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## THE TERAHERTZ FEATURES OF TRANSPORT OF NERVE IMPULSE ALONG THE NERVE SYSTEMS DRIVEN BY THE BIO-ENERGY IN LIFE SYSTEMS

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#### ABSTRACT

We here research the features of transport of nerve impulse along the nerve fiber using modern theory of molecular biology, in which we think this transport is due to the driving of bio-energy released from the hydrolyses reaction of ATP molecules in the cells. Because ATP molecules are often attached on the protein molecules, where the energy is transported along the protein molecules from the position of generation of hydrolyses reaction to the position used in virtue of transport of the soliton formed by the excitons through the mechanism of self-trapping, where the exciton is a quantum produced by the C=0 stretching (or amide-I) vibrations. We studied and obtained the properties of transport of bio-energy, which is carried by Pang's soliton, along  $\alpha$ -helical protein molecules and found further the lifetimes of Pang'soliton, which is between  $0.53 \times 10^{-10}$ S— $0.65 \times 10^{-10}$ S at physiological temperature T=300K. In this lifetime Pang's soliton can travel over several hundreds of amino acid residues. This implies that Pang 's theory is a relevant and correct model of bio-energy transport, then Pang's soliton is a real carrier of bio-energy transport in protein molecules. The bio-energy is transported into the nerve membrane to drive the works of sodium pump and potassium pump on the surface of membrane of cells, which drive also the transfer of the action electric-potential or the nerve impulse along the nerve membranes. We confirm that there is not the nerve impulse, or the action electric- potential without the works of sodium pump and potassium pump, or the bio-energy. This means that the nerve impulse can be transported along the nerve membrane, only if the bio-energy are absorbed really by the sodium pump and potassium pump. In order to obtain a stable nerve impulse we must ensure that the times forming it must be shorter than the lifetime of Pang's soliton and its experimental values, or else, the nerve impulse is not stable and is useless. Thus we can judge and affirm that the nerve impulse is a terahertz wave. Thus we can affirm and verified that the nerve impulse can be transport along the nerve systems in the terahertz wave, instead the millimeter wave. We here determinate and discuss further its features. This is first time to determinate the terahertz features of transport of the nerve impulse along the nerve fibers in life systems, which will promotes the development of the nerve science.

Keywords: Nerve impulse, nerve membrane, nerve fiber, bio-energy, soliton lifetime, protein molecule, ATP molecule, energy transport, carrier, terahertz wave, feature.

# INTRODUCTION, FORMATION OF NERVE IMPULSE IN LIFE SYSTEMS

It is well known, the distributions of  $Na^+$ ,  $K^+$  and  $Cl^-$  ions in the inner and the exterior of the neurons in the resting case are different, which are also same with general cells. their charges are all different, which results in the different of states of distribution for the charges, which are positive in the exterior and negative in the inner. Thus the resting potential of the neurons are about 40-70mV. which is just the membrane potential of the neurons we observed often. Its detailed reasons of form are just due to the differences of the permeability of the neurons for different ions. Therefore, the uneven of distribution and permeability of these ions in inside and outside of the membrane is just their basic feature. These ion channels in the neuron membranes are formed by a kind of transmembrane protein molecules. Just the existences of the channels, which promote to passive transfer and flow of these ions along the directions of the electrochemical gradients. But the transfer and flow have a observe the ion specificity, i.e., different ions have different channels.

Very clearly. The flow of these ions along these channel firm a current, this is just the electrical signal. It is controlled by the membrane potential. Thus we can say that the electrical signal is due to the changes of open or close of ion channels. Therefore we can affirm that there are changes of ion current in the nerve systems. However, to cause and to maintain the ion concentration gradient on both sides of the nerve membrane need supply constantly the energy, which can be carried out and guaranteed by the ionic pumps such as sodium pump and potassium pump on the membrane of neurons. These ionic pumps have obtained from the energy factory in life bodied through the metabolism or chemical reactions, which can release the energy, such as the hydrolysis reaction of ATP molecules.

