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## Research Article

# The production of Bio-energy and its properties of Transport in the Living Systems -

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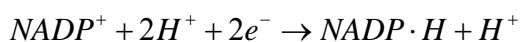
## ABSTRACT

We here introduced the form of bio - energy in living system and elucidated again the new theory of bio-energy transport along protein molecules in living systems based on the changes of structure and conformation of molecules arising from the energy, which is released by hydrolysis of Adenosine Triphosphate (ATP). In this theory, the Davydov's Hamiltonian and wave function of the systems are simultaneously improved and extended. A new interaction has been added into the original Hamiltonian. The original wave functions of the excitation state of single particles have been replaced by a new wave function of two-quanta quasicohherent state. In such a case, bio-energy is carried and transported by the new soliton along protein molecular chains. The soliton is formed through self - trapping of two excitons interacting amino acid residues. The exciton is generated by vibrations of amide - I (C = O stretching) arising from the energy of hydrolysis of ATP. The properties of the soliton are extensively studied by analytical method and its lifetime for a wide ranges of parameter values relevant to protein molecules is calculated using the nonlinear quantum perturbation theory. The lifetime of the new soliton at the biological temperature 300K is enough large and belongs to the order of  $10^{-10}$  second or  $\tau/T_0 \geq 700$ . The different properties of the new soliton are further studied. The results show that the new soliton in the new model is a better carrier of bio - energy transport and it can play an important role in biological processes. This model is a candidate of the bio-energy transport mechanism in protein molecules.

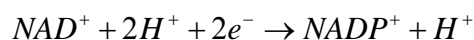
**Keywords:** Form; Living system; Bio – energy; Protein; Biological energy; Soliton; ATP hydrolysis; Amide; Exciton; Life time; Amino acid; Quasi - coherent state

## The Phosphorylation and De - Phosphorylation Reactions in the cell and the features of energy released in hydrolysis of ATP molecules

As it is known, Kal'kar first proposed the idea of aerobic phosphorylation, which is carried out by the phosphorylation coupled to the respiration. Belitser studied in detail the stoichiometric ratios between the conjugated bound phosphate and the absorption of oxygen and gave further the ratio of the number of inorganic phosphate molecules to the number of oxygen atoms absorbed during the respiration, which is not less than two. He thought also that the transfer of electrons from the substrate to the oxygen is a possible source of energy for the formation of two or more ATP molecules per atom of absorbed oxygen. Therefore Belitser and Kal'kar's research results are foundations establishing modern theory of oxidative phosphorylation of ATP molecules in the cell [1-3]. In such a case we must know clearly the mechanism and properties of the oxidation process, which involves the transfer of hydrogen atoms from the oxidised molecule to another molecule, in while there are always protons present in water and in the aqueous medium of the cell, thus we may only consider the transfer of electrons in this process. The necessary number of protons to form hydrogen atoms is taken from the aqueous medium. The oxidation reaction is usually proceeded inside the cell under the action of special enzymes, in which two electrons are transferred from the food substance to some kind of initial acceptor, another enzymes transfer them further along the electron transfer chain to the second acceptor etc. Thus a water molecule is formed in which each oxygen atom requires two electrons and two protons. The main initial acceptors of electrons in cells are the oxidised forms  $NAD^+$  and  $NADP^+$  of NAD (nicotine amide adenine dinucleotide or pyridine nucleotide with two phosphate groups) molecules and NADP (nicotine amide adenine nucleotide phosphate or pyridine nucleotide with three phosphate groups) as well as FAD (flavin adenine dinucleotide or flavoquinone) and FMN (flavin mononucleotide). The above oxidised forms of these molecules serve for primary acceptors of electrons and hydrogen atoms through attaching two hydrogen atoms [3], which is expressed by

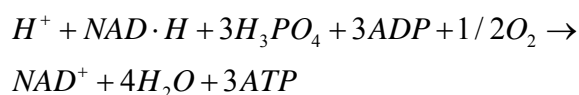


Where,  $NADP^+$  molecule becomes the reduced molecule  $NADP \cdot H$ . The  $NAD^+$  molecule has also the same active center as the  $NADP^+$  molecule; it can be converted to the reduced molecule  $NAD \cdot H$  under combining with two atoms of hydrogen according to the reaction [3]:

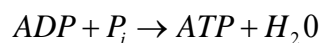


The  $NAD^+$  and  $NADP^+$  are the enzymes, which can perform the reaction of dehydrogenation on compounds containing the group of atoms through removing two hydrogen atoms.

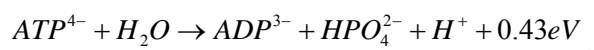
In the presence of enzymes, such as pyridine-dependent hydrogenases and with the participation  $NAD^+$  and  $NADP^+$  molecules two hydrogen atoms, including two protons and two electrons, are removed from this group of atoms. One proton and two electrons combine with the  $NAD^+$  or  $NADP^+$  molecule converting them to the reduced forms  $NADP \cdot H$  or  $NAD \cdot H$  and the second proton is released. This mechanism can be also used to oxidise lactic acid (lactate) with the formation of pyruvic acid (pyruvate) and  $NAD \cdot H$ , in which the reduced molecules  $NADP \cdot H$  and  $NAD \cdot H$  serve as electron donors (reducing agents) in other reactions. They are involved in a large number of biosynthetic processes, such as in the synthesis of fatty acids and cholesterol. Therefore, the molecule  $NAD \cdot H$  can serve as an electron donor in the process of oxidative phosphorylation, then the phosphorylation reaction is of [3]



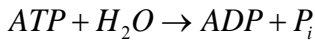
Where, ADP is called the adenosine diphosphate. The abbreviated form of this reaction can be written as



Thus three ATP molecules are formed in the reaction, in which the synthesis of ATP molecule are carried out through the transfer of two electrons from the  $NAD \cdot H$  molecule along the electron transport chain to the oxygen molecule in the mitochondria. In this way the energy of each electron is reduced by 1.14 eV. The reaction is called the phosphorylation of ADP molecules. However, an ATP molecule can reacts with water in an aqueous medium, which results in the energy release of about 0.43eV under normal physiological conditions by virtue of some special enzymes. The reaction can be represented by



Its abbreviated form is of



In this process ATP molecules are transformed as ADP molecules and the bio-energy of about 0.43eV is also released. Then it is referred to as de-phosphorylation reaction of ATP molecules. We know from the above representations that an increase in free energy  $\Delta G$  in reaction and its decrease in reaction depend on their temperatures, concentrations of the ions  $Mg^{2+}$  and  $Ca^{2+}$  and on the pH value of the medium. Under the standard conditions  $\Delta G_0 = 0.32 \text{ eV}$  ( $\sim 7.3 \text{ kcal/mole}$ ). If the appropriate corrections are made taking into consideration the physiological pH values and the concentration of  $Mg^{2+}$  and  $Ca^{2+}$  inside the cell as well as the normal values for the concentrations of ATP and ADP molecules and inorganic phosphate in the cytoplasm we can obtain a value of  $\sim 0.54 \text{ eV}$  ( $\sim 12.5 \text{ kcal/mole}$ ) for the free energy in the hydrolysis of ATP molecule. Hence the free energy for the hydrolysis of ATP molecules is not constant. But it is impossible the same at different sites of the same cell if these sites have different concentrations of ATP, ADP,  $P_i$ ,  $Mg^{2+}$  and  $Ca^{2+}$ .

On the other hand, cells contain a number of phosphorylated compounds the hydrolysis of which in the cytoplasm is associated with the release of free energy. Then the values for the standard free energy of hydrolysis for some of these compounds are also different. The enzymes carrying out the above synthesis of ATP molecules from ADP molecules and inorganic phosphate in the coupling membranes of mitochondria are the same as in the cytoplasmic membranes of bacteria, which are mainly composed of  $F^1$  and  $F^0$ , which are joined to each other by the small proteins  $F_5$  and  $F_6$ . These proteins form the  $F^1$ -  $F^0$  complex or the enzyme ATP - ase, in which  $F^1$  is composed of five protein subunits and has the shape of a sphere with a diameter of about 9nm which projects above the surface of the membrane in the form of a protuberance. In the coupling membrane of mitochondria and the cytoplasmic membrane of bacteria the complex  $F^1$ -  $F^0$  is positioned so that the enzyme  $F^1$  is on the inside of the membrane [1-3]. The enzyme  $F^0$  can extend from one side of the membrane to the other and has a channel which lets protons through. When two protons pass through the complex  $F^1$  -  $F^0$  in the coupling mitochondrial membrane one ATP molecule is synthesized inside the matrix from an ADP molecule and inorganic phosphate. This reaction is reversible. Under certain condition the enzyme transports protons from the matrix to the outside using the energy of dissociation of ATP molecules, which may be observed in a solution containing isolated molecules of enzyme  $F^1$  and ATP. The largest two proteins in  $F^1$ , which is composed of five protein molecules, take part in the synthesis and dissociation of ATP molecules, the other three are apparently inhibitors controlling these reactions. After removing enzyme  $F^1$  molecules from mitochondria the remaining  $F^0$  enzymes increase greatly the permeability of protons in the coupling membranes, which confirms that the enzyme  $F^0$  has really a channel for the passage of protons which is constructed by the enzyme  $F^1$ . However, the complete mechanism for the synthesis of ATP molecules by the enzyme ATP - ase is still not clearly known up to now.

### The Physical and Biological Foundations of Construction of New Theory

As it is known, many biological processes, such as muscle contraction, DNA reduplication, neuroelectric pulse transfer on the neurolemma and work of calcium pump and sodium pump, and so on, are associated with bioenergy transport through protein molecules, where the energy is released by the hydrolysis of Adenosine

Triphosphate (ATP) in the living systems. Thus there here are always a biological process of energy transport from production place to absorption place in the living systems. In general, the bioenergy transport is carried out by virtue of protein molecules. Therefore, the study of the bioenergy transport along protein molecules is a very interesting subject in biology and has important significance in life science. However, understanding the mechanism of bioenergy transport in biomacromolecular systems has been a long-standing problem that remains of great interest today. As an alternative to electronic mechanisms [1], one can assume that the energy is stored as vibrational energy in the  $C = 0$  stretching mode (amide-I) of a protein molecular chain of polypeptide. Following Davydov's idea [2], one takes into account the coupling between the amide-I vibrational quantum (exciton) and the acoustic phonon (molecular displacements) in the amino acid residues; Through the coupling, nonlinear interaction appears in the motion of the vibrational quanta, which could lead to a self-trapped state of the vibrational quantum. The latter plus the deformational amino acid lattice together can travel over macroscopic distances along the molecular chains, retaining the wave shape, energy, momentum and other properties of the quasiparticle. In this way, the bioenergy can be transported as a localized "wave packet" or soliton. This is just the Davydov's model of bioenergy transport in proteins, which was proposed in the 1970s [2,3]. Davydov model of bioenergy transport work at  $\alpha$  - helical proteins as shown in figure 1.

Following Davydov idea [3], the Hamiltonian describing such system has in the form of

$$H_D = \sum_n \left[ \epsilon_0 B_n^+ B_n - J (B_n^+ B_{n-1} + B_n B_{n+1}^+) \right] + \sum_n \left[ \frac{P_n^2}{2M} + \frac{1}{2} w (u_n - u_{n-1})^2 \right] + \sum_n \left[ \chi_1 (u_{n+1} - u_{n-1}) B_n^+ B_n \right] = H_{ex} + H_{ph} + H_{int}$$

where  $\epsilon_0 = 0.205 \text{ eV}$  is the amide-I quantum energy,  $-J$  is the dipole-dipole interaction energy between neighbouring sites,  $B_n^+$  ( $B_n$ ) is the creation (annihilation) operator for an amide - I quantum excitation (exciton) in the site  $n$ ,  $u_n$  is the displacement operator of amino acid residues at site  $n$ ,  $P_n$  is its conjugate momentum operator,  $M$  is the mass of an amino acid molecule,  $w$  is the elasticity constant of the protein molecular chains, and  $\chi_1$  is a nonlinear coupling parameter and represents the coupling size of the exciton-phonon interaction. The wave function of the systems proposed by Davydov is in the form of

$$|D_2(t)\rangle = |\varphi_D(t)\rangle |\beta(t)\rangle = \sum_n \phi_n(t) B_n^+ \exp\left(-\frac{i}{\hbar} \sum_n [\beta_n(t) P_n - \pi_n(t) u_n]\right) |I_0\rangle \quad (2)$$

(Or)

$$|D_1(t)\rangle = \sum_n \left\{ \phi_n(t) B_n^+ \exp\left(\sum_q [\alpha_{nq}(t) a_q^+ - \alpha_{nq}^*(t) a_n]\right) \right\} |I_0\rangle \quad (3)$$

where  $|I_0\rangle = |I_0\rangle_{ex} |I_0\rangle_{ph}$ ,  $|I_0\rangle_{ex}$  and  $|I_0\rangle_{ph}$  are the ground states of the exciton and phonon, respectively,  $a_q$  ( $a_q^+$ ) is

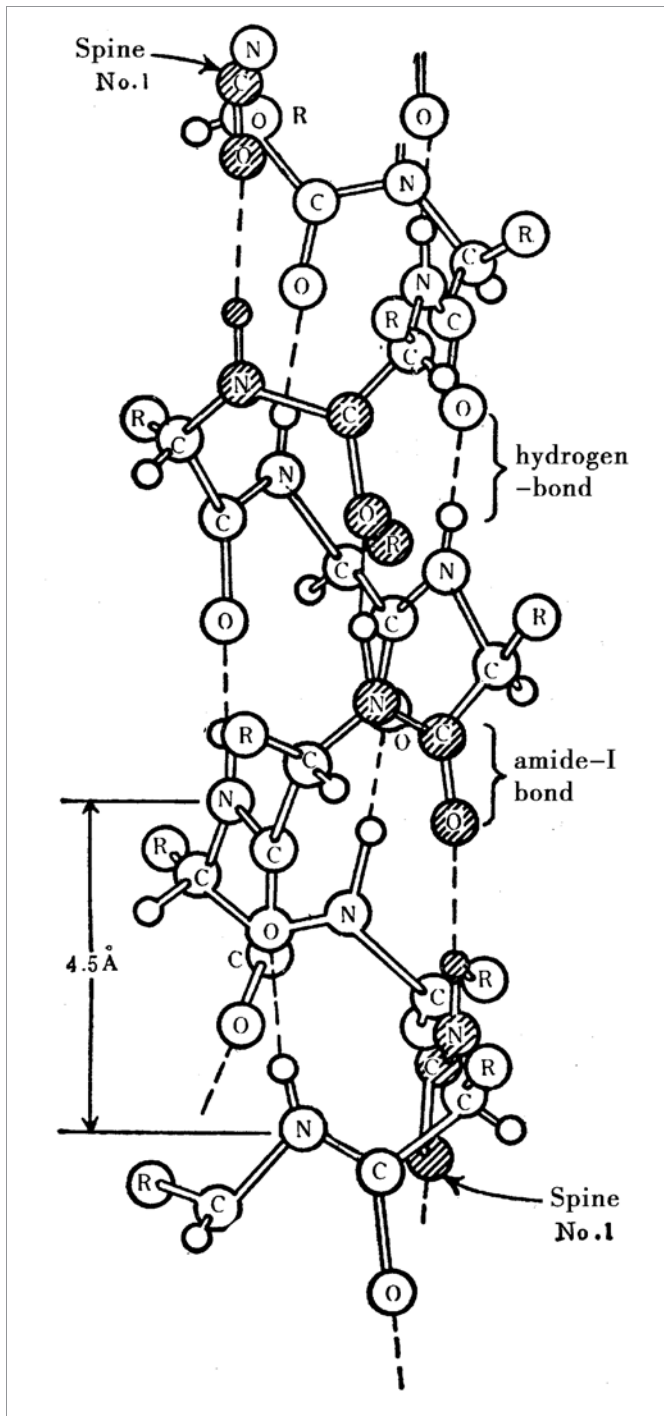


Figure 1: Structure of  $\alpha$ -helical protein.

annihilation (creation) operator of the phonon with wave vector  $q$ ,  $\phi_n(t)$  and  $\beta_n(t) \ll \Phi |u_n| \Phi$  and  $\pi_n(t) \ll |\Phi| P_n |\Phi$  and  $\alpha_q(t) \ll D_1(t) |a_q| D_1(t)$  are some undetermined functions of time. Obviously,  $|\phi_D(t)\rangle = \sum_n \phi_n(t) B_n^+ |0\rangle_{ex}$  in Eq.(2) is an eigenstate of the number operator,  $\hat{N} = \sum_n B_n^+ B_n$ , corresponding to

a single excitation, i.e.,  $\hat{N} |\phi_D(t)\rangle = |\phi_D(t)\rangle$ . The Davydov soliton obtained from Eqs. (1) - (2) in the semiclassical limit and using the continuum approximation has the form

$$\phi_D(x,t) = \left(\frac{\mu_D}{2}\right)^{1/2} \text{sech}\left[\frac{\mu_D}{r_0}(x-x_0-vt)\right] \exp\left\{i\left[\frac{\hbar v}{2Jr_0^2}(x-x_0) - E_v t/\hbar\right]\right\} \quad (4)$$

Corresponding to an excitation localized over a scale  $r_0/\mu_D$ , where

$$\mu_D = \frac{\chi_1^2}{(1-s^2)wJ}, \quad G_D = 4J\mu_D, \\ s^2 = \frac{v^2}{v_0^2}, \quad v_0 = r_0(w/M)^{1/2}$$

Is the sound speed in the protein molecular chains,  $v$  is the velocity of the soliton,  $r_0$  is the lattice constant. Evidently, the soliton contains only one exciton, i.e.,  $N = \langle \phi_D(t) | \hat{N} | \phi_D(t) \rangle = 1$ . This shows that the Davydov soliton is formed through self-trapping of one exciton with binding energy  $E_{BD}$ ,  $E_{BD} = \frac{-\chi_1^4}{3Jw^2}$ .

