ₁] term. This is, of course, a consequence of the breaking of the translation symmetry by the deformation. Consequently, we do not find the usual energy conservation. The terms $R_n(t)$ and $\xi_n(t)$ occur because the phonons in the initial and final states are defined relative to different deformations.

We should point out that the approximations made in the above calculation are physically justified because the transition and decay of the soliton is mainly determined by the energy of the thermal phonons absorbed. Thus the phonons with large wavevectors which fulfill wavevector conservation make a major contribution to the transition matrix element, while the contributions of the phonons with small wavevector which do not fulfill wavevector conservation are very small, and can be neglected.

From Eqs.(75) and (76) we see that the Γ_n and $R_n(t)$ and $\xi_n(t)$ and $\mu = n\mu_1$ mentioned above are all changed by increasing the number of quanta, n. Therefore, the approximation methods used to calculate Γ_n and related quantities (especially the integral contained in Γ_n) should be different for different n.

We now calculate the explicit formula of the decay rate of the new soliton with two-quanta (n=2) by using Eqs.(75)-(76). In such a case we can compute explicitly the expressions of this integral and $R_2(t)$ and $\xi_2(t)$ contained in Eqs.(75)-(76) by means of approximation. As a matter of fact, in Eq.(76) at n=2 the functions $R_2(t)$ and $\xi_2(t)$ can be exactly evaluated in terms of the digamma function and its derivative. In the case when the soliton velocity approaches zero and the phonon frequency ω_q is approximated by $\sqrt{w/M}\,|q|r_0$. For $t \to \infty$ (because we are interested in the long-time steady behaviour) the asymptotic forms of $R_2(t)$ and $\xi_2(t)$ are[112-120]

$$\mathbf{R}_2(\mathbf{t}) = -\mathbf{R}_0[\ln(\frac{1}{2}\omega_\alpha t) + 1.578 + \frac{1}{2}i\pi] \tag{77}$$

$$\xi_2(\mathbf{t}) \approx -\pi\mathbf{R}_0 \mathbf{k}_B \mathbf{T}t/\hbar \ \text{(where } \coth\frac{1}{2}\omega_\alpha t \sim 1) \tag{78}$$

i.e., $\displaystyle\lim_{t\to\infty}\xi_2(\mathbf{t}) = -\eta t$, $\eta = \pi\mathbf{R}_0/\beta\hbar = \pi\mathbf{R}_0\mathbf{k}_B\mathbf{T}/\hbar$ (79)

where
$$\mathbf{R}_0 = \frac{4(\chi_1 + \chi_2)^2}{\pi\hbar\mathbf{w}}(\mathbf{M}/\mathbf{w})^{1/2} = \frac{2\mathbf{J}\mu_p\mathbf{r}_0}{\pi\hbar\mathbf{v}_0},$$

$$\omega_\alpha = \frac{2\mu_p}{\pi}(\frac{\mathbf{w}}{\mathbf{M}})^{1/2}, \ \mathbf{T}_0 = \hbar\omega_\alpha/\mathbf{K}_B \tag{80}$$

At $R_0 < 1$ and $T_0 < T$ and $R_0 T/T_0 < 1$ for the protein molecules, one can evaluate the integral including in Eq.(75) by using the approximation. The result is

$$\frac{1}{\pi\hbar}\operatorname{Re}\int_0^\infty dt \exp\left\{ -i[2\mathbf{J}(\mathbf{k}'\mathbf{r}_0)^2 + \frac{4}{3}\mathbf{J}\mu_p^2 - \hbar\omega_k]t/\hbar + \right.$$

$$\mathbf{R}_2(\mathbf{t}) + \xi_2(\mathbf{t}) \Big\} \approx \frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-\mathbf{R}_0}\Gamma(1-\mathbf{R}_0)[\eta^2 +$$

$$(\delta(\mathbf{k},\mathbf{k}')/\hbar)^2]^{-(1-\mathbf{R}_0)/2}\left[1 - \frac{1}{2}\left[\frac{\pi\mathbf{R}_0}{2} + (1-\mathbf{R}_0)\left(\frac{\delta(\mathbf{k},\mathbf{k}')}{\eta\hbar}\right)\right]^2\right] \tag{81}$$

where $\delta(\mathbf{k},\mathbf{k}') = 2\mathbf{J}(\mathbf{k}'\mathbf{r}_0)^2 + \frac{4}{3}\mu_p^2\mathbf{J} - \hbar\omega_k$, $\Phi_1 = \frac{\mathbf{R}_0\pi}{2}$,

$$\Phi_2 = [(1-\mathbf{R}_0)\tan^{-1}\left(\frac{\delta(\mathbf{k},\mathbf{k}')}{\eta\hbar}\right)] \tag{82}$$