In general case the ion concentration on both sides of the membrane maintained always at a certain level. However, if the ion pumps are obtained the energy from the metabolic reactions, then they can put forth or pump out voluntarily some ions into the membrane to prompt the variations of the ion concentration on both sides of the membrane, thus their gradient of ion concentration on both sides will be changed, Thus, the potential of cell membrane, which is determined and controlled by the relative permeability of specific ions on the cell membrane, will be varied in this case. The changes of the potential are determined and concentration controlled by the and permeability of specific ions as well the energy imported from the factories, but their degree of influences are different for different ions. If the change of the potential of across the nerve membrane achieve and are more than its threshold values ,then the potential of nerve membrane having the features of great, severe of deformation and determination of outline will appear. Then the nerve excitement or nerve impulse as well its transport occurs in this case. Thus, a nerve impulse and its transport along the nerve membrane are also inducted and formed in this case.

From the investigations mentioned we know and affirm the conditions of form of the nerve impulse and its transport. They are described as follows

(1) The distributions of Na<sup>+</sup>and K<sup>+</sup> ions in the inner and the exterior of the nerve membrane are not same, their permeabilities are also different in the nerve membrane. In this case there are all channels of Na<sup>+</sup>and K<sup>+</sup> ions on the nerve membranes. (2) only if the bio-energy is provided and imported constantly to the nerve membrane to trigger the work of sodium pump and potassium pump, let the excitement of nerve membrane to produce and launch the nerve impulse, or else, the nerve impulse cannot be formed, produced and transported.

In practice, the changes of the potential of the neurons in the across membrane is controlled by many factors, such as variations the concentration and of permeability of sodium and potassium ions as well the energy imported from the energy factories. In this case meeting above two conditions the nerve excitement triggered by the action potential can also occur, if only different nerve membranes are in the excited states having a variety of forms and states. Then a nerve impulse will also be produced in the nerve membranes organism. If the nerve organism can obtain the bio-energy, then the nerve impulse with certain nerve information can transport along the nerve fiber organism. Therefore, the nerve impulse and its transport are always and closely related with the acquisition of the bio-energy. Then we can affirm that there are not the nerve impulse and its transport without import of the bio-energy in nerve fiber organizations.

### HODHKIN-HUXLEY MODEL FOR FORM OF NERVE IMPULSE AND ITS NECESSITY OF DEVELOPMENT

In accordance with these conditions and requests of form of nerve impulse and its features we can say that the famous Hodhkin-Huxley model of the nerve excitement (A. L. Hodgkin, et al. 1952; A. L. Hodgkinand and R. D. Keynes, 1955; A. L. Hodgkin and R. D. Keynes 1953) and transport of nerve impulse are not a complete theory. Why?

In fact, Hodhkin-Huxley proposed and established (A. L. Hodgkin, et al. 1952; A. L. Hodgkinand and R. D. Keynes, 1955; A. L. Hodgkin and R. D. Keynes 1953) first the model of the nerve impulse in the nerve membrane. In this case they assumed artificially that the possibility of potassium ions through their channel on the nerve membrane are controlled by four polar molecules with certain electric dipole moments, which are in the entrances of the channels. In this case they denoted the conductance of potassium ions appeared by

$$g_{K} = \overline{g}_{k} n^{4}$$

where  $g_k$  is maximal conductance of the solutions in the body, n is a characteristic constant of nerve membrane. Hodhkin-Huxley (A. L. Hodgkin, et al. 1952; A. L. Hodgkinand and R. D. Keynes, 1955; A. L. Hodgkin and R. D. Keynes 1953) assumedagain that n meets the equation:

$$\frac{dn}{dt} = \alpha_n (1-n) - \beta_n n$$

where  $\alpha_n$  and  $\beta_n$  are some rate contents for the sodium ions, they are related with the temperature of the nerve organism, the concentration of calcium ions and the potential V of the nerve membrane. If the potential is increased along the direction of its positive values, then the value of  $\alpha_n$  is increased, but  $\beta_n$  is decreased. If the potential is a content, then the solution of above equation can be denoted by  $n(t) = A - (A - n_0) \exp(t/t_0)$ , where  $n_0$  is its early value,  $A = \alpha_n (n_n + \beta_n)$ .