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 [3-28]. 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 extensively been studied by many scientists [7-26]. However, considerable controversy has arisen concerning whether the Davydov soliton is sufficiently stable in the region of biological temperature to provide a viable explanation for bio-energy transport. 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 [7-11,24-26]. Other simulations showed that the Davydov soliton is stable at 300K [10-24], but they were based on classical equations of motion which are likely to yield unreliable estimates for the stability of the soliton [3]. The simulations based on the  $ID_2$  state in Eq. (2) 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 Schrodinger 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. (3) with the thermal treatment of Davydov [3], where the equations of motion are derived from a thermally averaged Hamiltonian, yields the confusing 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 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, any exact fully quantum-mechanical treatment for the numerical simulation of the Davydov soliton does not exist. However, for the thermal equilibrium properties of the Davydov soliton, there is a quantum Monte Carlo simulation [13]. In the simulation, correlation characteristic of solitonlike quasiparticles occur only at low temperatures, about  $T < 10\text{k}$ , for widely accepted parameter values. This is consistent at a qualitative level with the result of Cottingham et al. [15,21]. 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 indicates clearly that the Davydov solution is not a true wave function of the systems. A thorough 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 [10-12]. 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 approximation. 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 [4,5]. 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 thought that the soliton with a multiquantum ( $n \geq 2$ ), for example, the coherent state of Brown et al. [4], the multiquantum state of Kerr et al. [12] and Schweitzer et al. [15,21], the two-quantum state of Cruzeiro-Hansson [18] and Forner [22], 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. 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. The assumption of a multiquantum state ( $n > 2$ ) 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. On the other hand, the numerical result shows that the soliton of two-quantum state is more stable than that with a one-quantum state. Cruzeiro - Hansson [18] 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 [18]:

$$|\phi(t)\rangle = \sum_{n,m=1}^N \varphi_{nm}(\{u_1\}, \{P_1\}, t) B_n^+ B_m^+ |0\rangle_{ex} \quad (5)$$

Where,  $B_n(B_n^+)$  is the annihilation (creation) operator for an amide - I vibration quantum (exciton),  $u_1$  is the displacement of the lattice molecules,  $P_1$  is its conjugate momentum, and  $|0\rangle_{ex}$  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  $\ln\beta(\beta = 1 / K_B T)$  in the so-called two-quantum state. Eq. (5), where  $\chi_1$  is a nonlinear coupling parameter related to the interaction of the exciton-phonon in the Davydov model. Their energies and stability are compared with those 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 that 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. (5), we can find that the Cruzeiro-Hansson wave function [18,24-26] does not represent exactly the two-quantum state. To find out how many quanta the state Eq.(1), indeed contains, the expectation value of the exciton number operator has to be computed.  $N = \sum_n B_n^+ B_n$ , in this state Eq.(5), and sum over the sites, i.e., the exciton numbers N are

$$\begin{aligned} N &= \langle \phi | \sum_n B_n^+ B_n | \phi \rangle = \\ &= \sum_{ijklmn} \varphi_{im}^* \varphi_{jl} \langle 0 | B_i B_m B_n^+ B_n B_j^+ B_l^+ | 0 \rangle_{ex} \\ &= \sum_{nj} (\varphi_{nj}^* \varphi_{jn} + \varphi_{jn}^* \varphi_{jn}) + \sum_{nl} (\varphi_{nl}^* \varphi_{nl} + \varphi_{ln}^* \varphi_{nl}) = 4 \end{aligned} \quad (6)$$

Where, we use the relations

$$[B_n, B_j^+] = \sigma_{nj}, \sum_{nl} |\varphi_{nl}|^2 = 1 \quad (7)$$

$$\begin{aligned} \langle 0 | B_n^+ | 0 \rangle_{ex} &= \langle 0 | B_n^+ B_n | 0 \rangle_{ex} \\ &= \langle 0 | B_n^+ B_n B_1 | 0 \rangle_{ex} = \dots = 0 \end{aligned} \quad (8)$$

Therefore, the state Eq. (5), as it is put forward in Ref.[10], deals with four excitons (quanta), instead of two excitons, in contradiction to the author's statements. Obviously, it is impossible 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 to protein molecules, and his discussion and conclusion are all unreliable and implausible in that paper [10]. It is believed that the physical significance of the wave function, Eq. (5), is also unclear, or at least is very difficult to understand. As far as the physical meaning of Eq. (5) is concerned, it represents only a combinational state of single-particle excitation with two quanta created at sites  $n$  and  $m$ ;  $\varphi_{nm}(\{u_1\}, \{P_1\}, t)$  [18,26] is the probability amplitude of particles occurring at the sites  $n$  and  $m$  simultaneously. In general,  $n \neq m$  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 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. On the basis of the work of Cruzeiro-Hansson [18], Forner [12,13,22], Schweitzer [21] and Pang [24-26] proposed a new model of the bioenergy transport in the protein molecules, in which both the Hamiltonian and the wave function of the Davydov model [24] have been improved. A new coupling interaction between the acoustic and amide - I vibrational modes was added to the original Davydov's Hamiltonian which takes into account relative displacement of the neighbouring amino acids resulting from dipole - dipole interaction of the neighbouring amide - I vibrational quanta. Davydov's wave function has been also replaced with a quasi-coherent two-quanta state to exhibit the coherent behaviors of collective excitations of the excitons and phonons [25,26] which are a feature of the energy released in ATP hydrolysis in the systems. The equation of motion and the properties of the new soliton in the new model are different from those in the Davydov model and as a result the soliton lifetime and stability are greatly enhanced. It is suggested that this model can resolve the controversy on the thermal stability and lifetime of the soliton excited in the protein molecules. The quantum properties of the new soliton will be studied here, but here attention is paid also to the problem of its lifetime and thermal stability at biological temperature 300K and the lifetime of the new soliton at 300K is calculated in detail by using the generally accepted values of the parameters appropriate to  $\alpha$ -helical protein molecules in terms of the quantum perturbation theory developed by Cottingham et al. [15], which can take simultaneously into account the quantum and thermal effects. It can be seen that the lifetime of the new soliton at 300K is long enough to provide a viable explanation of the bioenergy transport in the proteins. The plan of this paper is as follows. In Section 2, the new model, including the extended Hamiltonian and the wave function, is presented. The equations of motion and the new soliton solution in this model are given in Section 3. In Section 4, the properties and thermal stability of the new soliton are discussed, and the possibility of the soliton being a suitable candidate for the mechanism of bioenergy transport in protein molecules is predicted on the basis of results obtained in this paper. In Section 5, the properties of the new soliton are described and its lifetime is calculated by using quantum-mechanical perturbation method. The detailed discussion of the properties and changes of the lifetimes of the soliton for a large range of parameter values is presented. The conclusions of this investigation are also given in this section.

### Establishment of New theory of Bio - energy Transport in the Protein Molecules

Results obtained by many scientists over the years indicate that the Davydov model, whether it is the wave function or the Hamiltonian, is indeed too simple, i.e., it does not denote the elementary properties of the collective excitations occurring in protein molecules, and many improvements of 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 [24]. 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-bonded

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 [25,26]. Therefore, it is worth studying how we can physically describe these properties. It is noted that Davydov operation is not strictly correct. Therefore, it is believed 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  $|D_1 >$  and  $|D_2 >$ , are concerned [3], 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 [24-26], i.e., the excitonic part in it should also be coherent or quasicohherent to represent the coherent feature of collective excitation in protein molecules. However, the standard coherent [4] and large - n excitation states [12,22] are not appropriate for the protein molecules due to the reasons mentioned above. Similarly, Forner's and Cruzeiro-Hansson's two-quantum states do not fulfill the above request. In view of the above discussion, we proposed the following wave function of the protein molecular systems:

$$\Phi(t) = |\varphi_p(t) > |\beta(t) > = \frac{1}{\lambda} \left[ I + \sum_n \varphi_n(t) B_n^+ + \frac{1}{2!} \left( \sum_n \varphi_n(t) B_n^+ \right)^2 \right] |0 >_{ex} \times \exp \left( -\frac{i}{\hbar} \sum_n [\beta_n(t) P_n - \pi_n(t) u_n] \right) |0 >_{ph} \quad (9)$$

Where,  $B_n^+$  and  $B_n$  are boson creation and annihilation operators for the exciton,  $|0 >_{ex}$  and  $|0 >_{ph}$  are the ground states of the exciton and phonon, respectively  $u_n$  and  $P_n$  are the displacement and momentum operators of the amino acid residue at site  $n$  respectively. The  $\phi_n(t) \cdot \beta_n(t) = \langle \Phi(t) | u_n | \Phi(t) \rangle$  and  $\pi_n(t) = \langle \Phi(t) | P_n | \Phi(t) \rangle$  are there sets of unknown functions,  $\lambda$  is a normalization constant. It is assumed hereafter that  $\lambda = 1$  for convenience of calculation, except when explicitly mentioned. A second problem arises for the Davydov Hamiltonian [24-26,28]. The Davydov Hamiltonian takes into account the resonant or dipole-dipole interaction of the neighboring amide - I vibrational quanta in neighboring amino acid residues with an electrical moment of about 3.5D, but why do we not consider the changes of relative displacement of the neighboring amino acid residues arising from this interaction? It is reasonable to add the new interaction term  $\chi_2 (u_{n+1} - u_n) (B_{n+1}^+ B_n + B_m^+ B_{n+1})$

into the Davydov's Hamiltonian to represent correlations of the collective excitations and collective motions in the protein molecules, as mentioned above [24-26]. Although the dipole-dipole interaction is small as compared with the energy of the amide-I vibrational quantum, the change of relative 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 matter and bio-self-organization. Thus, the Davydov Hamiltonian is replaced by

$$H = H_{ex} + H_{ph} + H_{int} = \sum_n \left[ \varepsilon_0 B_n^+ B_n - J (B_n^+ B_{n+1} + B_n B_{n+1}^+) \right] + \sum_n \left[ \frac{P_n^2}{2M} + \frac{1}{2} w (u_n - u_{n-1})^2 \right] + \sum_n \left[ \chi_1 (u_{n+1} - u_n) \right] B_n^+ B_n + \chi_2 (u_{n+1} - u_n) \times (B_{n+1}^+ B_n + B_n^+ B_{n+1}) \quad (10)$$

Where  $\varepsilon_0 = 0.205\text{eV}$  is the energy of the exciton (the  $C=O$  stretching mode). The present nonlinear coupling constants are  $X_1$  and  $X_2$ . 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 Eqs.(6) are the same as those in the above explanations. The Hamiltonian and wave function shown in Eqs.(9)-(10) are different from Davydov's. We add a new interaction term,  $\sum_n \chi_2 (u_{n+1} - u_n) (B_{n+1}^+ B_n + B_n^+ B_{n+1})$ ,

into the original Davydov Hamiltonian. Thus the Hamiltonian now has better correspondence between the interactions and can also 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 Pang [24-26] and others [27-28] 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. (9,10). Evidently, the present wave function of the exciton in Eq. (9) is not an excitation state of a single particle, but rather a coherent state, more precisely, a quasicohent state, because it retain only fore three terms of the expansion of a standard coherent state, which can be viewed as an effective truncation of a standard coherent state. When  $\varphi_n(t)$  is small, i.e.,  $|\varphi_n(t)| \ll 1$ , Pang represented the wave function of the excitons,  $|\varphi_p(t)\rangle$ , in Eq.(9) as

$$|\varphi_p(t)\rangle \approx \frac{1}{\lambda} \left[ 1 + \sum_n \varphi_n(t) B_n^+ + \frac{1}{2!} \left( \sum_n \varphi_n(t) B_n^+ \right)^2 \right] |0\rangle_{ex} \sim \frac{1}{\lambda} \exp\left[-\frac{1}{2} \sum_n |\varphi_n(t)|^2\right] \times \exp\left\{ \sum_n \varphi_n(t) B_n^+ \right\} \quad (11)$$

$$|0\rangle_{ex} = \frac{1}{\lambda} \exp\left\{ \sum_n [\varphi_n(t) B_n^+ - \varphi_n^*(t) B_n] \right\} |0\rangle_{ex}$$

The last representation in Eq. (11) is a standard coherent state. Therefore, the state of exciton denoted by the new wave function  $|\varphi(t)\rangle$  has a coherent feature. Thus the wave function in Eq. (11) is normalized at  $\lambda = 1$ . Since  $\sum_n |\varphi_n(t)|^2 = 1$  is required in the calculation, then this condition of  $|\varphi_n(t)| \ll 1$  is naturally satisfied for the proteins consisting of several hundreds of amino acids. Just so, the wave function denoted in Eq.(9) represents exactly the coherent features of collective excitations of both the excitons and phonons caused by the nonlinear exciton - phonon interaction, this indicates that the wave function in Eq.(9) is justified for the proteins. However, it is not an eigenstate of the number operator,  $\hat{N} = \sum_n B_n^+ B_n$ , because of

$$\hat{N}|\varphi_p\rangle = \sum_n B_n^+ B_n |\varphi_p\rangle = \left\{ \sum_n \varphi_n(t) B_n^+ + \left( \sum_n \varphi_n(t) B_n^+ \right)^2 \right\} |0\rangle_{ex} = 2|\varphi_p\rangle - \left( 2 + \sum_n \varphi_n(t) B_n^+ \right) |0\rangle_{ex} \quad (12)$$

Therefore, the  $|\varphi_p\rangle$  represents a coherent superposition of the excitonic state with two quanta and the ground state of the exciton, but it has a determinate number of quanta. From the expectation value of number operator  $\hat{N}$  we find that this state contains the number of exciton is

$$N = \langle \varphi_p | \hat{N} | \varphi_p \rangle = \sum_n \langle \varphi_p | B_n^+ B_n | \varphi_p \rangle = \left\{ \sum_n |\varphi_n(t)|^2 + \left( \sum_n |\varphi_n(t)|^2 \right) \left( \sum_m |\varphi_m(t)|^2 \right) \right\} = \left( \sum_n |\varphi_n(t)|^2 \right) \left( 1 + \sum_m |\varphi_m(t)|^2 \right) = 2 \quad (13)$$