The decay rate of the new solition with two-quanta, in such an approximation, can be represented, from

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Eqs.(75) and (81)[112-120], by

$$\Gamma_2 = \lim_{t \to \infty} \frac{d\overline{W}}{dt} = \frac{2}{\mu_p}\left(\frac{\pi}{N}\right)^2 \sum_{kk'}\left[\frac{(kr_0)^2 |g_1(k) + 2g_2(k)|^2 \operatorname{sech}^2[(\pi r_0/2\mu_p)(k-k')]}{[\mu_p^2 + (k'r_0)^2][\exp(\beta\hbar\omega_k)-1]}(2.43\omega_\alpha)^{-R_0}\right.$$

$$\left\{\frac{\left(\eta^2 + \frac{1}{\hbar^2}[\frac{4}{3}\mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k]^2\right)^{(1+R_0)/2}}{\hbar^2\eta^2 + [\frac{4}{3}\mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k]^2}\right\}\left\{1 - \frac{1}{2}\left[\frac{R_0\pi}{2} + (1-R_0)\left[\frac{\frac{4}{3}\mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k}{\hbar\eta}\right]\right]^2\right\} \qquad (83)$$

In fact, Cottingham et al[65,66] found out the decay rate of Davydov's solition using the quantum perturbation method, which is represented as

$$\Gamma_D = \frac{1}{\hbar^2}\frac{\chi_1^2}{\mu_D}\left(\frac{2\pi}{N}\right)^2\sum_{kk'}\left(\frac{\hbar}{2M\omega_k}\right)$$

$$\frac{(kr_0)^2 \sin^2(kr_0)\operatorname{sech}^2[(\pi r_0/2\mu_D)(k-k')]}{[\mu_D^2 + (k'r_0)^2][\exp(\beta\hbar\omega_k)-1]}\left(\frac{\omega_\alpha^D}{\eta_D}\right)^{-R_0^D} \cdot$$

$$\frac{\hbar^2\eta_D}{\hbar^2\eta_D^2 + [J\mu_D^2/3 + J(k'r_0)^2 - \hbar\omega_k]} \qquad (84)$$

where

$$\eta_D = \pi R_0^D K_B T/\hbar, \quad R_0^D = \frac{2\chi_1^2}{\pi\hbar w}(\frac{M}{w})^{1/2}, \quad \omega_\alpha^D = \frac{2\mu_D}{\pi}(\frac{M}{w})^{1/2} \quad (85)$$

Equation (84) can also be found out from Eq.(74) at n=1.

Comparing Eq.(83) with Eq.(84) we find that the decay rate of the new solition with two-quanta is considerably different from that in the Davydov model not only for the parameter's values, but also the factors contained in them. In Eq.(83) the factor,

$$\left\{1 - \frac{1}{2}\left[\frac{R_0\pi}{2} + (1-R_0)\left[(\frac{4}{3}\mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k)/\hbar\eta\right]\right]^2\right\} \text{ is}$$

added, while in Eq.(84) the factor, $(\frac{\omega_\alpha}{\eta_D})^{-R_0^D}\eta_D$ replaces

the term $(2.43\omega_d)^{-R_0}\cdot(\eta^2 + \frac{1}{\hbar^2}[\frac{4}{3}\mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k]^2)^{(\frac{1+R_0}{2})})$ in Eq.(83) due to the two-quanta nature of the new wavefunction and the additional interaction term in the new Hamiltonian. In Eq. (83) the $\cdot$, R_0 and T_0 are not small, unlike in the Davydov model. Using Eq.(50) and TABLE 1 we find out the values of η, R_0 and To at T=300K in both models, which are listed in TABLE 2. From this table we see that the η, R_0 and T_0 in Pang's model are about 3 times larger than the corresponding values in the Davydov model due to the increases of μ_p and of the nonlinear interaction coefficient G_p. Thus the approximations used in the Davydov model by

Cottingham, et.al[65,66] can not be applied in our calculation of lifetime of the new soliton, although we utilized the same quantum-perturbation scheme. Hence we can audaciously suppose that the lifetimes of the quasi-coherent soliton will greatly change.