For the motions of sodium ions, their possibility along the channels on the nerve membrane, Hodhkin-Huxley assumed still that they are controlled by four polar molecules, in which but three polar molecules carrier only a pair of charge, respectively, but other molecule carries three pairs charges. When the channels have not be opened, the positive charges of the above three polar molecules can be turned to the out parts of the mouths of the channels to stop the import of the sodium ions, thus the channels are closed, or speaking, the activity of the channels are lost, thus the possibility along the channels are now in the states of negative charges. then can also come into the channels under the action of the electric field. In this case the negative charges can come into the mouths of the channels to attract the sodium ions. Thus, the sodium ions can come into the channels in this case. However, the molecular dipoles with three pairs of charge turn immediately to the positive charges to face the entrance of these channels from 3 pairs original negative charges turn to the positive charges to face the entrance. Then the activity of the channels is lost in this case. This is called h process in this case.

In this case, the probability of Na<sup>+</sup> ions across the nerve membrane are determined together by the probability appearing the open state related to the three processes of m and the probability appearing the closed state related to the process of h=1-m. Thus the conductance of sodium ions can be represented by the equation:

$$g_{Na} = \overline{g}_{Na} m^3 h$$

where  $g_{Na}$  is the maximal conductance of the sodium ions, m and h are some general contents, they meet following equations :

$$\frac{dm}{dt} = \alpha_m (1-m) - \beta_m m ,$$

$$\frac{dh}{dt} = \alpha_h (1-h) - \beta_h h$$

where  $\alpha_m$ ,  $\alpha_h$ ,  $\beta_m$  and  $\beta_h$  are some

contents, which are related with the temperature of nerve membrane and concentration of the calcium ion and the potential of nerve membranes. If the fibrous inner potential are changed along the positive direction, then  $\alpha_m$  and  $\alpha$  will be increased, but  $\beta m$  aad  $\beta_h$  are decreased.

If m and n are known, then from Equations above mentioned we can obtain sodium conductance. the potassium and membranes conductance the conductance in these cases of depolarization of cell membranes. Some researchers measured really the nerve membrane conductance, depolarization of cell membranes, sodium conductance and potassium conductance and their changes in the squid. These results obtained from experiments in the squid are basically consistent the theoretical results bv Hodhkin-Huxley's model. This manifest that Hodhkin-Huxley's model is successful.

However, we knew clearly from above investigation that Hodhkin-Huxley's model (A. L. Hodgkin, et al. 1952; A. L. Hodgkinand and R. D. Keynes, 1955; A. L. Hodgkin and R. D. Keynes 1953) is only a simple description of the properties of nerve impulse and it has not elucidated the form of the nerve impulse and its feature of transport along the nerve membranes. Strictly speaking, Hodhkin-Huxley's model is only a static theory of the nerve impulse, can describe only the form and features of the action potential because it has not researched the properties of transport of nerve impulse along the nerve fibers triggered by the work of sodium pump and potassium pump under the drive of the bioenergy importing from biological organisms .

However, the transports of nerve impulse are widely existent in the life systems, there are not life activity without the transports of nerve impulse. Therefore, to investigate the form of nerve impulse and its features of transports have very important significances in life sciences. Then we can affirm that Hodhkin-Huxley model is only an approximate theory, it cannot describe and elucidate correctly the form and transport of nerve impulse along the nerve fibers. This means that the Hodhkin-Huxley model must be developed forward to built complete the theory of transport of nerve impulse in life systems.

In the following sections we will research and elucidate completely and in detail the form of nerve impulse and its features of transports driven by the works of sodium pump and potassium pump, which are triggered by the bio-energy. The energy are released from the hydrolysis reaction of the adenosine phosphate (ATP) molecules in the mitochondrion in the cells. The energy are transported to the sodium pump and potassium pump through the protein molecules. We should investigate in detail these processes and properties of transport of the bio-energy. These investigations are described as follows.