Namely, it contains only two quanta. Where we utilize Eq. (8) and the following relation [24] is:

$$\sum_n |\varphi_n(t)|^2 = 1, \sum_m |\varphi_m(t)|^2 = 1, [B_n, B_m^+] = \delta_{nm} \quad (14)$$

$$\begin{aligned} &_{ex} \langle 0 | B_n^+ | 0 \rangle_{ex} = {}_{ex} \langle 0 | B_n^+ B_n | 0 \rangle_{ex} = {}_{ex} \langle 0 | B_n^+ B_m | 0 \rangle_{ex} \\ &= {}_{ex} \langle 0 | B_n^+ B_m B_l | 0 \rangle_{ex} = {}_{ex} \langle 0 | B_n^+ B_m B_l^+ B_n | 0 \rangle_{ex} \\ &= {}_{ex} \langle 0 | B_n^+ B_m B_l^+ B_l B_j | 0 \rangle_{ex} \\ &= {}_{ex} \langle 0 | B_n^+ B_m B_l^+ B_l B_j B_n | 0 \rangle_{ex} \dots = 0 \end{aligned}$$

Therefore, the new wave function is 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, but the former is not. The new state is a quasicohent state. It contains only two excitons, which come from the second and third terms in Eq. (9), in which each term contributes only an exciton, but it is not an excitation state of two single parties. Hence, as far as the form of new wave function in Eq. (9) is concerned, it is either two - quanta states proposed by Forner [21] and Cruzeiro-Hansson [10,18] or a standard coherent state proposed by Brown et al. [4,2] and Kerr et al's [13] and Schweitzer et al's [15,21] multiquanta states. Therefore, the wave function, Eq. (9), is new for the protein molecular systems. It not only exhibits the coherent feature of the collective excitation of excitons and phonons caused by the nonlinear interaction generated by the exciton-phonon interaction, which, thus, also makes the wave

function of the states of the system symmetrical, but it 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 which, thus, can also make the numbers of excitons maintain conservation in the Hamiltonian, Eq. (10). 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. (9) and (10), but the wave function of the states of the system in other models could not, including the one-quanta state [3] and the two-quanta state [12,22]. Therefore, the above Hamiltonian and wave function, Eqs. (9) and (10), are reasonable and appropriate to the protein molecules.

**The Dynamic Equation of Bio - energy Transport**

We now derive the equations of motion from Pang’s model. First of all, we give the interpretation of  $\beta_n(t)$  and  $\pi_n(t)$  in Eq. (9). We know that the phonon part of the new wave function in Eq. (9) depending on the displacement and momentum operators is a coherent state of the normal model of creation and annihilation operators. A coherent state for the mode with wave vector  $Q$  is [3,12,24-26]

$$|\alpha(t)\rangle = \exp\left(\sum_q [\alpha_q(t)a_q^+ - \alpha_q^*(t)a_q]\right) |0\rangle_{ph} \quad (15)$$

Utilizing the standard transformations

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

$$P_n = i \sum_q \left[ \frac{M\hbar\omega_q}{2N} \right]^{1/2} e^{iqnr_0} (a_{-q}^+ - a_q) \quad (16)$$

We can get [12,23]  $|\alpha(t)\rangle = |\beta(t)\rangle$ , where  $|\beta(t)\rangle$  is in Eq. (9),

and  $\omega_q = 2(w/M)^{1/2} \sin(r_0q/2)$ ,  $r_0$  is the distance between neighboring amino acid molecules, and  $a_q$  ( $a_q^+$ ) is the annihilation (creation) operator of the phonon with wave vector  $Q$ , where

$$\langle \alpha(t) | a_q | \alpha(t) \rangle = a_q(t)$$

$$= \left( \frac{M\omega_q}{2\hbar} \right)^{1/2} \beta_q(t) + i \left( \frac{1}{2M\hbar\omega_q} \right)^{1/2} \pi_q(t)$$

$$\beta_q(t) = \frac{1}{\sqrt{N}} \sum_n e^{-iqnr_0} \beta_n(t) \quad \pi_q(t) = \frac{1}{\sqrt{N}} \sum_n e^{-iqnr_0} \pi_n(t)$$

$$\langle \Phi(t) | P_n | \Phi(t) \rangle = \pi_n(t) \quad (17)$$

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  $|\Phi(t)\rangle$ .

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

$$i\hbar \frac{\partial}{\partial t} \langle \Phi(t) | P_n | \Phi(t) \rangle = \langle \Phi(t) | [P_n, H] | \Phi(t) \rangle \quad (18)$$

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

$$M\ddot{\beta}_n(t) = w[\beta_{n+1}(t) - 2\beta_n(t) + \beta_{n-1}(t)]$$

$$+ 2\chi_1 \left[ |\varphi_{n+1}(t)|^2 - |\varphi_{n-1}(t)|^2 \right]_+$$

$$2\chi_2 \left\{ \phi_n^*(t) [\phi_{n+1}(t) - \phi_{n-1}(t)] \right.$$

$$\left. + \varphi_n(t) [\varphi_{n+1}^*(t) - \varphi_{n-1}^*(t)] \right\} \quad (19)$$

From Eq. (19) 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.

We now derive the equation of motion for the  $\varphi_n$ . A basic assumption in the derivation is that  $|\Phi(t)\rangle$  in Eq. (9) is a solution of the time-dependent Shrodinger equation [24-26]:

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = H |\Phi(t)\rangle \quad (20)$$

The left-hand side of Eq. (16) has [12,23]

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

$$\left\{ i\hbar \left( \sum_n \dot{\phi}_n(t) B_n^+ + \sum_n \dot{\phi}_n(t) \phi_n(t) B_n^+ B_n^+ |0\rangle_{ex} \right) \right\} |\beta(t)\rangle$$

$$+ |\varphi_p(t)\rangle \left\{ \sum_n \left[ \frac{\beta_n(t) P_n - \pi_n(t) u_n +}{2} \left[ \beta_n(t) \dot{\pi}_n(t) - \dot{\beta}_n(t) \pi_n(t) \right] \right] \right\} |\beta(t)\rangle \quad (21)$$

Now left-multiplying the both sides of Eq. (21) by  $\langle \Phi(t) |$ , the left-hand side of Eq. (21) can be

$$i\hbar \langle \Phi(t) | u_n | \Phi(t) \rangle =$$

$$i\hbar \sum_n \varphi_n^*(t) \varphi_n(t) \left( \sum_m \varphi_m^*(t) \varphi_m(t) + I \right)$$

$$= \frac{5}{4} \sum_n \left[ \dot{\beta}_n(t) \pi_n(t) - \dot{\pi}_n(t) \beta_n(t) \right] \sum_n |\varphi_n(t)|^2 \quad (22)$$

Similarly, for the right-hand side of Eq. (20) we can have [12,23]

$$\langle \Phi(t) | (H_{ex} + H_{ph} + H_{int}) | \Phi(t) \rangle =$$

$$\left\{ \sum_n \left[ \varepsilon_0 |\varphi_n(t)|^2 - J \varphi_n^*(t) [\varphi_{n+1}(t) - \varphi_{n-1}(t)] \right] \right\}$$



$$\begin{aligned} & \times \left( 1 + \sum_m |\varphi_m(t)|^2 \right) \\ & + \left\{ \sum_n \left[ \chi_1 [\beta_{n+1}(t) - \beta_{n-1}(t)] \varphi_n(t) \right]^2 + \chi_2 [\beta_{n+1}(t) - \beta_{n-1}(t)] \right. \\ & \left. \times \varphi_n^*(t) [\varphi_{n+1}(t) - \varphi_{n-1}(t)] \right\} \left( 1 + \sum_m |\varphi_m(t)|^2 \right) \\ & + \frac{5}{2} W(t) \sum_n |\varphi_n(t)|^2 \end{aligned} \quad (23)$$

Where,

$$W(t) = \langle \beta(t) | H_{\text{ph}} | \beta(t) \rangle = \sum_n \left( \frac{1}{2M} \pi_n^2(t) + \frac{1}{2} w [\beta_n(t) - \beta_{n-1}(t)]^2 \right) + \sum_q \frac{1}{2} \hbar \omega_q \quad (24)$$

And utilizing Eqs. (8) and (12) - (14) and the relationships can be obtained:

$$\begin{aligned} & \sum_n [\beta_{m+1}(t) - 2\beta_m(t) + \beta_{m-1}(t)] \beta_m(t) = \\ & - \sum_n [\beta_{m+1}(t) - \beta_{m-1}(t)]^2, \\ & \left\langle \Phi(t) \left| \sum_n (B_n^+ B_{n-1} + B_n B_{n-1}^+) \right| \Phi(t) \right\rangle = \\ & \sum_n [\phi_n^*(t) \phi_{n+1}(t) + \phi_{n-1}^*(t) \phi(t)] \left( 1 + \sum_m |\phi_m(t)|^2 \right), \\ & \left\langle \Phi(t) \left| \sum_n (u_{n+1} - u_{n-1}) (B_n^+ B_n) \right| \Phi(t) \right\rangle \\ & = \sum_n \left\{ [\beta_{m+1}(t) - \beta_{m-1}(t)] |\phi_n(t)|^2 \right\} \left( 1 + \sum_m |\phi_m(t)|^2 \right), \\ & \left\langle \Phi(t) \left| \sum_n (u_{n-1} - u_n) (B_n^+ B_{n-1} + B_n B_{n-1}^+) \right| \Phi(t) \right\rangle \\ & = \sum_n \left\{ [\beta_{m+1}(t) - \beta_{m-1}(t)] [\phi_n^*(t) \phi_{n+1}(t) + \phi_{n-1}^*(t) \phi(t)] \right\} \\ & \times \left( 1 + \sum_m |\varphi_m(t)|^2 \right) \end{aligned} \quad (25)$$

From Eqs. (20) - (23) we can obtain

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi_n(t) &= \varepsilon_0 \phi_n(t) - \\ J [\phi_{n+1}(t) + \phi_{n-1}(t)] &+ \chi_1 [\beta_{n+1}(t) + \beta_{n-1}(t)] \phi_n(t) \\ - \chi_2 [\beta_{n+1}(t) + \beta_n(t)] &\times [\varphi_{n+1}(t) + \varphi_{n-1}(t)] \end{aligned}$$

$$+ \frac{5}{2} \left( \frac{W(t) - \frac{1}{2}}{\sum_m [\dot{\beta}_m(t) \pi_m(t) - \dot{\pi}_m(t) \beta(t)]} \right) \phi_n(t) \quad (26)$$

In the continuum approximation we get from Eqs. (19) and (26)

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi(x, t) &= R(t) \phi(x, t) - \\ J r_0^2 \frac{\partial^2}{\partial x^2} \phi(x, t) &- G_p |\phi(x, t)|^2 \phi(x, t) \end{aligned} \quad (27)$$

And

$$\frac{\partial \beta(x, t)}{\partial \xi} = \frac{\partial \beta(x, t)}{\partial x} = - \frac{4(\chi_1 + \chi_2)}{w(1-s^2) r_0} |\phi(x, t)|^2 \quad (28)$$

Here,

$$\xi = x - v_t$$

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

and  $s = v/v_0$ . The soliton solution of Eq. (27) is thus

$$\begin{aligned} \phi(x, t) &= \left( \frac{\mu_p}{2} \right)^{1/2} \sec h \left[ (\mu_p / r_0) (x - x_0 - V_t) \right] \times \\ \exp \left\{ i \left[ \frac{\hbar v}{2J r_0^2} (x - x_0) - E_v \frac{t}{\hbar} \right] \right\} \end{aligned} \quad (29)$$

$$\text{With } \mu_p = \frac{2(\chi_1 + \chi_2)^2}{w(1-s^2)J}, \quad G_p = \frac{8(\chi_1 + \chi_2)^2}{w(1-s^2)} \quad (30)$$

Although forms of the above equations of motion and the corresponding solution, Eqs. (27)- (30), are quite similar to that of the Davydov soliton, the properties of new soliton have very large differences from the latter because the parameter values in the equation of motion and the solution Eqs. (27) and (29), including  $R(t)$ ,  $G_p$ , and  $\mu_p$ , have obvious distinctions from that in the Davydov model. A straightforward result of 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 the amplitude of the new soliton and decrease its width due to an increase of [24-26] when compared with Davydov soliton [3], 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 mode[3-8]. Thus the localized feature of the new soliton is enhanced. Therefore its stability against the quantum fluctuation and thermal perturbations increased considerably as compared with the Davydov soliton.

**The Properties of Carrier of Bio - energy Transport**

The energy of soliton in Pang’s model becomes [24-26]

$$E = \langle \Phi(t) | H | \Phi(t) \rangle = \frac{1}{r_0} \int_{-\infty}^{\infty} 2 \left[ J r_0^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + R |\phi(x,t)|^2 - G_p |\phi(x,t)|^4 \right] dx + \frac{1}{r_0} \int_{-\infty}^{\infty} \frac{1}{2} \left[ M \left( \frac{\partial \beta(x,t)}{\partial t} \right)^2 + w r_0 \left( \frac{\partial \beta(x,t)}{\partial x} \right)^2 \right] dx$$

$$= E_0 + \frac{1}{2} M_{sol} v^2 \tag{31}$$

The rest energy of the new soliton is

$$E_0 = 2(\epsilon_0 - 2J) - \frac{8(x_1 + x_2)^4}{3w^2 J} = E_s^0 - W \tag{32}$$

Where,  $W = [2(x_1 + x_2)^4] / 3w^2 J$  is the energy of deformation of the lattice. The effective mass of the new soliton is

$$M_{sol} = 2m_{ex} + \frac{8(x_1 + x_2)^4 (9s^2 + 2 - 3s^4)}{3w^2 J (1 - s^2)^3 v_0^2} \tag{33}$$

We utilize Eqs. (8) and (12) (14) in the above calculations. In such a case, the binding energy of the new soliton is

$$E_{BP} = \frac{-8(x_1 + x_2)^4}{3Jw^2} \tag{34}$$

$E_{BP}$  Is larger than that of the Davydov soliton. The latter is

$E_{BD} = -x_1^4 / 3Jw^2$ . They have the following relation:

$$E_{BP} = 8E_{BD} \left[ 1 + 4 \left( \frac{x_2}{x_1} \right) + 6 \left( \frac{x_2}{x_1} \right)^2 + 4 \left( \frac{x_2}{x_1} \right)^3 + \left( \frac{x_2}{x_1} \right)^4 \right] \tag{35}$$

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.

$\sum_i \chi_2 (\mathbf{u}_{n+1} - \mathbf{u}_n) (\mathbf{B}_{n+1}^+ \mathbf{B}_n + \mathbf{B}_n^+ \mathbf{B}_{n+1})$ , in the Hamiltonian of the systems, Eq. (10). However, we see from Eq. (35) 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 Pouthier and Spatchek et al [32-35] and Scott [6] again, it is convenient to define another composite parameter [3,24-26] that can

be written as

$$4\pi\alpha_p = (\chi_1 + \chi_2)^2 / 2w\hbar\omega_D \tag{36}$$

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 [2-23],

$$J = 1.55 \times 10^{-22} \text{ J} \quad w = (13 - 19.5) \text{ N/m}.$$

$$M = (1.17 - 1.91) \times 10^{-25} \text{ kg}$$

$$\chi_1 = 62 \times 10^{-12} \text{ N} \quad \chi_2 = (10 - 18) \times 10^{-12} \text{ N}.$$

$$r_0 = 4.5 \times 10^{-10} \text{ m}.$$

$$\tag{37}$$

We can estimate that the coupled constant lies in the region of  $4\pi\alpha_p = 0.11 - 0.273$ , which is not a weakly coupled theory, the coupling strength is enhanced as compared with the Davydov model, the latter is  $4\pi\alpha_D = 0.036 - 0.045$ . Using the notation of Bullough et al. [29,30], Teki et al. [31,32], and Pouthier, et al. [33-35].

$$\gamma = J / 2\hbar w_D \tag{38}$$

In terms of the two composite parameters,  $4\pi\alpha_p$  and  $\gamma$ , the soliton binding energy for Pang’s model can be written by

$$E_{BP} / J = 8(4\pi\alpha_p / \gamma)^2 / 3,$$

$$M_{sol} = 2m_{ex} \left[ 1 + 32(4\pi\alpha_p)^2 / 3 \right] \tag{39}$$

From the above parameter values, we find  $\gamma = 0.08$ . Utilizing this value, the  $E_{BP} / J$  versus  $4\pi\alpha$  relations in Eq. (39) are plotted in figure 1.

$$\text{However, } E_{BP} / J = (4\pi\alpha_p / \gamma)^2 / 3$$

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  $4\pi\alpha$  [24-26].