**TABLE 2 : Comparison of characteristic parameters in the Davydov model and in our new model**

	R_0	T_0 (K)	$\eta(\times 10^{13}/s)$
New model	0.529	294	6.527
Davydov model	0.16	95	2.096

The above expression, Eq.(83), allows us to compute numerically the decay rate, Γ_2, and the lifetimes of the new soliton, $\tau = 1/\Gamma_2$, for values of the physical parameters appropriate to α-helical protein molecules. Using the parameter values given in Eq.(50), TABLES 1 and 2, $v=0.2v_0$ and assuming the wavevectors are in the Brillouin zone we obtain values of Γ_2 between $1.54\times10^{10}S^{-1}$-$1.89\times10^{10}S^{-1}$. This corresponds to the soliton lifetimesτ, of between $0.53\times10^{-10}S$-$0.65\times10^{-10}S$ at T=300K, or τ/τ_0=510-630, where $\tau_0 = r_0/v_0$ is the time for travelling one lattice spacing at the speed of sound, equal to $(M/w)^{1/2}$=0.96×10^{-13}S. In this amount of time the new soliton, travelling at two tenths of the speed of sound in the chain, would travel several hundreds of lattice spacings, that is several hundred times more than the Davydov soliton for which τ/τ_0<10 at 300K[65,66].

Cottingham et al.[65,66] obtained from Eq.(83) that the lifetime of Davydov soliton is only $10^{-12} - 10^{-13}$ Sec., i.e., Davydov soliton traveling at a half of the sound speed can cover less than 10 lattice spacing in its lifetime. This shows that the lifetime of Davydov soliton is too small (about) to be useful in biological processes. This shows clearly that the Davydov solution is not a true wave function of the systems. However, the lifetime is sufficiently long for the new soliton excitation to be a carrier of energy. Therefore the quasi-coherent soliton is a viable

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mechanism for the energy transport at biological temperature in the above range of parameters.

We are very interested in the relation between the lifetime of the quasi-coherent soliton and temperature. Figure 5 shows the relative lifetimes τ/τ_0 of the new soliton versus temperature T for a set of widely accepted parameter values as shown in Eq.(50). 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 $L = Nr_0$ is the typical length of the protein molecular chains. Hence for $L/r_0 H \approx 100$, $\tau/\tau_0 > 500$ is a reasonable criterion for the soliton to be a possible mechanism of the energy transport in protein molecules. The lifetime of the quasi-coherent soliton shown in Figure 5 decreases rapidly as temperature increases, but below T=310K it is still large enough to fulfill the criterion. Thus the new soliton can play an important roles in biological processes[112-120].
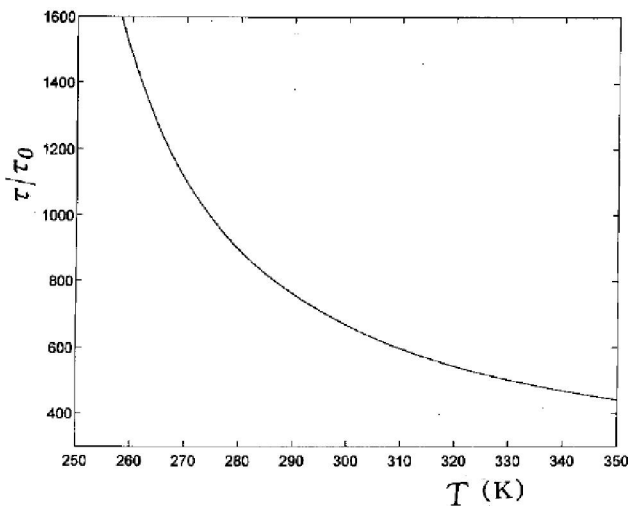
Figure 5 : Soliton lifetime τ relatively to τ_0 as a function of the temperature T for parameters appropriate to the α-helical molecules in the new model in Eq.(31)