## THE THEORY OF BIO-ENERGY TRANSPORT ALONG THE PROTEIN MOLECULES AND ITS C PROPERTIES

## The Theory of Bio-energy Transport along the Protein Molecule in the Living System

As it is known from the above investigation that life or life activity is just processes mutual changes of and coordination and unity for the bio-material, bio-energy and bio-information in the live systems. Their synthetic movements and cooperative changes are just total life activity, where the bio-material is the foundation if life, the bio-energy is its center, the bioinformation is its key, the transfer of bioinformation are always accompanied by the transport of bio-energy in living systems

(PangXiao-Feng 2007). Thus, the bio-energy and its transport are an fundamental and important process in life activity. In this case the bio-energies are mainly provided by that released in adenosine phosphate (ATP) hydrolysis in the living systems. Namely, an ATP molecule reacts with water, which results in the energy release of 0.43eV under normal physiological conditions as mentioned above. The reaction is represented in Eq.(18) in chapter1.The bioenergies needed in biological processes in the bio-tissues come basically from this energy, namely, it is mainly used in these processes, such as the muscle contraction, DNA duplication and the neuroelectric pulse transfer on the membranes of neurocytes as well as work of calcium pump and sodium pump. Therefore, there is always a process of bio-energy transport from the producing place to required organisms in the living systems. However, understanding of mechanism of the bio-energy transport in the living systems is a long standing problem which retains interesting up now. Plenty of the mechanisms of bio-energy transport were proposed, but most of them are not successful (PangXiao-Feng 2007; D.A. Baylor, et al. A.F. Huxley 1957; G..E. Schulz and R.H. Schirmar 1979). It is known that ATP molecules bind often to a specific site on the protein molecule, the energy supply for most protein activity and functions is provided by the ATP hydrolysis. Thus the transport of bio-energy released by ATP hydrolysis is always related to the protein molecules and their changes of conformation and configuration.

As it is known, the protein molecules are composed of more than twenty different kinds of individual building blocks called amino acids. Each amino acid is again constructed by an amino group( $NH_2$ ), a carboxyl group (COOH), and a side group, or radical attached to an  $\alpha$  carbon atom. The radical is what distinguishes one amino acid from another. Amino acids polymerize to form long chains of residues that constitute a protein molecule. When two amino acids join together, they release one water molecule and form a peptide bond. When the polypeptide chain has been formed, it can fold into a variety of complex threedimensional conformations. Of particulars are the three structural configurations that recur over and over in proteins: the  $\alpha$  –helix, the β-sheet and globular conformation. In the  $\alpha$ -helix the polypeptide chain is tightly coiled about its longitudinal axis. In theßsheet the chain can be visualized as pleated strands of protein. The globular conformation is most complex since the chains are folded irregularly into a compact near- spherical shape. Part of the chain can often be in the  $\alpha$ -helix or the  $\beta$ sheet configuration (PangXiao-Feng 2007; G..E. Schulz and R.H. Schirmar 1979; A. S. Davydov 1982; C.W.F. McClare 1974).

Generally speaking, the energy can be converted to a particular vibrational excitation within a protein molecule. A likely recipient exchange is the amide-I vibration. Their vibration is primarily a stretch and contraction of the C= O bond of the peptide groups. The amide-I vibration is also a prominent feature in infrared and Raman spectra of protein molecules. Experimental measurement shows that one of the fundamental frequencies of the amide-I vibration is about 0.205eV. This energy is about half the energy released during the ATP hydrolysis. Moreover, it remains nearly constant from protein to protein, indicating that it is rather weakly coupled to other degrees of freedom. All these factors can lead to the assumption that the energy released by ATP hydrolysis might stay localized and stored in the amide-I vibration excitation. A biological role for vibrational excited states was first proposed by McClare in connection with a possible crisis in bioenergetics (A.F. Huxley 1957) (for more information about McClare's work see the article by Luca Turin, in this issue (G.E. Schulz and R.H. Schirmar 1979). Then, as an alternative to electronic mechanisms, one can assume that the energy is stored as vibrational energy in the C=O stretching model (amide-I) of polypeptide chains in the protein molecules. In view of the features of bio-energy some theoretical models of the bio-energy transport have been proposed subsequently. We here will survey these theoretical models as well as their properties and correctness.