Also, we see clearly from Eqs. (28) (32) and (35) that the localized feature of the new soliton is enhanced due to increases of the nonlinear interaction and of the binding energy of the new soliton resulting from the increases of exciton-phonon interaction in Pang’s model. Thus, the stability of the soliton against quantum and thermal fluctuations is also enhanced considerably [24-26]. As a matter of fact, the nonlinear interaction energy forming the new soliton 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 linear dispersion energy,  $J = 1.55 \times 10^{-32} J$ , i.e., the nonlinear interaction in Pang's model is so large that it can actually cancel or suppress the linear dispersion effect in the equation of motion, thus the new soliton is stable in such a case according to the soliton theory [2,33-35]. On the other hand, 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 as compared with 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. (31), 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  $\omega_D$  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 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  $\mu_p$  and  $T_0 = \hbar V_0 \mu_p / K_B \pi$  increase at a given temperature) [15] and the above obtained results, an inference could roughly be drawn that the lifetime of the new soliton will increase considerably as compared with that of the Davydov soliton due to the increase of  $\mu_p$  and  $T_0$  because the latter are about three times larger than that of the Davydov model. On the other hand, 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 it indicates

that the Davydov soliton has a very small lifetime, and it is unstable at the biological temperature  $300K$ . This conclusion is consistent at a qualitative level with the results of Wang *et al.* [13,14] and Cottingham *et al.* [15,21]. One can sum up the differences between Pang's model and Davydov's model, Eqs. (1) - (4), as follows. First, the parameter

$\mu_p$  is increased ( $\mu_p = 2\mu_D \left[ 1 + 2\left(\frac{\chi_2}{\chi_1}\right) + \left(\frac{\chi_2}{\chi_1}\right)^2 \right]$ ). Secondly the nonlinear coupling energy becomes  $G_p = \frac{\chi_1 8(\chi_1 + \chi_2)^2}{w(1 - s^2)}$  ( $G_p = 2G_D$ )

$\left[ 1 + 2\left(\frac{\chi_2}{\chi_1}\right) + \left(\frac{\chi_2}{\chi_1}\right)^2 \right]$ , where  $G_D = \frac{4\chi_1^2}{w(1 - s^2)}$  is the nonlinear

interaction in the Davydov model, resulting from the two - quanta nature and the enhancement of the coupling the coefficient ( $\chi_1 + \chi_2$ ). For  $\alpha$ -helical protein molecules, and using the parameter values listed in Eq. (37) the values of the main parameters in Pang's model can be calculated. These values and the corresponding values in the Davydov model are simultaneously listed in table 1. From table 1 we can see clearly that the new model produces considerable changes in the properties of the new soliton, such as large increase of the nonlinear interaction, binding energy and amplitude of the soliton, and decrease of its width as compared to that of the Davydov soliton. This indicates that the soliton in Pang's model is more localized and more robust against quantum and the thermal stability has been enhanced [2,27,28] which implies an increase in lifetime for the new soliton. From Eq. (19) it can also be found 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.

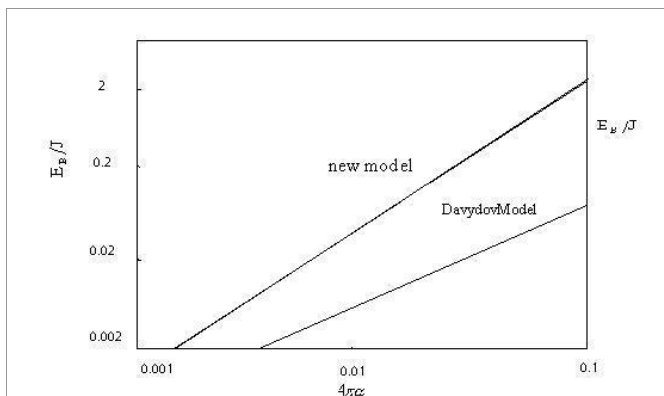
In the above studies, the influences of quantum and thermal effects on soliton state, which are expected to cause the soliton to decay into delocalized states, we postulate that the model Hamiltonian and the wavefunction in Pang's model together give a complete and realistic picture of the interaction 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 fulfil the fact that the energy released by the ATP hydrolysis can only excite two quanta. In such a case, using a standard calculating method [2,26] 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. (29) in its rest frame as

$|\varphi(x)|^2 = \frac{\mu_p}{2} \sec^2 h^2 \left( \frac{\mu_p x}{r_0} \right)$ . 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 the continuous approximation used in the calculation is valid. Therefore we should believe that the above calculated results obtained from Pang's model is correct.



**Figure 2 :** Binding energy ( $E_B$ ) of the solitons in our model and the Davydov model in units of dipole-dipole interaction energy ( $J$ ) vs The coupled constant,  $4\pi\alpha$ , relationship.

**Table 1: Comparison of parameters used in the Davydov model and our new model.**

Parameters Models	$\mu$	G ( $\times 10^{-21}$ J)	Amplitude of soliton A'	Width of soliton $\Delta X$ ( $\times 10^{-10}$ m)	Binding energy of soliton $E_b$ ( $\times 10^{-21}$ J)
Our Model	5.94	3.8	1.72	4.95	- 7.8
Davydov model	1.90	1.18	0.974	14.88	- 0.188

**The lifetime of the carrier of Bio-Energy transport at biological temperature**

**Partially Diagonalized Form of the Model Hamiltonian:** The lifetime of the soliton in the protein molecules is an centre 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. Therefore, to calculate the lifetime of the new soliton in Pang's model has important significance. For convenience of calculation, we here represent the wave function of the system in Eq. (9) by [24-26]

$$|\Phi(t)\rangle = |\varphi(t)\rangle |\beta(t)\rangle = U_1 |10\rangle_{ex} U_2 |10\rangle_{ph}, \tag{40}$$

Where, 
$$U_1 = \frac{1}{\lambda} [1 + \sum_n \varphi_n(t) B_n^+ + \frac{1}{2!} (\sum_n \varphi_n(t) B_n^+)^2], \tag{40a}$$

$$U_2 = \exp\left\{-\frac{i}{\hbar} \sum_n [\beta_n(t) P_n - \pi_n(t) u_n]\right\} \tag{40b}$$

$$= \exp\left\{\frac{1}{\sqrt{N}} \sum_q \alpha_q(t) a_q^+ - \alpha_q^*(t) a_q\right\} \tag{40c}$$

Where, we assume  $\sum_i |\varphi_i|^2 = n$ , where n is an integer, denotes the number of particle. The wave function, Eq.(40), does not only exhibit coherent properties, but also agrees with the fact that the energy released in the ATP hydrolysis (about 0.43eV) excites only two amide-I vibrational quanta, instead of multi-quanta ( $n > 2$ ) [24-26]. Therefore, the Hamiltonian and wave function of the systems, Eqs. (9) - (10), or (40) are reasonable and appropriate to the protein molecules. Using the standard transformation in Eq. (16), where,

$$\omega_q = 2(w/M)^{1/2} \sin\left(\frac{r_0 q}{2}\right), \text{ Eq.(10) becomes}$$

$$H = \sum_n [\varepsilon_0 B_n^+ B_n - J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)] + \sum_q \hbar \omega_q (a_q^+ a_q + \frac{1}{2}) + \frac{1}{\sqrt{N}} \sum_{q,n} [g_1(q) B_n^+ B_n + g_2(q) (B_n^+ B_{n+1} + B_n^+ B_{n+1})] (a_q + a_{-q}^+) e^{i n r_0 q} \tag{41}$$

Where,

$$g_1(q) = 2\chi_1 i \left[\frac{\hbar}{2M\omega_q}\right]^{1/2} \sin r_0 q; \quad g_2(q) = \chi_2 \left[\frac{\hbar}{2M\omega_q}\right]^{1/2} (e^{i r_0 q} - 1) \tag{42}$$

In a semiclassical and continuum approximations, from Eq. (41) we can obtain the envelope soliton solution Eq. (29) in Pang's model, we now represent Eq. (29) by the following form [24-26]

$$\phi(x,t) = \left(\frac{\mu_p}{2}\right)^{1/2} \text{Sech}\left[\frac{\mu_p}{r_0}(x-vt)\right] \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 v x}{2Jr_0^2} - E_{sol} t\right)\right] \tag{43}$$

where 
$$\mu_p = \frac{2(\chi_1 + \chi_2)^2}{w(1-s^2)J} \tag{44}$$

The energy of the new soliton is

$$E_{sol} = 2\left[(\varepsilon_0 - 2J) + \frac{\hbar^2 v^2}{4Jr_0^2} - \frac{2\mu_p^2}{3} J\right] \tag{45}$$

Thus we can also find out that

$$\alpha_q(t) = \frac{i\pi(\chi_1 + \chi_2)}{w\mu_p(1-v^2/v_0^2)} \left[\frac{M}{2\hbar\omega_q}\right]^{1/2} \tag{46}$$

$$(\omega_q + qv) \text{csc} h(\pi q r_0 / 2\mu_p) e^{i q v t} = \alpha_q e^{i q v t}$$

This treatment yields a localized coherent structure of the excitons with size of order  $2\pi r_0/v_p$  that propagates with velocity v and can transfer energy  $E_{sol} < 2\varepsilon_0$ . Unlike bare excitons that are scattered by the interactions with the phonons, 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 the vibration of amino acids (lattices), and can maintain its form, energy, momentum and other quasiparticle properties moving over a macroscopic distance. The bell-shaped form of the soliton Eq. (43) 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 they do not emit phonons, i.e., their kinetic energy is not transformed into thermal energy. This is one important reason for the high stability of the new soliton. In addition the energy of the 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 soliton state to a bare exciton state, i.e, the destruction of the 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 such a soliton is stable enough to propagate through the length of a typical protein structure. However, the thermal stability of the soliton state must be calculated quantitatively. The following calculation addresses this point explicitly [24-26]. We now diagonalize partially the model Hamiltonian in order to calculate the lifetime of the soliton, Eq. (43), using the quantum perturbation method [14]. 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,  $\tilde{H} - vP$ , where P is the total momentum, and  $P = \sum_q \hbar q (a_q^+ a_q - B_q^+ B_q)$ , Where,

$$B_q^+ = \frac{1}{\sqrt{N}} \sum_n e^{i q n r_0} B_n^+. \text{ Also, in order to have simple analytical}$$

expressions we make the usual continuum approximation. This gives

$$\tilde{H} = \int_0^L dx 2 \left[ \left( \varepsilon_0 - 2J \right) \phi^+(x) \phi(x) + Jr_0^2 \frac{\partial \phi^+}{\partial x} \frac{\partial \phi}{\partial x} - \frac{i\hbar v}{2} \left( \frac{\partial \phi^+}{\partial x} \phi(x) - \phi^+(x) \frac{\partial \phi}{\partial x} \right) \right] + \sum_q \hbar(\omega_q - qv) a_q^+ a_q + \frac{1}{\sqrt{N}} \sum_q 2[g_1(q) + 2g_2(q)] (a_{-q}^+ + a_q) \int_0^L dx e^{iqx} \phi^+(x) \phi(x) \quad (47)$$

Where,  $\phi(x)$  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  $\Omega_q \approx (w/M)^{1/2} r_0 |q|$ ,  $x = nr_0$ . Since the soliton excitation is connected with the deformation of intermolecular spacing, it is necessary to pass in Eq. (47) to new phonons taking this deformation into account. Such a transformation can be realized by means of the following transformation of phonon operators [29].

$$b_q = a_p - \frac{1}{\sqrt{N}} \alpha_q, \quad b_q^+ = a_q^+ - \frac{1}{\sqrt{N}} \alpha_q^* \quad (48)$$

Which describe phonons relative to a chain with a particular deformation, where  $b_q$  ( $b_q^+$ ) is the annihilation (creation) operator of new phonon. The vacuum state for the new phonons is

$$|\tilde{0}\rangle_{ph} = \exp \left[ \frac{1}{\sqrt{N}} \sum_q (\alpha_q(t) a_q^+ - \alpha_q^*(t) a_q) \right] |0\rangle_{ph} \quad (49)$$

Which is a coherent phonon state [30], i.e.,  $b_q |\tilde{0}\rangle_{ph} = 0$ . The Hamiltonian  $\tilde{H}$  can now be rewritten [24-26] as

$$\tilde{H} = \int_0^L dx \phi(x) [\varepsilon_0 - 2J + V(x) - Jr_0^2 \frac{\partial^2}{\partial x^2} + i\hbar \frac{\partial}{\partial x}] \phi(x) + \sum_q \hbar(\omega_q - qv) [b_q^+ b_q + \frac{1}{\sqrt{N}} (\alpha_q b_q^+ + \alpha_q^* b_q^+)] + W' + \frac{1}{\sqrt{N}} \sum_q 2[g_1(q) + 2g_2(q)] (b_{-q}^+ + b_q) \int_0^L dx e^{iqx} \phi^+(x) \phi(x) \quad (50)$$

Where,

$$W' = \frac{1}{N} \sum_q \hbar(\omega_q - qv) |\alpha_q|^2, \quad V(x) = \frac{1}{N} \sum_q [g_1(q) + 2g_2(q)] (\alpha_{-q}^* + \alpha_{-q}) e^{iqx} \quad (51)$$

To describe the deformation corresponding to a soliton in the subspace where there is

$$\int_0^L dx \phi^+(x) \phi(x) = 1$$

From Eq (45) in such a case. From the above formulae we can obtain

$$V(x) = -2J\mu_p^2 \sec^2(\mu_p x / r_0) \quad (52)$$

In order to partially diagonalize the Hamiltonian Eq.(50) we introduce the following canonical transformation<sup>[14,23]</sup>

$$\phi(x) = \sum_j A_j C_j(x) \quad \phi^+(x) = \sum_j C_j^*(x) A_j^+ \quad (53)$$

Where,

$$\int C_i^*(x) C_j(x) dx = \delta_{ij}, \quad \sum_j C_j^*(x') C_j(x) = \delta(x-x'), \quad \int dx |C_j(x)|^2 = 1 \quad (54)$$

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. The detailed calculation of the partial diagonalization and of corresponding  $C_s(x)$  and  $C_k(x)$  are described in Appendix A. The partially diagonalized Hamiltonian obtained is as follows

$$\tilde{H} = W' + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - qv) b_q^+ b_q +$$

$$\frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - qv) (b_q^+ \alpha_q + \alpha_q^* b_q) (1 - A_s^+ A_s) + \frac{1}{\sqrt{N}}$$

$$\sum_{kk'q} F(k, k', q) (b_{-q}^+ + b_q) A_k^+ A_k - \frac{1}{\sqrt{N}}$$

$$\sum_{kq} \tilde{F}(k, q) (b_{-q}^+ + b_q) (A_s^+ A_{-k} - A_k^+ A_s)$$

and

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

with

$$E_s = 2 \left[ \varepsilon_0 - 2J - \frac{\hbar^2 v^2}{2Jr_0^2} - \mu_p^2 J \right] \quad (56a)$$

$$C_k(x) = \frac{\mu_p \tanh(\mu_p x / r_0) - ikr_0}{\sqrt{Nr_0} [\mu_p - ikr_0]} \exp[ikx + \frac{i\hbar vx}{2Jr_0^2}], \quad (56b)$$

$$\text{with } E_k = 2 \left[ \varepsilon_0 - 2J - \frac{\hbar^2 v^2}{2Jr_0^2} - J(kr_0)^2 \right]$$