For comparison we plotted simultaneously log (τ / τ_0) versus the temperature relations for the Davydov soliton and the new soliton with a quasi-coherent two-quanta state in Figure 6. The temperature-dependence of log (τ / τ_0) of the Davydov soliton is obtained from Eq. (84). We find that the differences of values of τ / τ_0 between the two models are very large. The value of τ / τ_0 of the Davydov soliton really is too small, and it can only travel fewer than ten lattice spacings in half the speed of sound in the protein chain[65]. Hence it is true that the Davydov soliton is ineffective for biological processes[65,66].
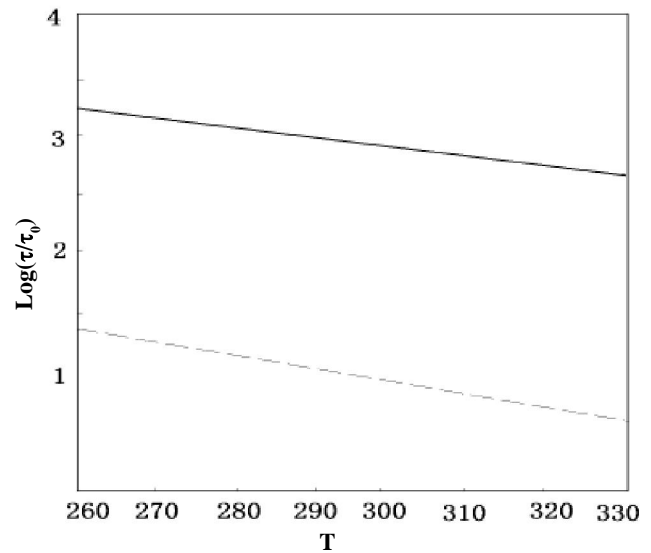
Figure 6 : Log(τ/τ_0) versus the temperature for the soliton. The solid line is the result of the new model, the dashed line is the result of the Davydov model.

We can also study the dependency of the soliton lifetime on the other parameters by using Eq.(83). We chose parameter values near the above accepted values shown in Eq. (50). In Pang's model we know from Eq.(83) that the lifetime of the soliton depends mainly on the following parameters: coupling constants $(\chi_1 + \chi_2)$, M, w, J, phonon energy $\hbar\omega_k$, as well as on the composite parameters $\mu(\mu = \mu_p)$, R_0 and T/T_0. At a given temperature, τ/τ_0 increases as μ and T_0 increase. The dependences of the lifetime τ/τ_0, at 300K on $(\chi_1 + \chi_2)$ and μ are shown in Figures 7 and 8, respectively[112-120]. Since μ is inversely proportional to the size of the soliton, and determining the binding energy in Pang's model, therefore it is an important quantity. We regard it as an independent variable. In such a case the other parameters in Eq. (83) adopt the values in Eq. (50). It is clear from Figures 7 and 8 that the lifetime of the soliton, τ/τ_0, increases rapidly with increasing μ and $(\chi_1 + \chi_2)$. Furthermore, when $\mu \geq 5.8$ and $(\chi_1 + \chi_2) \geq 7.5 \times 10^{-11}$N, which are values appropriate to Pang's model, we find $\tau/\tau_0 > 500$. For comparison we show in Figure 8 the corresponding result obtained using Eq.(83).

For the original Davydov model as a dashed line in Figure 8. Here we see that the increase in lifetime of the Davydov soliton with increasing μ is quite slow and the difference between the two models increases rapidly with increasing μ. The same holds for the dependency on the parameter $(\chi_1 + \chi_2)$ but the result

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for the Davydov soliton is not drawn in Figure 7. These results show again that the new soliton in Pang's model is a likely candidate for the mechanism of energy transport in the protein molecules. In addition it shows that a basic mechanism for increasing the lifetime of the soliton in protein molecules is to enhance the strength of the exciton-phonon interaction.
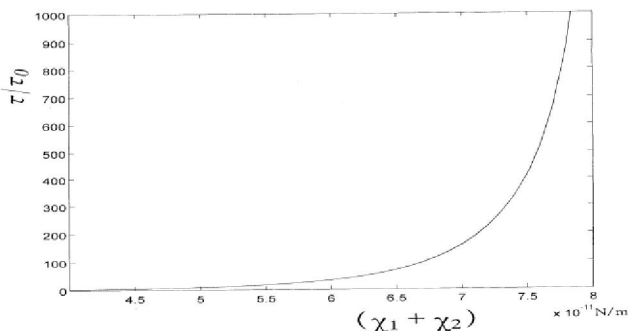