## Davydov's theory

As it is well known, an inspection of the  $\alpha$ -helix structure reveals three channels of hydrogen-bonded peptide groups approximately in the longitudinal direction with the sequence :

:....H-N-C=O...H-N-C=O...H-N-C=O...H-N-C=O...., where the dotted lines indicate the hydrogen bond, Davydov worked out this idea in the  $\alpha$ -helix protein molecules, which is shown in Fig. 1, based on McClare's proposal for explaining the conformational changes responsible for muscle contraction (A. S. Davydov, A.D. Suprun 1973; A. S. Davydov 1973), where the trigger is the energy donating reaction of ATP hydrolysis. His theory has shown how a soliton could travel along the hydrogen-bonded spines of the  $\alpha$ -helix protein molecular chains. Davydov's assumption was that the first event after the ATP hydrolysis is the storing of the energy released by the chemical reaction in a vibrational mode of the peptide group. In 1973 Davydov suggested that the amide-I energy could stay localized through the nonlinear interactions of the vibrational excitation with the deformation in the protein structure caused by the presence of the excitation. The excitation and the deformation balance each other and form a soliton. Thus the bio-energy can transport along the protein molecules in virtue of the motion of the soliton. This mechanism can be described classically as follows. Vibrational energy of the C=0 stretching (or amide-I) oscillators that it localized on the helix chains acts, through a phonon coupling effect, to deform the structure of the amino acid residue, the deformation of amino acid residues reacts, again through phonon coupling, to trap the amide-I vibrational guanta and prevent its dispersion. Thus a soliton is formed in this process. This effect is called self-trapping of the amide-I vibrational quantum (or exciton). The soliton can moves over a macroscopic distances along the molecular chains keeping its shape and energy and momentum and other quasi-particle properties. This is just Davydov theory of bioenergy transport in αhelical protein molecules, which was proposed by Davydov in1973 (A. S. Davydov 1973; A. S. Davydov 1991; A. S. Davydov 1979; A.S. Davydov 1983; A. S. Davvdov The mathematical 1982). techniques that are used to analyze Davydov's soliton are analogous to some that have been developed for the "polaron' effect suggested by Landau (L. D. Landau, and E. M. Lifshitz 1987; L. D. Landau 1933) and studied by Pekar (S. Pekar 1946), (Frohlich 1952; W. F"orner 1991), Holstein (1959) and many others.

Therefore, Davydov's first main addition to McClare's proposal was to point out a specific vibrational band that is found in proteins and that is ideal for the storage and propagation of energy. His second main contribution to the field of bioenergetics was to realize that the amide-I energy depends on the strength of the hydrogen bond that may exist between the oxygen of one peptide group and the nitrogen of another, Thus Davydov took into account the coupling between the amide-I vibration (intramolecular excitation or exciton) and deformation of amino acid residues (or, acoustic phonon) in the  $\alpha$ -helix proteins and gave further the Hamiltonian of the system (A. S. Davydov 1973; A. S. Davydov 1991; A. S. Davydov 1979; A.S. Davydov 1983; A. S. Davydov 1982), which is as follows

$$H = H_{ex} + H_{ph} + H_{int}.$$
 (1)

with

$$H_{ex} = \sum_{n} \left[ \left( \mathcal{E}_{0} - D \right) B_{n}^{+} B_{n} - J \left( B_{n}^{+} B_{n+1} + B_{n+1}^{+} B_{n} \right) \right]$$
(2)

$$H_{ph} = \sum_{n} \left[ \frac{P_{n}^{2}}{2M} + \frac{1}{2} w(u_{n} - u_{n-1}) \right] \text{ and }$$
$$H_{int} = \sum_{n} \chi(u_{n+1} - u_{n-1}) B_{n}^{+} B_{n}$$
(3)

which are the Hamiltonians of the excitons with energy  $\mathcal{E}_0$ , the vibration of amino acid residue and their interaction, respectively, where  $B_n^+(B_n)$  is the exciton creation (annihilation) operator at the *n*th site with an energy  $\mathcal{E}_0 = 0.205$  eV. They satisfy the commutation relation:

$$\begin{bmatrix} B_n, B_m^+ \end{bmatrix} = \delta_{nm}, \begin{bmatrix} B_n, B_m \end{bmatrix} = \begin{bmatrix} B_n^+, B_m^+ \end{bmatrix} = 0.$$
(4)