Where,

$$F(k, k', q) = 2[g_1(q) + 2g_2(q)] \int_0^L dx e^{iqx} C_k^*(x) C_k(x) \approx 2[g_1(q) + 2g_2(q)] \left\{ 1 - \frac{i\mu_p q r_0}{[\mu_p + i(k+q)r_0][\mu_p - ikr_0]} \right\} \approx F[k, (k+q), q] \delta_{kk+q} \quad (57)$$

$$\tilde{F}(k, q) = 2[g_1(q) + 2g_2(q)] \int_0^L dx e^{iqx} C_k^*(x) C_s(x) = \frac{2\pi}{\sqrt{2\mu_p}} [g_1(q) + 2g_2(q)] \left\{ \frac{iqr_0}{[\mu_p + ikr_0]} \right\} \sec h[\pi(k-q)r_0 / 2\mu_p] \quad (58)$$

Where,  $\alpha_q$  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.(55). Thus we find

$$\alpha_q = \frac{i\pi(\chi_1 + \chi_2)}{w\mu_p(1-s^2)} \left[ \frac{M}{2\hbar\omega_q} \right]^{1/2} (\omega_q + qv) \text{csc} h(\pi q r_0 / 2\mu_p) \quad (59)$$

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

For this  $\alpha_q$  the  $|\tilde{0}\rangle_{ph}$  in Eq.(49) is just the coherent phonon state introduced by Davydov. However, the bound state  $C_s(x)$  in Eq.(56a), unlike the unbounded state  $C_k(x)$  in Eq.(56b), is self-consistent with the deformation. Such a self-consistent state of the intramolecular excitation and deformation forms a soliton which in the intrinsic reference frame is stationary. For the new soliton described by the state vector  $|\psi\rangle = \frac{1}{\sqrt{2!}} (A_s^+)^2 |0\rangle_{ex} |\tilde{0}\rangle_{ph}$  the average energy of  $\tilde{H}$  in Eq.(55) is

$$\langle \psi | \tilde{H} | \psi \rangle = 2(\epsilon_0 - 2J - \frac{\hbar^2 v^2}{4Jr_0^2}) - \frac{4}{3} J \mu_p^2 \quad (60)$$

Evidently, the average energy of  $\tilde{H}$  in the soliton state  $|\psi\rangle$ , Eq.(60), is just equal to the above soliton energy  $E_{sol}$ , or the sum of the energy of the bound state in Eq.(56a),  $E_s$ , and the deformation energy of the lattice,  $W'$ , i.e.,  $\langle \psi | \tilde{H} | \psi \rangle = E_{sol} = E_s + W'$ . This is an interesting result, which shows clearly that the quasi-coherent soliton formed by this mechanism is just a self-trapping state of the two excitons plus the corresponding deformation of the amino acid lattice. However, it should be noted that  $|\psi\rangle$  is not an exact eigenstate of  $\tilde{H}$  owing to the presence of the terms in  $\tilde{H}$  with  $A_k^+$ ,  $A_s$  and  $A_s^+ A_k$ . BA

**Transition Probability and Decay Rate of the New Soliton:** 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. [14], 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. (55) into  $H_0 + V_1 + V_2$ , where

$$H_0 = W' + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - vq) b_q^+ b_q +$$

$$\frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - vq) (\alpha_q b_q^+ + \alpha_q^* b_q) (1 - A_s^+ A_s) \quad (61)$$

$$V_1 = \frac{1}{\sqrt{N}} \sum_{kkq} F(k, k+q, q) (b_{-q}^+ + b_q) A_k^+ A_k \quad (62)$$

$$V_2 = \frac{1}{N} \sum_{kkq} \tilde{F}(k, q) (b_{-q}^+ + b_q) (A_s^+ A_k - A_s^+ A_{-k}), \quad V = V_1 + V_2 \quad (63)$$

Where,  $H_0$  describes the relevant quasi-particle excitations in the protein. This is a soliton together with phonons relative to the distorted amino acid 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. (61) and  $V_2$  in Eq. (63) 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. (40a) is replaced by (n+1) terms of the expression of a coherent state,  $\exp\left\{\sum_n [\varphi_n(t) B_n^+ - \varphi_n^*(t) B_n]\right\} |0\rangle_{ex}$ .

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,  $|n\rangle$  has energy  $W' + nE'_s$  in the subspace of excitation number equal to n, i.e.,  $\langle n | \sum_i B_i^+ B_i | n \rangle = n \langle (A_s^+ A_s + \sum_k A_k^+ A_k) | n \rangle = n$ . In this subspace the eigenstates have the simple form

$$\tilde{\lambda} |n-m, k_1 k_2 \dots k_m, \{n_q\}\rangle = \frac{1}{\sqrt{(n-m)!}} (A_s^+)^{n-m} A_{k_1}^+ A_{k_2}^+ \dots A_{k_m}^+ |0\rangle_{ex} \prod_q \frac{(d_q^+)^{n_q}}{\sqrt{n_q!}} |\tilde{0}\rangle_{ph}^{n-m} \quad (64)$$

Where,

$$d_q = b_q + \frac{m}{n} \frac{1}{\sqrt{N}} \alpha_q = a_q - \frac{n-m}{n} \frac{1}{\sqrt{N}} \alpha_q \quad (65)$$

( $m \leq n$ , n and m are all integers)

With,  $d_q |\tilde{0}\rangle_{ph}^{n-m} = 0$ . The corresponding energy of the systems is

$$E_{n-m; k_1 \dots k_m; \{n_q\}}^{(0)} = (1 - (m/n)^2) W' + (n-m) E'_s + \sum_{j=1}^m E'_{k_j} + \sum_q \hbar(\omega_q - vq) n_q \quad (66)$$

$E'_s$  is the energy of a bound state with one exciton,  $E'_k$  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:

$$\tilde{\lambda} |n\rangle = \frac{1}{\sqrt{n!}} \prod_q \frac{(b_q^+)^{n_q}}{(n_q!)^{1/2}} (A_s^+)^n |0\rangle_{ex} |\tilde{0}\rangle_{ph} \quad (67)$$

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:

$$\tilde{\lambda} | \alpha k \rangle = \prod_q \frac{(a_q^+)^{n_q}}{\sqrt{n_q!}} |0\rangle_{ph} (A_k^+)^n |0\rangle_{ex} \quad (68)$$

With corresponding energy  $E_k \{n_q\} = E'_k + \sum_q \hbar(\omega_q - \nu q)$   $n_q$  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

$$\bar{W} = \frac{1}{\hbar^2} \int_0^t dt' \int_0^{t'} dt'' \left\{ \sum_{\alpha k'} \sum_l P_l^{(ph)} \langle n | \exp\left(\frac{iH_0 t''}{\hbar}\right) V_2 \exp\left(\frac{-iH_0 t'}{\hbar}\right) | \alpha k' \rangle \right. \quad (6)$$

$$\left. \langle \alpha k' | \exp\left(\frac{iH_0 t'}{\hbar}\right) V_2 \exp\left(\frac{-iH_0 t''}{\hbar}\right) | n \rangle \right\}$$

We should calculate the transition probability of the soliton resulting from the perturbed potential,  $(V_1 + V_2)$ , at first-order in perturbation theory. Following Cottingham and Schweitzer [14] 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. (58) 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 excitations in the weak coupling limit ( $J\mu_p / K_B T_0 \ll 1$ , 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  $V_1$ . The sum over  $l$  in Eq. (69) indicates a sum over an initial set of occupation numbers for phonons relative to the distorted amino acid lattice with probability distribution  $P_l^{(ph)}$ , which is taken to be the thermal equilibrium distribution for a given temperature  $T$ . Since

$$e^{-iH_0 t} | n, \{n_q\} \rangle = \exp\{-i(W' + nE'_q)\}$$

$$t / \hbar - i \sum_q (\omega_q - \nu q) b_q^\dagger b_q t \} | n, \{n_q\} \rangle$$

and

$$e^{iH_0 t} | n-1, \{n'_q\} \rangle = \exp$$

$$\left\{ -i \left[ \left(1 - \frac{1}{n^2}\right) W' + (n-1) E'_s + E'_k \right] \right.$$

$$\left. t / \hbar - i \sum_q (\omega_q - \nu q) d_q^\dagger d_q t \right\} | n-1, \{n'_q\} \rangle$$

Where,  $d_q = b_q + \frac{1}{n} \frac{1}{\sqrt{N}} \alpha_q$ ,

Using the explicit form for  $V_2$  and the fact that the sum over states  $| k', \{n'_q\} \rangle$  contains a complete set of phonons for each values of  $k'$ , one can rewrite  $\bar{W}$  as

$$\bar{W} = \frac{1}{\hbar^2} \frac{\pi^2}{2n\mu_1 N^2} \sum_k \sum_{k'} [g_1^*(k) + 2g_2^*(k)] [g_1(k'') + 2g_2(k'')] \frac{(kr_0)(k'r_0)}{(n\mu_1)^2 + (k'r_0)^2} \text{Sech} \left[ \frac{\pi r_0}{2n\mu_1} (k-k') \right] \cdot \text{sech} \left[ \frac{\pi r_0}{2n\mu_1} (k''-k') \right] \int_0^t dt' \int_0^{t'} dt'' \left\{ \exp \left[ \frac{-i}{\hbar} \left( n(n^2 - \frac{2}{3}n) \mu_1^2 J + nJ(k'r_0)^2 \right) (t'-t'') \right] \right. \quad (70)$$

$$\left. \langle \langle \exp [i \sum_q (\omega_q - \nu q) b_q^\dagger b_q (t'-t'')] (b_k^+ + b_{-k}) \rangle \rangle \exp [i \sum_q (\omega_q - \nu q) a_q^\dagger a_q (t'-t'')] (b_{-k'}^+ + b_{k'}) \rangle \rangle \right\}$$

Where,

$$g_1(k) + 2g_2(k) = 2\chi_1 \left( \frac{\hbar}{2M\omega_k} \right)^{1/2} [A(\cos(r_0 k) - 1) + i(A+1)\sin(r_0 k)] \approx 2i(A+1)(r_0 k) \chi_1 \left( \frac{\hbar}{2M\omega_k} \right)^{1/2},$$

$$\mu_1 = \frac{\chi_1^2(1+A^2)}{\omega(1-s^2)J}, \quad A = \chi_2 / \chi_1 \quad (71)$$

Here,  $A$  is a new parameter introduced to describe the rate between the new nonlinear interaction term and the one in the Davydov's model. To estimate the lifetime of the soliton we are interested in the long-time behavior of  $\frac{d\bar{W}}{dt}$ . By straightforward calculation, the average transition probability or decay rate of the soliton is given by

$$\Gamma_n = \lim_{t \rightarrow \infty} \frac{d\bar{W}}{dt} = \frac{4}{\hbar} \left[ \frac{\pi^2}{2n\mu_1 N^2} \right] \sum_{kk''} [ [g_1^*(k) + 2g_2^*(k)] [g_1(k'') + 2g_2(k'')] \frac{(kr_0)(k'r_0)}{(n\mu_1)^2 + (k'r_0)^2} \cdot \text{sech} \left[ \frac{\pi r_0}{2n\mu_1} (k-k') \right] \cdot \text{sech} \left[ \frac{\pi r_0}{2n\mu_1} (k''-k') \right] \cdot \text{Re} \left\{ \int_0^\infty dt \exp \left[ -\frac{i}{\hbar} \left( n(n^2 - \frac{2}{3}n) \mu_1^2 J + nJ(k'r_0)^2 \right) t \right] \right\} \cdot \langle \langle \exp [i \sum_q (\omega_q - \nu q) b_q^\dagger b_q t] (b_k^+ + b_{-k}) \rangle \rangle \exp [ -i \sum_q (\omega_q - \nu q) a_q^\dagger a_q t ] (b_{-k'}^+ + b_{k'}) \rangle \rangle \left. \right\} \quad (72)$$

Where, the thermal average is

$$U(k, k'', t) = \langle \langle \exp [i \sum_q (\omega_q - \nu q) b_q^\dagger b_q t] (b_k^+ + b_{-k}) \rangle \rangle \exp [ -i \sum_q (\omega_q - \nu q) a_q^\dagger a_q t ] (b_{-k'}^+ + b_{k'}) \rangle \rangle$$

With

$$\langle \langle A \rangle \rangle = \text{Tr} \{ A \exp [ -\beta \sum_q \hbar(\omega_q - \nu q) b_q^\dagger b_q ] / \text{Tr} \{ \exp [ -\beta \sum_q \hbar(\omega_q - \nu q) b_q^\dagger b_q ] \} \} / Z_{ph} \quad (73)$$

and  $Z_{ph} = \prod_q (1 - \exp [ -\beta \hbar(\omega_q - \nu q) ])^{-1}$ ,  $(\beta = \frac{1}{K_B T})$

This rather unusual expression of  $\Gamma_n$  occurs because the phonons in the final state are related to a different deformation. However, the analytical evaluation of  $U(k, k'', t)$  is a critical step in the calculation of the decay rate  $\Gamma_n$ . It is well known that the trace contained in  $U(k, k'', t)$  can be approximately calculated by using the occupation number states of single-particles and coherent state. However the former is both a very tedious calculation, including the

summation of infinite series, and also not rigorous because the state of the excited quasiparticles is coherent in Pang's model. Here we use the coherent state to calculate the  $\mathbf{U}(\mathbf{k}, \mathbf{k}', t)$  as it is described in Appendix B. The decay rate obtained finally is,

$$\Gamma_n = \lim_{t \rightarrow \infty} \frac{d\bar{W}}{dt} = \frac{2}{n\mu_1\hbar^2} \frac{\pi^2}{N^2} \sum_{kk'} \frac{[|g_1(k) + 2g_2(k)|^2 \sec^2 h^2[\pi(k-k')r_0/2n\mu_1] \text{Re} \int_0^\infty dt \cdot \left\{ \exp[-i(nJ(k'r_0)^2 + n(n^2 - \frac{2}{3}n)\mu_1^2 J t / \hbar + R_n(t) + \xi_n(t)] \frac{\exp[i(\omega_k - kv)t]}{\exp[\beta\hbar(\omega_k - kv)] - 1} \right\}]}{(n\mu_1)^2 + (k'r_0)^2} \quad (74)$$

Where,

$$R_n(t) = -\frac{1}{n^2 N} \sum_k |\alpha_k|^2 \{i - \exp[-i(\omega_k - kv)t]\}, \quad (75)$$

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

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. (75) is absorbed, the delocalized excitation produced does not need to have wavevector equal to k. The wavevector here is only approximately conserved by the  $\text{sech}^2[\pi(k-k')r_0/2n\mu_1]$  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 [24-26]. 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 fulfil wavevector conservation, make a major contribution to the transition matrix element, while the contributions of the phonons with small wavevector, which do not fulfil wavevector conservation, are very small, and can be neglected.