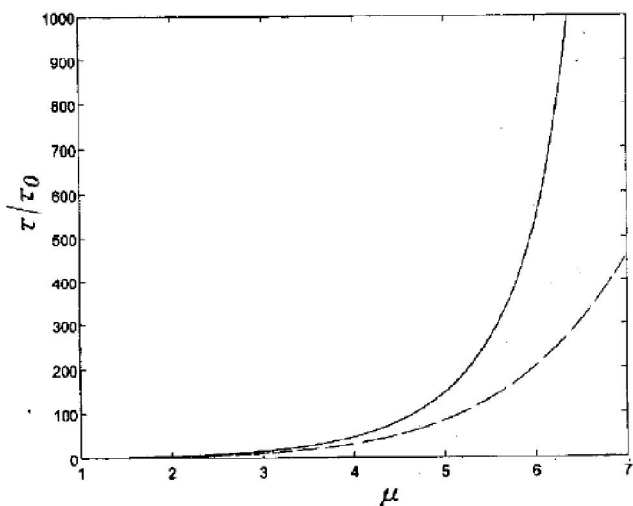**Figure 7 : τ/τ_0 versus $(\chi_1+\chi_2)$ relation in Eq.(83)**

Figure 8 : τ/τ_0 versus μ relation. The solid and dashed lines are results of Eq.(83) and Eq.(84), respectively
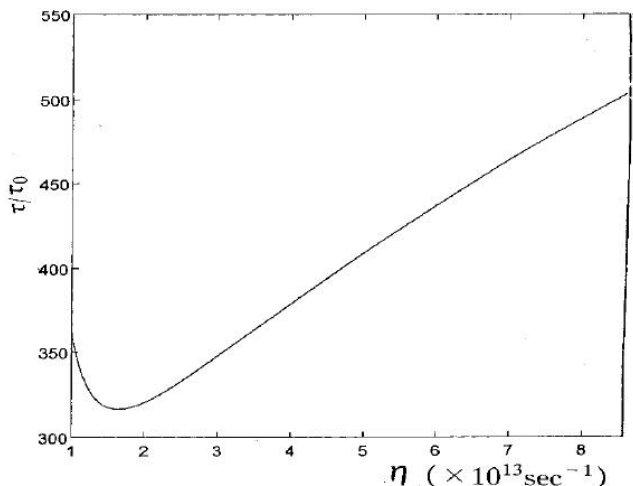

Figure 9 : τ/τ_0 versus η relation in Eq.(83)

In Figure 9 we plot τ/τ_0 versus η. Since $-\eta$ designates the influence of the thermal phonons on the soliton, it is also an important quantity. Thus, we regard it here as an independent variable. The other parameters in Eq.(83) take the values in Eq.(50). From this figure we see that τ/τ_0 increases with increasing η. Therefore, to enhance η can also increase the value of τ/τ_0.

CONCLUSION

As it is known, the energy transport is a basic problem in life science and related to many biological processes. Therefore it is very necessary to establish the mechanism of energy transport and its theory, where the energy is released by ATP hydrolysis. Scientists established different theories of energy transport based on different properties of structure of α–helical protein molecules, for example, Davydov's, Takeno's, Yomosa's, Brown et al's, Schweitzer's, Cruzeiro-Hansson's, Forner's and Pang's models, and so on. We first review past researches on different models or theories. Subsequently we studied and reviewed systematically the properties, thermal stability and lifetimes at physiological temperature 300K for the carriers (solitons) transporting the energy in Pang's and Davydov's theories. From these investigations we know that the carrier (soliton) of energy transport in Pang's model has a higher binding energy, higher thermal stability and larger lifetime at 300K relative to those of Davydov's model, in which the lifetime of the new soliton at 300K is enough large and belongs to the order of 10^{-10} second or $\tau/\tau_0 \geq 700$. Thus we can conclude that the new soliton in Pang's model is exactly the carrier of energy transport, Pang's theory is appropriate to α–helical protein molecules.

Why then does the quasi-coherent soliton have such high lifetime? From Eqs. (47) and TABLES 1 and 2 we see that the binding energy and localization of the new soliton increase due to the increase of the nonlinear interactions of exciton-phonon interaction, i.e., the new wave function with two-quanta state and the new Hamiltonian with the added interaction produce considerable changes to the properties of the soliton. In fact, the nonlinear interaction energy in Pang's model is $G_p=8(\chi_1+\chi_2)^2/(1-s^2)w=3.8\times10^{-21}J$, and it is larger than the linear dispersion energy, $J=1.55\times10^{-22}J$, i.e., the nonlinear interaction is so large that it can really cancel