From Eqs. (74) and (75) we see that the  $\Gamma_n$  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  $\Gamma_n$  and related quantities (especially the integral contained in  $\Gamma_n$ ) 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. (74)-(75) in Pang's model. In such a case we can compute explicitly the expressions of this integral and  $R_2(t)$  and  $\xi_2(t)$  contained in Eqs.(74)-(75) by means of approximation. As a matter of fact, in Eq.(75) 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  $\omega_q$  is approximated by  $\sqrt{w/M} |q|r_0$ , as it is shown in Appendix C. For  $t \rightarrow \infty$  (because we are interested in the long-time steady behaviour) the asymptotic forms of  $R_2(t)$  and  $\xi_2(t)$  are

$$R_2(t) = -R_0 \left[ \ln\left(\frac{1}{2} \omega_\alpha t\right) + 1.578 + \frac{1}{2} i\pi \right] \quad (76)$$

$$\xi_2(t) \approx -\pi R_0 k_B T t / \hbar \quad (\text{where } \coth \frac{1}{2} \omega_\alpha t \sim 1) \quad (77)$$

$$\text{i.e., } \lim_{t \rightarrow \infty} \xi_2(t) = -\eta t, \quad \eta = \pi R_0 / \beta\hbar = \pi R_0 k_B T / \hbar \quad (78)$$

Where,

$$R_0 = \frac{4(\chi_1 + \chi_2)^2}{\pi \hbar w} (M/w)^{1/2} = \frac{2J\mu_p r_0}{\pi \hbar v_0}, \quad (79)$$

$$\omega_\alpha = \frac{2\mu_p}{\pi} \left(\frac{w}{M}\right)^{1/2}, \quad T_0 = \hbar\omega_\alpha / K_B$$

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.(74) by using the approximation which is shown in Appendix C. The result is

$$\frac{1}{\pi\hbar} \text{Re} \int_0^\infty dt \exp \left\{ -i \left[ 2J(k'r_0)^2 + \frac{4}{3} J\mu_p^2 - \hbar\omega_k \right] t / \hbar + R_2(t) + \xi_2(t) \right\} \approx \frac{1}{\pi\hbar} (2.43\omega_\alpha)^{-R_0} \Gamma(1-R_0) [\eta^2 + (\delta(k, k')/\hbar)^2]^{-(1-R_0)/2} \left[ 1 - \frac{1}{2} \left[ \frac{\pi R_0}{2} + (1-R_0) \left( \frac{\delta(k, k')}{\eta\hbar} \right)^2 \right] \right] \quad (80)$$

Where,

$$\delta(k, k') = 2J(k'r_0)^2 + \frac{4}{3} \mu_p^2 J - \hbar\omega_k, \quad \Phi_1 = \frac{R_0\pi}{2},$$

$$\Phi_2 = \left[ (1-R_0) \tan^{-1} \left( \frac{\delta(k, k')}{\eta\hbar} \right) \right] \quad (81)$$

The decay rate of the soliton, in such an approximation, can be represented, from Eqs. (74) and (80), by

$$\Gamma_2 = \lim_{t \rightarrow \infty} \frac{d\bar{W}}{dt} = \frac{2}{\mu_p} \left( \frac{\pi}{N} \right)^2 \sum_{kk'} \left\{ \frac{(kr_0)^2 |g_1(k) + 2g_2(k)|^2 \sec^2 h^2[(\pi r_0/2\mu_p)(k-k')]}{[\mu_p^2 + (k'r_0)^2] [\exp(\beta\hbar\omega_k) - 1]} (2.43\omega_\alpha)^{-R_0} \left[ \frac{\left( \eta^2 + \frac{1}{\hbar^2} \left[ \frac{4}{3} \mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k \right]^2 \right)^{(1+R_0)/2}}{\hbar^2 \eta^2 + \left[ \frac{4}{3} \mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k \right]^2} \right] \left[ 1 - \frac{1}{2} \left[ \frac{R_0\pi}{2} + (1-R_0) \left[ \frac{\frac{4}{3} \mu_p^2 J + 2(k'r_0)^2 J - \hbar\omega_k}{\hbar\eta} \right]^2 \right] \right] \right\} \quad (82)$$

This is the final analytical expression for the decay rate of the quasi-coherent soliton with two-quanta. Evidently, it is different from that in the Davydov model [15,21]. To emphasize the difference of the decay rate between the two models we rewrite down the corresponding quantity for the Davydov soliton [15,21]



$$\Gamma_D = \frac{1}{\hbar^2} \frac{\chi_1^2}{\mu_D} \left( \frac{2\pi}{N} \right)^2 \sum_{kk'} \left( \frac{\hbar}{2M\omega_k} \right) \frac{(kr_0)^2 \sin^2(kr_0) \sec^2 h^2 [(\pi r_0 / 2\mu_D)(k - k')] \left( \frac{\omega_\alpha^D}{\eta_D} \right)^{-R_0^D}}{[\mu_D^2 + (k'r_0)^2] [\exp(\beta \hbar \omega_k) - 1]} \frac{\hbar^2 \eta_D}{\hbar^2 \eta_D^2 + [J\mu_D^2 / 3 + J(k'r_0)^2 - \hbar \omega_k]} \quad (83)$$

Where,  $\eta_D = \pi R_0^D K_B T / \hbar$ ,  $R_0^D = \frac{2\chi_1^2}{\pi \hbar w} \left( \frac{M}{w} \right)^{1/2}$ ,  $\omega_\alpha^D = \frac{2\mu_D}{\pi} \left( \frac{M}{w} \right)^{1/2}$  (84)

Equation (83) can also be found out from Eq. (74) at  $n = 1$  by using the Cottingham et al's approximation. The two formulae above, Eqs. (82) and (83), are completely different, not only for the parameter's values, but also the factors contained in them. In Eq.(82) the factor,

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

is added, while in Eq.(83) the factor,  $(2.43\omega_d)^{-R_0} \cdot \left( \eta^2 + \frac{1}{\hbar^2} \left[ \frac{4}{3} \mu_p^2 J + 2(k'r_0)^2 J - \hbar \omega_k \right]^2 \right)^{\left( \frac{1+R_0}{2} \right)}$  in Eq. (82) due to the two-quanta

nature of the new wavefunction and the additional interaction term in the new Hamiltonian. In Eq. (82) the  $\eta$ ,  $R_0$  and  $T_0$  are not small, unlike in the Davydov model. Using Eq. (72) and table 1 we find out the values of  $\eta$ ,  $R_0$  and  $T_0$  at  $T = 300K$  in both models, which are listed in table 2. From this table we see that the  $\eta$ ,  $R_0$  and  $T_0$  for Pang's model are about 3 times larger than the corresponding values in the Davydov model due to the increases of  $\mu_p$  and of the non-linear interaction coefficient  $G_p$ . Thus the approximations used in the Davydov model by Cottingham, et.al [14] 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.

**Discussion for the Lifetime of the New Soliton and Results:**

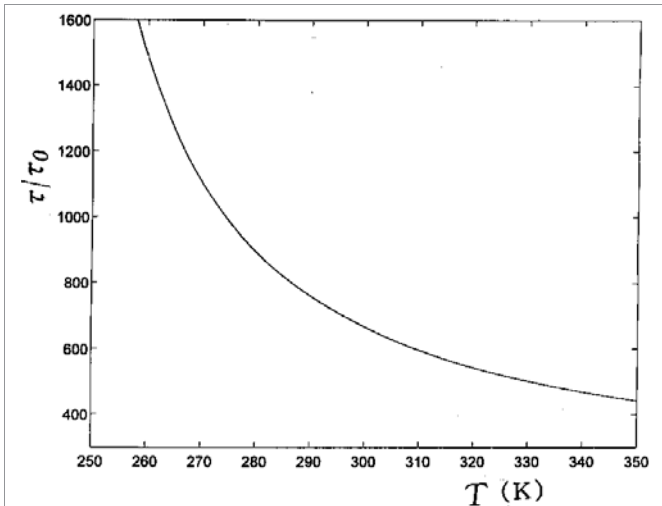
The above expression, Eq. (82), allows us to compute numerically the decay rate,  $\Gamma_2$ , and the lifetimes of the new soliton,  $\tau = 1/\Gamma_2$ , for values of the physical parameters appropriate to  $\alpha$ -helical protein molecules. Using the parameter values given in Eq. (37), tables 1 and 2,  $v = 0.2 v_0$  and assuming the wavevectors are in the Brillouin zone, the values of  $\Gamma_2$  between  $1.54 \times 10^{10} S^{-1}$  -  $1.89 \times 10^{10} S^{-1}$  can be obtained. This corresponds to the soliton lifetime  $\tau$ , of between

$0.53 \times 10^{-10} S$  -  $0.65 \times 10^{-10} S$  at  $T = 300K$ , or  $\tau/\tau_0 = 510$ - $630$ , where  $\tau_0 = r_0/v_0$  is the time for travelling one lattice spacing at the speed of sound, equal to  $(M/w)^{1/2} = 0.96 \times 10^{-13} S$ . 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 amino acid lattice spacings, that is several hundred times more than the Davydov soliton for which  $\tau/\tau_0 < 10$  at  $300K$  [15,21] (i.e., the Davydov soliton traveling at a half of the sound speed can cover less than 10 lattice spacing in its lifetime). The lifetime is sufficiently long for the new soliton excitation to be a carrier of bio-energy. Therefore the quasi-coherent soliton is a viable mechanism for the bio-energy transport at biological temperature in the above range of parameters. Attention is being paid to the relationship between the lifetime of the quasi-coherent soliton and temperature. Fig.3 shows the relative lifetimes  $\tau/\tau_0$  of the new soliton versus temperature  $T$  for a set of widely accepted parameter values as shown in Eq. (37). Since one assumes that  $v < v_0$ , the soliton will not travel the length of the chain unless  $\tau/\tau_0$  is large compared with  $L/r_0$ , where  $L = Nr_0$  is the typical length of the protein molecular chains. Hence for  $L/r_0 \approx 100$ ,  $\tau/\tau_0 > 500$  is a reasonable criterion for the soliton to be a possible mechanism of the bio-energy transport in protein molecules. The lifetime of the quasi-coherent soliton shown in Figure 4 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. For comparison,  $\log(\tau/\tau_0)$  versus the temperature relationships was plotted simultaneously for the Davydov soliton and the new soliton with a quasi-coherent two-quanta state in Fig.4. The temperature-dependence of  $\log(\tau/\tau_0)$  of the Davydov soliton is obtained from Eq. (83). We find that the differences of values of  $\tau/\tau_0$  between the two models are very large. The value of  $\tau/\tau_0$  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. Hence it is true that the Davydov soliton is ineffective for biological processes [3-23].

The dependency of the soliton lifetime on the other parameters can also be studied by using Eq. (82). Parameter values near the above accepted values shown in Eq. (37) are chosen. In Pang's model we know from Eq. (82) that the lifetime of the soliton depends mainly on the following parameters: coupling constants  $(\chi_1 + \chi_2)$ ,  $M$ ,  $w$ ,  $J$ , phonon energy  $\omega_k$ , as well as on the composite parameters  $\mu$  ( $\mu = \mu_p$ ),  $R_0$  and  $T/T_0$ . At a given temperature,  $\tau/\tau_0$  increases as  $\mu$  and  $T_0$  increase. The dependences of the lifetime  $\tau/\tau_0$ , at  $300K$  on  $(\chi_1 + \chi_2)$  and  $\mu$  are shown in Figs.5 and 6, respectively. Since  $\mu$  is inversely proportional to the size of the soliton, and determines the binding energy in the new model, it is an important quantity. It is regarded as an independent variable. In such a case the other parameters in Eq. (82) adopt the values in Eq. (37). It is clear from Figs.5 and 6 that the lifetime of the soliton,  $\tau/\tau_0$ , increases rapidly with increasing  $\mu$  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 the new model, we find  $\tau/\tau_0 > 500$ . For comparison, the corresponding result obtained using Eq. (83) is shown for the original Davydov model as a dashed line in figure 6. Here we see that the increase in lifetime of the Davydov soliton with increasing  $\mu$  is quite slow and the difference between the two models increases rapidly with increasing  $\mu$ . The same holds for the dependency on

**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



**Figure 3:** Soliton lifetime  $\tau$  relatively to  $\tau_0$  as a function of the temperature  $T$  for parameters appropriate to the  $\alpha$ -helical molecules in Pan's model in Eq. (9).

the parameter  $(\chi_1 + \chi_2)$ , but the result for the Davydov soliton is not drawn in figure 5. These results show again that the quasi-coherent soliton in Pang's model is a likely candidate for the mechanism of bio-energy transport in the protein molecules. In addition it shows that a basic mechanism for increasing the lifetime of the soliton in the biomacromolecules is to enhance the strength of the exciton-phonon interaction.

In figure 7  $\tau/\tau_0$  versus  $\eta$  is plotted. Since  $-\eta$  designates the influence of the thermal phonons on the soliton, it is also an important quantity. Thus, it is regarded here as an independent variable. The other parameters in Eq. (82) take the values in Eq. (37). From this figure we see that  $\tau/\tau_0$  increases with increasing  $\eta$ . Therefore, to enhance  $\tau$  can also increase the value of  $\tau/\tau_0$ . In order to understand the behavior of the quasi-coherent soliton lifetime in very wide ranges, it is necessary to study  $\tau/\tau_0$  in the limit  $\omega_a t \rightarrow 0$  in Eq. (75) or Eqs. (C1) and (C3) (i.e., this is in the initial case) in which we can evaluate analytically the values of  $R_2(t)$  and  $\xi_2(t)$ . In fact, for  $\omega_a t < 1$  both  $R_2(t)$  and  $\xi_2(t)$  have power-series expansions. To the lowest order as  $\omega_a t \rightarrow 0$ , it can be found from Eq. (75)

$$R_2(t) \approx -R_0 [i\pi^2 \omega_a t / 6 + 3\zeta(3)(\omega_a t)^2] \tag{85}$$

$$\xi_2(t) \approx -\frac{R_0 K_B^2 T_0 \pi^2}{3\hbar^2} t^2, \tag{86}$$

$$\text{using } \coth(\pi\omega_a t) \approx [(\pi\omega_a t)^{-1} + \frac{\pi}{3}\omega_a t]$$

Thus,

$$\frac{1}{\pi\hbar} \text{Re} \int_0^\infty dt \exp \left\{ -i \left[ 2J(k'r_0)^2 + \frac{4J\mu_p^2}{3} - \hbar\omega_k \right] \right\} \approx \left[ \frac{t/\hbar + R_2(t) + \xi_2(t)}{4\pi(3\zeta(3)R_0K_B^2T_0^2 + R_0\pi^2K_B^2TT_0/3)} \right]^{-1/2} \exp \left\{ -\frac{[2J(k'r_0)^2 + \frac{4}{3}\mu_p^2J - \hbar\omega_k + \hbar(R_0\pi^2K_B T)^2]}{4[3\zeta(3)R_0K_B^2T_0^2 + R_0\pi^2K_B^2TT_0/3]} \right\} \tag{87}$$

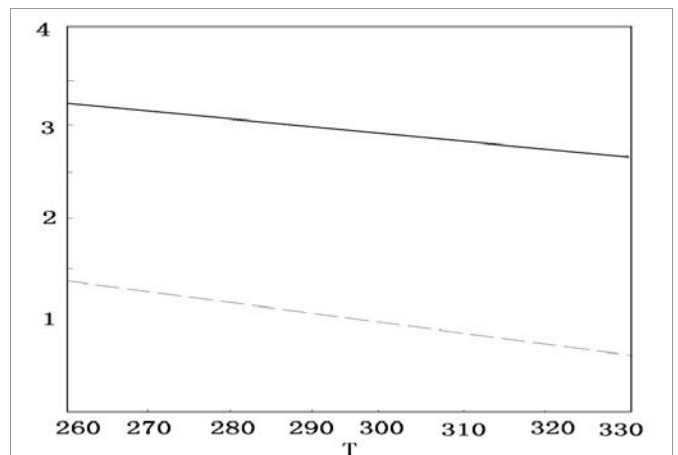
When,  $T/T_0 > 1$  and  $\pi^4 R_0 T / 2\mu T_0 > 1$ . The above integral is a generalization of the usual  $\delta$ -function for energy conservation in zero-temperature perturbation theory. Thus we can obtain from Eqs. (74) and (87) at  $n=2$  the decay rate of the soliton as

$$\Gamma_2 = \frac{2\pi^3}{\mu_p \hbar N^2 K_B} \left( \frac{\pi}{R_0 T_0 [3\zeta(3)T_0 + \pi^2 T / 3]} \right)^{-1/2} \sum_{kk'} \frac{(kr_0)^2 |g_1(k) + 2g_2(k)|^2}{\mu_p^2 + (k'r_0)^2} \sec^2 h^2 \left[ \frac{\pi r_0}{2\mu_p} (k - k') \right] \left\{ \exp \left[ \frac{[2J(\mu_p r_0)^2 + \frac{4}{3}\mu_p^2 J - \hbar\omega_k + \frac{1}{6}R_0\pi^2 K_B T_0]^2}{4[3\zeta(3)R_0K_B^2T_0^2 + R_0\pi^2K_B^2TT_0/3]} [\exp(\beta\hbar\omega_k) - 1] \right] \right\}^{-1} \tag{88}$$

The expression of the decay rate of the quasi-coherent soliton in this limit is different from Eq. (84). Therefore, studying properties of the lifetime of the new soliton in such a case helps in understanding the behavior of the soliton. A summary of the results obtained from Eq. (88) are given in figures 8-11. The dependency of lifetime on temperature  $T$  is shown in figure 8, which has been obtained from the numerical evaluation of Eq. (88).

$\frac{2}{0} = 4.10$  at 300K and  $\mu = 5.81-5.96$  depending on whether the widely accepted or the "three-channel" parameter values for the protein are assumed. From these results, it is clear that using widely accepted and realistic parameter values, the new model can satisfy the relation  $\tau/\tau_0 \geq 500$  at 300K and large  $\mu$  and large  $T_0$ . Hence the proposed new soliton model provides a viable candidate for the biological processes.

Here a new theory of bio-energy transport is proposed to study the properties of the nonlinear excitation and motion of the soliton along protein molecules. In this theory, Davydov's Hamiltonian and wave function of the systems are simultaneously improved and extended, a new interaction is added into the original Hamiltonian, and the original wave function of the excitation state of single particles is replaced by a new wave function of a two-quanta quasi-coherent state. From this model, a lot of interesting and new results are obtained. The soliton has sufficiently long lifetime and can play an important role in biological processes. Therefore, it is an exact carrier of bio-energy in living systems. Present problem is why the quasi-coherent soliton has such long lifetime? From Eqs. (35) and (45) and tables 1 and 2 it can be seen that the binding energy and



**Figure 4:**  $\log(\tau/\tau_0)$  versus the temperature. The solid line is the result of Pang's model, the dashed line is the result of the Davydov model.



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 the new model is  $G_p = 8(\chi_1 + \chi_2)^2 / (1-s^2)w = 3.8 \times 10^{-21} J$ , and it is larger than the linear dispersion energy,  $J = 1.55 \times 10^{-22} J$ , i.e., the nonlinear interaction is so large that it can really cancel or suppress the linear dispersion effects in the equation of motion of this model. From this point the soliton is stable according to the conditions of formation and stability of the soliton in the soliton theory [27,28]. By comparison, the non-linear 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  $G_p$ . Thus the stability of the Davydov soliton is weak compared to that of the new soliton. Moreover, the binding energy of the quaasi-coherent soliton in Pang's model is  $E_{BP} = 4\mu_p^2 J/3 = 7.8 \times 10^{-21} J$  in Eq. (19), 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  $\omega_D$  is Debye frequency), and it is approximately equal to  $\mathcal{E}_0 / 4 = 8.2 \times 10^{-21} J$ , i.e., it has same order of magnitude of the energy of the amide-I vibrational quantum,  $\mathcal{E}_0$ . This shows that the quasi-coherent soliton is robust against the quantum fluctuation and thermal perturbation of the systems due to the large energy gap between the soliton state and the delocalized state. In contrast,

the binding energy of the Davydov soliton is only  $E_{BD} = \frac{\chi_1^4}{3w^2 J} = 0.188 \times 10^{-21} J$ , which is about 41 times smaller than that of the new soliton, about 23 times smaller than  $K_B T$  and about six times smaller than  $K_B \Theta = \omega_D = 1.2 \times 10^{-21} J$ , 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 [15-18,24-26]. Therefore, the quasi-coherent soliton can provide a realistic mechanism for the bio-energy transport in protein molecules. The two-quanta nature of the quasi-coherent soliton plays a more important role in the increase of lifetime relative to that of the

added interaction because of the following facts. (1) The change of the

$$\text{nonlinear interaction energy } G_p = 2G_D \left[ 1 + 2\left(\frac{\chi_2}{\chi_1}\right) + \left(\frac{\chi_2}{\chi_1}\right)^2 \right] \text{ by } \mu_p$$

produced the added interaction in the new model are  $\Delta G = G_p(\chi_2 \neq 0) - G_p(\chi_2 = 0) = 1.08G_D < G_p(\chi_2 = 0) = 2G_D$  and  $\Delta\mu = \mu_p(\chi_2 \neq 0) - \mu_p(\chi_2 = 0) = 1.08\mu_p < \mu_p(\chi_2 = 0) = 2\mu_p$ , respectively, i.e., the roles of the added interaction on  $G_p$  and  $\mu_p$  are smaller than that of the two-quanta nature. The two parameters  $G_p$  and  $\mu_p$  are responsible for the lifetime of the soliton. Thus the effect of the former on the lifetimes is smaller than the latter. (2) The contribution of the added interaction to the binding energy

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

which is smaller than that of the two-quanta nature which is  $E''_{BD} = 16E_{BD}$ . Putting them together in Eq. (35) we see that  $E_{BP} \approx 41E_{BD}$ . (3) From the  $(\chi_1 + \chi_2)$ -dependence of  $\tau/\tau_0$  in figure 5,  $\tau/\tau_0 \approx 100$  has already been found directly 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

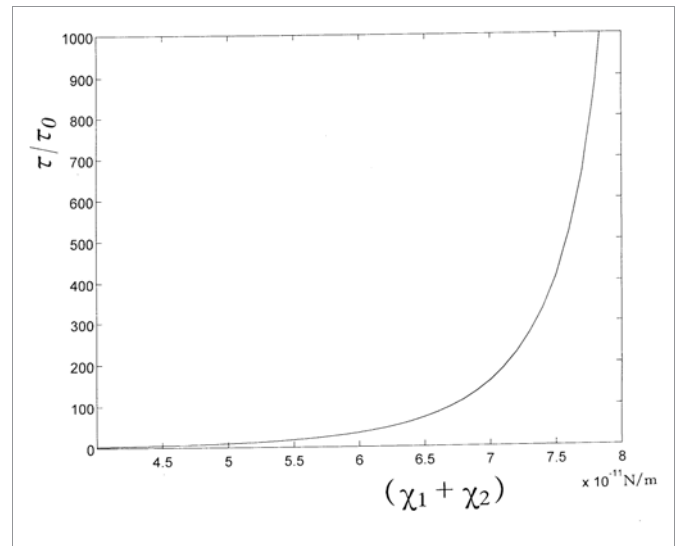


Figure 5:  $\tau/\tau_0$  versus  $(\chi_1 + \chi_2)$  relation in Eq. (82).

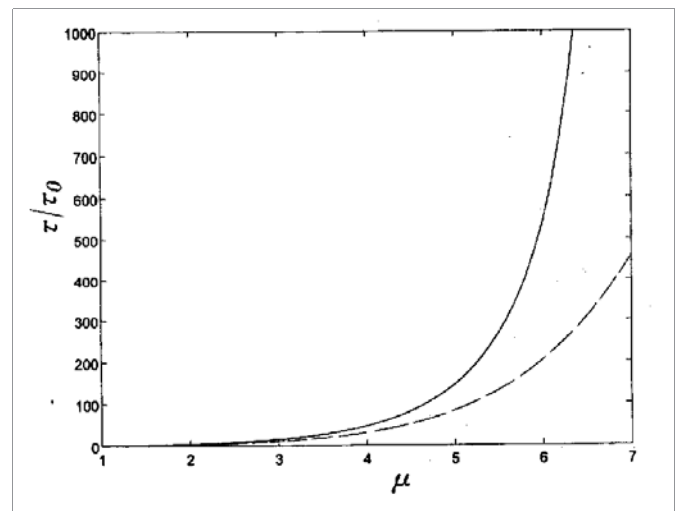


Figure 6:  $\tau/\tau_0$  versus  $\mu$  relation. The solid and dashed lines are results of Eq. (82) and Eq. (83), respectively.

wave function. Therefore, it is very reasonable to refer to the new soliton as the quasi-coherent soliton [30-35]. The above calculation helps to resolve the controversies on the lifetime of the Davydov soliton, which is too small in the region of biological temperature. However, by modifying the wave function and the Hamiltonian of the model, a stable soliton at biological temperatures could be produced. This result was obtained considering a new coupled interaction between the acoustic and amide-I vibration modes and a wave function with quasi-coherent two-quanta state. In such a way, the quasi-coherent soliton is a viable mechanism for the bio-energy transport in living systems. Therefore, it can be seen that Pang's model is completely different from the Davydov's model. Thus, the equation of motion and properties of the soliton occurring in Pang's model are also different from that in the Davydov's model. The distinction of features of the solitons between the two models is shown in table 3 [15]. From the table 3 we know that our new model repulse and refuse the shortcomings of the Davydov model [3], the new soliton in Pang's model is thermal stable at biological temperature 300K, and has so enough long lifetime, thus it can plays important role in biological processes.

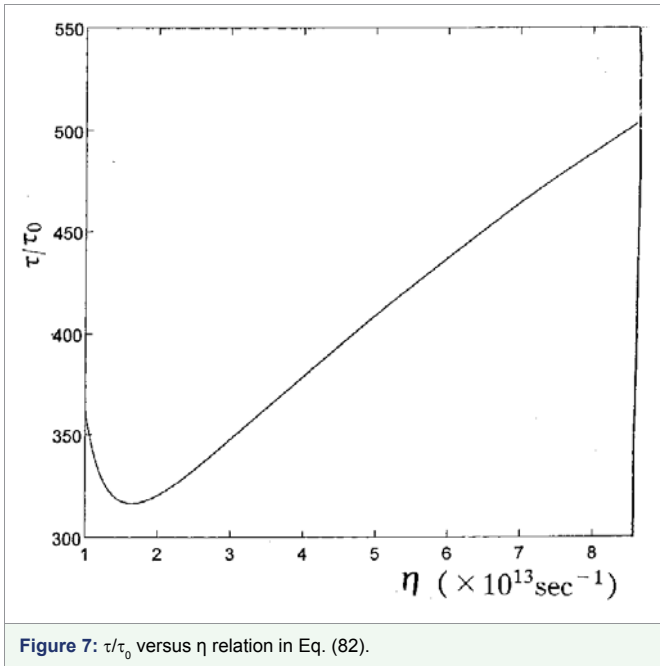


Figure 7:  $\tau/\tau_0$  versus  $\eta$  relation in Eq. (82).

**Appendix A:** The partial diagonalization of the Hamiltonian implies the diagonalization of that part of the Hamiltonian in Eq. (50) which does not involve the creation and annihilation operators of new phonons Eq. (48). Thus the condition imposed into the functions  $C_j(x)$  contained in Eq. (53) to realize such a diagonalization are equivalent, in the continuum approximation, to the following problems of eigenfunctions  $C_j(x)$  and eigenvalues  $E_j$  determined by

$$2 \left[ -Jr_0^2 \frac{\partial^2}{\partial x^2} + i\hbar v \frac{\partial}{\partial x} + \varepsilon_0 - 2J + V(x) \right] C_j(x) = E_j C_j(x) \quad (A1)$$

For the above expression of  $V(x)$  in Eq. (52) there is only one bound state in Eq. (A1)

$$C_s(x) = \left( \frac{\mu_p}{2r_0} \right)^{1/2} \text{sech}(\mu_p x / r_0) \exp[i\hbar v x / 2Jr_0^2] \quad (A2)$$

$$\text{With, energy } E_s = 2 \left[ \varepsilon_0 - 2J - \frac{\hbar^2 v^2}{4Jr_0^2} - J\mu_p^2 \right] \quad (A3)$$

and unbounded (delocalized) states

$$C_k(x) = \frac{\mu_p \tanh(\mu_p x / r_0) - ikr_0}{\sqrt{Nr_0[\mu_p - ikr_0]}} \exp[ikx + i\hbar v x / 2Jr_0^2] \quad (A4)$$

$$\text{With, energy } E_k = 2 \left[ \varepsilon_0 - 2J - \frac{\hbar^2 v^2}{2\mathbf{f}_0^2} + J(\mathbf{k}_0)^2 \right] \quad (A5)$$

The energy of the lowest unbounded state is greater than that of the bounded state by the value  $2\mu^2 J$ . The functions  $C_k(x)$  are normalized as follows:

$$\int_{-\infty}^{\infty} dx C_k^*(x) C_{k'}(x) = \delta(kr_0 - k'r_0),$$

$$\int_{-\infty}^{\infty} dx |C_k(x)|^2 = 1, \int_{-\infty}^{\infty} dx C_s^*(x) C_k(x) = 0$$

Therefore,  $A_s^+$  is an excitation which is localized at the lattice

distortion, while  $A_k^+$  creates an unbounded excitation with wave vector  $k$ . In getting Eq. (A1) the variable  $x$  was assumed to be continuous and the chain length to tend to infinity  $L = Nr_0 \rightarrow \infty$ . Thus this wave vector  $k$  has a continuous value between  $-\infty$  and  $\infty$ . In subsequent calculation we mainly use a discrete description. The continuous description is transformed into a discrete one according to the rules

$$\int_{-\infty}^{\infty} dx / r_0 \rightarrow \sum_n, \int_{-\infty}^{\infty} dx \rightarrow \frac{2\pi}{Nr_0} \sum_k, \delta(kr_0 - k'r_0) \rightarrow \frac{N}{2\pi} \delta_{kk'}, C_s(x) \rightarrow C_s(n), C_k(x) \rightarrow \left( \frac{N}{2\pi} \right)^{1/2} C_k(n)$$

Utilizing Eqs. (50) - (51), (53) and (54), then the partially diagonalized Hamiltonian in the new representation is just Eq. (55).

**Appendix B:** We now calculate  $U(k, k', t)$  in Eq.(72) utilizing the coherent state  $|u\rangle$  defined by  $b_q|u\rangle = u_q|u\rangle$  with

$$\langle u | u' \rangle = \exp \left\{ \sum_q \left[ u_q^* u'_q - \frac{1}{2} |u_q|^2 - \frac{1}{2} |u'_q|^2 \right] \right\},$$

$$|u\rangle = \exp \sum_q (u_q b_q^+ - u_q^* b_q) |0\rangle$$

Utilizing the coherent state  $|u\rangle$ , the  $U(k, k', t)$  in Eq. (72) can be represented by

$$U(k, k', t) = \frac{1}{Z_{ph}} \int d\Omega(u) \int d\Omega(u'') (u_k^* + u''_k) (u_{-k}^* + u_{-k}'')$$

$$\langle u | \exp \sum_q (\omega_q - qv) (-\beta\hbar + it) b_q^+ b_q \rangle |u''\rangle$$

$$\langle u'' | \exp \left\{ -i \sum_q (\omega_q - qv) \left[ \begin{matrix} (b_q^+ b_q + \frac{1}{n\sqrt{N}}) \\ (b_q^+ \alpha_q + \alpha_q^* b_q) + \frac{1}{n^2} \frac{1}{N} |\alpha_q|^2 \end{matrix} \right] t \right\} |u\rangle \quad (B1)$$

Where, the integration measure is defined as,

$$\int d\Omega(u) = \prod_k \frac{1}{\pi} dx_k dy_k, \text{ with } x_k + iy_k = u_k$$

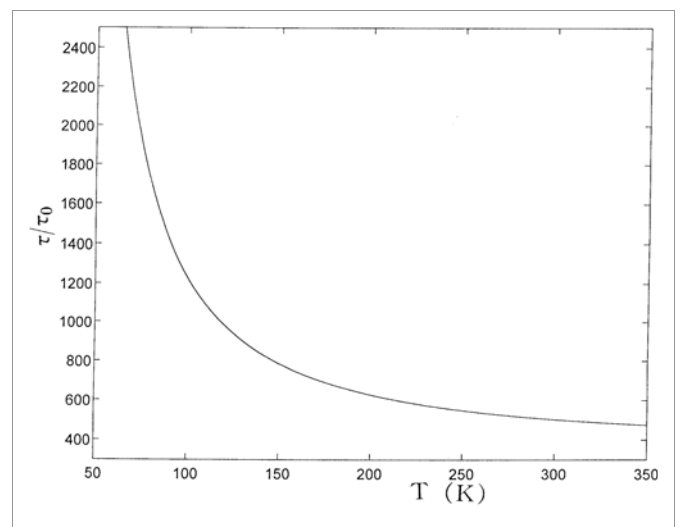


Figure 8:  $\tau/\tau_0$  vs  $T$  relation in Pang's model in Eq. (88).