or suppress the linear dispersion effects in the dynamic equation in this model. Thus we can conclude that the new soliton is stable and localized according to the soliton theory[26,149]. However, the nonlinear interaction energy in the Davydov model is $G_D = 4\chi_1^2/(1-s^2)w \approx 1.18 \times 10^{-21}$J and it is 3-4 times smaller than G_p. Then the stability of the Davydov soliton is weak compared to that of the new soliton. Moreover, the binding energy of the new soliton in Pang's model is $E_{BP}=4\mu_p^2 J/3=7.8 \times 10^{-21}$J in Eq.(47), which is about 2 times larger than the thermal energy, $K_B T = 4.14 \times 10^{-21}$J, at 300K, and about 6 times larger than the Debye energy, $K_B \Theta = \hbar\omega_D = 1.2 \times 10^{-21}$J (here ω_D is Debye frequency), and it is approximately equal to $\varepsilon_0/4=8.2 \times 10^{-21}$J, i.e., it has same order of magnitude of the energy of the amide-I vibrational quantum, ε_0. This shows that the new soliton is robust due to the large energy gap between the solitonic ground state and the delocalized state. In contrast the binding energy of the Davydov soliton is only

$$E_{BD} = \frac{\chi_1^4}{3w^2 J} = 0.188 \times 10^{-21} \text{ J}$$

which is about 41 times smaller than that of the new soliton, about 23 times smaller than $K_B T$ and about 6 times smaller than $K_B\Theta$, respectively. Therefore, it is easily destroyed by thermal and quantum effects. Hence the Davydov soliton has very small lifetime (about $10^{-12} \sim 10^{-13}$s), and it is unstable at 300K[65,66]. Thus the new soliton can provide a realistic mechanism for the energy transport in protein molecules.

The two-quanta nature for the quasi-coherent soliton in Pang's model plays a more important role in the increase of lifetime than that of the added interaction because of the following facts.

(1) The changes of the nonlinear interaction energy

$$G_P=2G_D\left[1+2\left(\frac{\chi_2}{\chi_1}\right)+\left(\frac{\chi_2}{\chi_1}\right)^2\right]$$ and μ_p produced by the

added interaction in the Hamiltonian in Pang's model are $\Delta G = G_P(\chi_2 \neq 0) - G_P(\chi_2=0) = 1.08\ G_D < G_P(\chi_2=0) = 2G_D$ and $\Delta\mu=\mu_p(\chi_2\neq0)-\mu_p(\chi_2=0) =$ $1.08\mu_D<\mu_p(\chi_2=0) = 2\mu_D$, respectively, where $\Delta G =2G_D$ and $\Delta\mu=2\mu_D$ are just the results caused by the two-quanta feature in Pang's model. This means that the effects of the added interaction on G_p and μ_p are smaller those of the two-quanta nature. Since the two parameters G_p and μ_p are responsible for the lifetime of the soliton, then we can conclude that the effect of the former on the lifetimes is smaller than the latter.

(2) The contribution of the added interaction to the binding energy of the new soliton is about

$$E'_{BP} = E_{BD}\left[1+\left(\frac{\chi_2}{\chi_1}\right)\right]^4 = 2.6E_{BD} \text{ , which is smaller than}$$

that of the two-quanta nature which is $E''_{BD} = 8E_{BD}$. Putting them together in Eq.(47) we see that $E_{BP} \approx 41E_{BD}$.

(3) From the $(\chi_1+\chi_2)$-dependence of τ/τ_0 in Figure 7 we find that $\tau/\tau_0 \approx 100$ at $\chi_2=0$ which is about 20 times larger than that of the Davydov soliton under the same conditions. This shows clearly that the major effect in the increase of the lifetime is due to the modified wave function. Therefore, it is very reasonable to refer to the new soliton as the quasi-coherent soliton.

The above calculation is helpful to resolve the controversies on the lifetime of the Davydov soliton, which is too small in the region of biological temperature. In fact, modifying the wave function and the Hamiltonian of the Davydov's model, we find that the stability and lifetime of the soliton at 300K in Pang's model increase considerably relative to those in Davydov's model, which are shown in TABLE 3. TABLE 3 shows that Pang's model repulse and refuse the shortcomings of the Davydov model, the new soliton is thermal stable at 300K and has so enough long lifetime, thus it can plays important role in biological processes, it is possibly an actually carrier of energy transport in the protein molecules. Thus the quasi-coherent soliton is a viable mechanism for the energy transport, Pang's model is appropriate to α–helical protein molecules.

TABLE 3 : Comparison of features of the solitons between our model and Davydov model

Model	Nonlinear interaction $G(10^{-21}J)$	Amplitude	Width 10^{-10}m	Binding energy $(10^{-21}J)$	Lifetime at 300K (S)	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}	320	Several handreds
Davydov model	1.18	0.974	14.88	-0.188	10^{-12}-10^{-13}	<200	Less than 10

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