Since we can show that,

$$\exp(\tau b_k^+ b_k) |u_k\rangle = \exp\left\{\frac{1}{2}|u_k|^2 (e^{\tau+\tau^*} - 1)\right\} |e^\tau u_k\rangle$$

It, follows that the first matrix element in Eq. (B1) equals

$$\langle u_k | \exp\left[\sum_q (\omega_q - qv)(-\beta\hbar + it)b_q^+ b_q\right] |u_k''\rangle = \exp\left\{-\sum_k \left(\frac{1}{2}|u_k|^2 + \frac{1}{2}|u_k''|^2 - u_k^* u_k'' \exp[(\omega_q - qv)(-\beta\hbar + it)]\right)\right\}$$

The second matrix element in Eq. (B1) can be represented as a path integral that can be evaluated exactly. Utilizing the general relationship between the matrix element and the path integral:

$$\langle u_k'' | \exp[-i\omega(b_k^+ b_k + \tau^* b_k + b_k^+ \tau + \tau^* \tau)] |u_k\rangle = \exp\left[-\frac{1}{2}(|u_k''|^2 + |u_k|^2 - i\omega|\tau|^2 t)\right] \quad (B2)$$

$$\int_{y^*(t)=u_k''}^{y(0)=u_k} D(y^*, y) \exp[iT(y^*, y)]$$

Where,

$$T(y^*, y) = \int_0^t dt' \left\{ iy^*(t') \frac{dy}{dt'} - \omega[y^*(t)y] - iu_k''^* y(t) [(t') + \tau^* y(t') + y^*(t')\tau] \right\}$$

We can evaluate the path integral by standard techniques. The result for Eq. (B2) is

$$\begin{aligned} & \bar{A} \exp \left\{ -\frac{1}{2} (|u_k''|^2 + |u_k|^2 + u_k''^* u_k e^{-i\omega t} \right. \\ & \left. - (1 - e^{-i\omega t})(u_k''^* \tau + \tau^* u_k + |\tau|^2) \right\} \end{aligned} \quad (B3)$$

Substituting above the matrix elements obtained into Eq. (B1) we get

$$U(k, k'', t) = \frac{e^{R_n(t)}}{Z_{ph}} \int d\Omega(u) \int d\Omega(u'') (u_k''^* + u_{-k}'') (u_{-k}^* + u_{k'})$$

$$\begin{aligned} & \bar{A} \exp \left\{ -\sum_q (|u_q|^2 + |u_q''|^2 - u_q^* u_q'' \exp[(\omega_q - qv)(-\beta\hbar + it)] - u_q^* u_q \cdot \right. \\ & \left. \exp[-i(\omega_q - qv)t] + \frac{1}{n} \frac{1}{\sqrt{N}} (u_q'' \alpha_q + u_q^* \alpha_q^*) (1 - \exp[i(\omega_q - qv)t]) \right\} \end{aligned} \quad (B4)$$

Where,

$$R_n(t) = \frac{-1}{n^2 N} \sum_k |\alpha_k|^2 (1 - \exp[-i(\omega_k - kv)t]) \quad (B5)$$

The  $u''$  and  $u$  integrations can easily be finished. For instance, the contribution from the term with the  $u_k''^* u_{k'}$  factor, which we can denote by  $U_a(k, k'', t)$  since it is associated with the absorption of a phonon, is

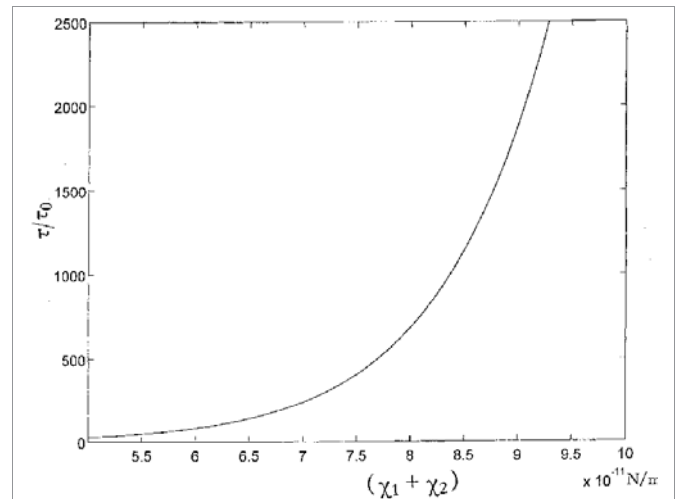


Figure 9:  $\tau/\tau_0$  versus  $(\chi_1 + \chi_2)$ , relations in the new model in Eq. (88).

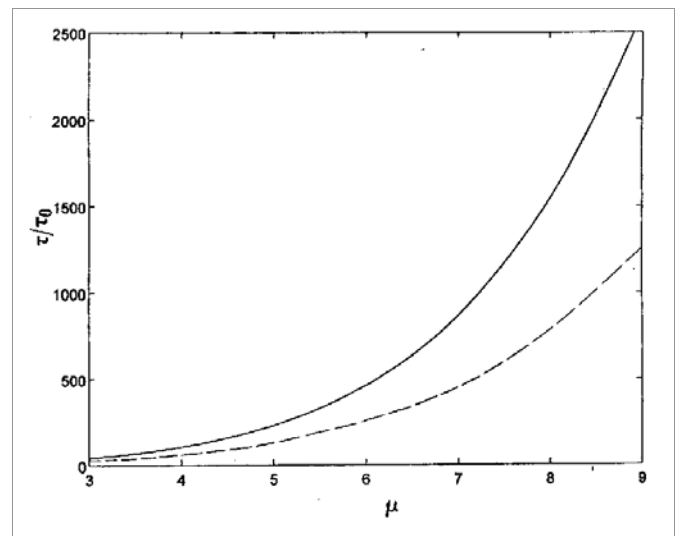


Figure 10:  $\tau/\tau_0$  versus  $\mu$  relation in the new model in Eq. (88).

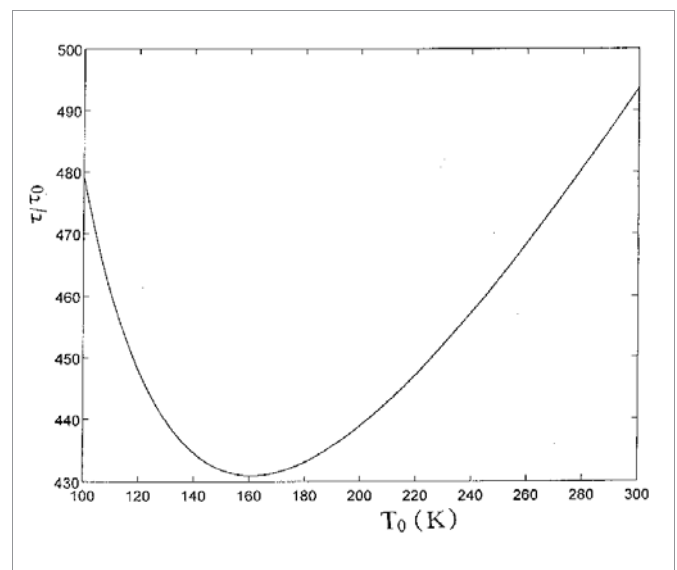


Figure 11:  $\tau/\tau_0$  versus  $T_0$  relation. Here the solid and dashed lines are the results in the new model in Eq. (88) and in the Davydov model, respectively.



$$U_a(k, k'', t) = \frac{\exp[i(\omega_k - kv)t + R_n(t) + \xi_n(t)]}{\exp[\beta\hbar(\omega_k - vk)] - 1} \cdot \left\{ \delta_{kk''} - \frac{\frac{1}{n^2} \frac{1}{N} \alpha_k^* \alpha_{k''} (\exp[i(\omega_k - k''v)t] - 1)(\exp[-i(\omega_k - kv)t] - 1)}{\exp[\beta\hbar(\omega_k - vk)] - 1} \right\} \quad (B6)$$

Where,

$$\xi_n(t) = \frac{-4}{n^2 N} \sum_k \frac{|\alpha_k|^2 \sin^2\left(\frac{1}{2}(\omega_k - vk)t\right)}{\exp[\beta\hbar(\omega_k - vk)] - 1} \quad (B7)$$

We note that the breaking of the translational symmetry by the deformation leads to off-diagonal terms corresponding to violation of wavevector conservation. However, we can prove that these terms are proportional to  $\frac{1}{N} \alpha_k^* \alpha_{k''}$  which can be neglected when

either  $|k|$  or  $|k''|$  is large as compared to  $4\mu_p/\pi a_0$  as can be seen in the definition of  $\alpha_k$  in Eq. (59). Furthermore, when  $-\pi \leq kr_0 \leq \pi$  and  $\mu_p < \pi^2$  the off-diagonal terms are negligible except for a small region at the center of the Brillouin zone. Since the small wavevector terms do not significantly contribute to  $\Gamma_n$  due to the  $k$ -dependence of  $\tilde{F}(q, k)$ , and thus the off-diagonal terms can be neglected in  $U_a(k, k'', t)$  in the calculation of  $\Gamma_n$ . The energy of the soliton state is less than that of the unlocalized exciton in the uniform lattice. Therefore, the parts of  $U_a(k, k'', t)$  corresponding to the absorption of a phonon make the major contributions to the sum in Eq. (72) at the temperature and parameter values of interest, and their off-diagonal terms may also be neglected just as above. Using the result of the  $U_a(k, k'', t)$  obtained from the above formulae of Eq (72) the decay rate Eq. (74) can be obtained.

**Appendix C:** If the soliton velocity approaches zero we can get an analytical expression for  $R_2(t)$  and  $\xi_2(t)$  at  $n = 2$  defined in Eq. (75) or Eqs. (B5) and (B7) through inserting Eq. (59) into Eqs. (B5) and

(B7) and applying the relation of  $\frac{1}{N} \sum_q \rightarrow \frac{r_0}{2\pi} \int_{-\infty}^{\infty} dq$ , i.e.,

$$\lim_{v \rightarrow 0} R_2(t) = -R_0 \int_{-\infty}^{\infty} \frac{y}{sh^2 y} \left\{ [1 - \cos(\omega_\alpha ty)] + i \sin(\omega_\alpha ty) \right\} dy \quad (\text{here } y = \frac{\pi q r_0}{2\mu_p}) \quad (C1)$$

$$= -R_0 [ix' \psi'(1 + ix') + \psi(1 + ix') - \psi(1)]$$

Where,

$$R_0 = \frac{4(\chi_1 + \chi_2)^2}{\pi \hbar w} \left(\frac{M}{w}\right)^{1/2} = \frac{2J\mu_p r_0}{\pi \hbar v_0}, \quad \omega_\alpha = \frac{2\mu_p}{\pi} \left(\frac{w}{M}\right)^{1/2} \quad (C2)$$

$\Psi$  Is the digamma function,  $\Psi'$  is its derivative and  $x' = \omega_\alpha t = K_B T_0 t / \hbar$ .

$\xi_2(t)$  Can be easily evaluated when  $v=0$  and  $R_0 < 1$  at sufficiently high temperature

$T > T_0 (T_0 = \hbar \omega_\alpha / K_B)$ . In this case it is

$$\xi_2(t) = \frac{-R_0}{\omega_\alpha} \left[ \frac{T}{T_0} \right] \int_0^\infty d\omega_k \frac{\sin^2\left[\frac{1}{2}\omega_k t\right]}{sh^2(\omega_k / \omega_\alpha)} = \frac{R_0 T}{T_0} [1 - \pi \omega_\alpha t \coth(\pi \omega_\alpha t)] \quad (C3)$$

Where, we use the relation  $\exp(\beta\hbar\omega_k) \approx 1 + \beta\hbar\omega_k$ .

As  $t \rightarrow \infty$  (because we are interested in the long-time steady behaviour) the leading terms in the above asymptotic formulae of  $R_2(t)$  and  $\xi_2(t)$  can be represented by

$$R_2(t) = -R_0 \left[ \ln\left(\frac{1}{2} \omega_\alpha t\right) + 1.578 + \frac{1}{2} i\pi \right] \quad (C4)$$

$$\xi_2(t) \approx -\pi R_0 k_B T t / \hbar \quad (C5)$$

(Where, we approximated  $\coth\left(\frac{1}{2} \omega_\alpha t\right) \sim 1$ ), i.e.,

$$\lim_{t \rightarrow \infty} \xi_2(t) = -\eta t, \quad \eta = \pi R_0 / \beta \hbar = \pi R_0 k_B T / \hbar \quad (D6)$$

Except at low temperature, the  $x' (= \omega_\alpha t)$  - dependent term in the real part of  $R_2(t)$  is small with respect to  $\xi_2(t)$  for parameter values of interest and can be neglected. Furthermore, since  $R_0 < 1$  (but it is not very small, about  $R_0 \approx 0.529$ ) and  $T_0 < T$  (but it is not too small, about  $T_0 \approx 294K$ ) and  $R_0 T/T_0 < 1$  for the protein molecules, then one can evaluate the integral in Eq. (72) by using the following approximation and utilizing the above results of Eqs. (C4-C6)

$$\frac{1}{\pi \hbar} \text{Re} \int_0^\infty dt \exp \left\{ -i \left[ 2J(k'r_0)^2 + \frac{4}{3} J \mu_p^2 - \hbar \omega_k \right] t / \hbar + R(t) + \xi(t) \right\} \approx \frac{1}{\pi \hbar} (2.43 \omega_\alpha)^{-R_0} \Gamma(1 - R_0) [\eta^2 + (\delta(k, k') / \hbar)^2]^{-(1-R_0)/2} \left\{ \cos\left(\frac{\pi R_0}{2}\right) \cos \left[ (1 - R_0) \tan^{-1} \left( \frac{\delta(k, k')}{\eta \hbar} \right) \right] - \sin\left(\frac{\pi R_0}{2}\right) \sin \left[ (1 - R_0) \tan^{-1} \left( \frac{\delta(k, k')}{\eta \hbar} \right) \right] \right\} = \frac{1}{\pi \hbar} (2.43 \omega_\alpha)^{-R_0} \Gamma(1 - R_0) [\eta^2 + (\delta(k, k') / \hbar)^2]^{-(1-R_0)/2} \cos(\Phi_1 + \Phi_2) \approx \frac{1}{\pi \hbar} (2.43 \omega_\alpha)^{-R_0} \Gamma(1 - R_0) [\eta^2 + (\delta(k, k') / \hbar)^2]^{-(1-R_0)/2} \left[ 1 - \frac{1}{2} \left[ \frac{\pi R_0}{2} + (1 - R_0) \left( \frac{\delta(k, k')}{\eta \hbar} \right) \right]^2 \right]$$

Where,

$$\delta(k, k') = 2J(k'r_0)^2 + \frac{4}{3} \mu_p^2 J - \hbar \omega_k, \quad \Phi_1 = \frac{R_0 \pi}{2},$$

$$\Phi_2 = \left[ (1 - R_0) \tan^{-1} \left( \frac{\delta(k, k')}{\eta \hbar} \right) \right] \quad (C8).$$

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