Fig. 1. structure of  $\Omega$  — helical protein (A. C. Scott 1982; A. C. Scott 1984; A.H. Rornero 1999; D. W. Brown 1986; D. W. Brown 1987; D. W. Brown 1988; D. W. Brown 1990; D. W. Brown 1986; D. W. Brown 1988; D. W. Brown and Z. Ivic 1989; K. Lindenberg 1990; M. J. Skrinjar 1988; A. C. Scott 1987; A. C. Scott 1990; Pang Xiao-Feng 1986; Pang Xiao-Feng 1986)

Also in Eq. (84), the  $\mathcal{E}_0 B_n^+ B_n$  denotes the kinetic energy of the exciton.  $J(B_n^+ B_{n+1}^- + B_{n+1}^+ B_n^-)$ represents the resonant (or dipole-dipole) interaction between neighboring excitons,  $J = 2\vec{d}^2/r_0^3$ (or dipole-dipole) the resonance is interaction that determines the transition of an exciton from one molecule to another. Then  $DB_n^+B_n$  denotes the interaction of the exciton with the lattice or peptide groups. D is the deformation excitation energy, and is approximately a constant,  $u_n$  and  $P_n$  are the displacement of the peptide groups and its conjugate moment, M is the mass of the peptide group, w is the spring constant of the molecular chains and  $\chi = \partial J / \partial u_n$  is the coupling constant between the exciton and vibrational quantum of the peptide group (phonon). Obviously, the Hamiltonian in Eq.(1) represents the elementary motions of the exciton and phonon as well as their interactions in the systems.

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

$$|D_{2}(t)\rangle = |\varphi(t)\rangle |\beta(t)\rangle =$$

$$\sum_{n} \varphi_{n}(t)B_{n}^{+} \exp\left(-\frac{i}{\hbar}\sum_{n} [\beta_{n}(t)P_{n} - \pi_{n}(t)u_{n}]\right)|0\rangle.$$
(5a)
or
$$\left(a_{n}(t)B_{n}^{+} \exp\left(-\frac{i}{\hbar}\sum_{n} [\beta_{n}(t)P_{n} - \pi_{n}(t)u_{n}]\right)|0\rangle.$$

$$|D_{1}(t)\rangle = \sum_{n} \left\{ \begin{cases} \varphi_{n}(t)B_{n}^{*} \exp \\ \left(\sum_{q} \left[\alpha_{nq}(t)a_{q}^{*} - \alpha_{nq}^{*}(t)a_{n}\right]\right) \right\} |0\rangle \end{cases}$$
(5b)

where

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

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

Obviously, the Davydov wave functions, both  $|D_1 > and |D_2 >$ , are concerned, they are all not true solutions of the protein molecules., in the meanwhile, 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.

Using the functional  $\langle \Phi(t) | H | \Phi(t) \rangle$ and the variational approach, Davydov et al (A. S. Davydov 1973; A. S. Davydov 1991; A. S. Davydov 1979; A.S.Davydov 1983; A. S. Davydov 1982) got:

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

and

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

where,

$$\begin{split} \beta_n(t) &= \left\langle \Phi(t) \left| u_n \right| \Phi(t) \right\rangle, \pi_n = \left\langle \Phi(t) \left| P_n \right| \Phi(t) \right\rangle = M \; \frac{\partial \beta_n}{\partial t} \\ W &= \frac{1}{2} \sum_n \left[ M \left( \frac{\partial \beta_n}{\partial t} \right)^2 + w \left( \beta_n - \beta_{n-1} \right)^2 \right]. \end{split}$$

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

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

and

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

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

$$\phi(x,t) = \sqrt{\frac{\mu_D}{2}} \sec h \left[ \frac{\mu_D}{r_0} (x - x_0 - vt) \right] \exp\left\{ \frac{\hbar v}{2Jr_0^2} (x - x_0) - \frac{E_D t}{\hbar} \right\}$$
(11)

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

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

Equations (11)-(12) show clearly that the bio-energy transports along the protein molecular chains in the form of bell-type of soliton in Eq.(11). The soliton is localized over a scale  $r_0/\mu_D$ , where,  $\mu_D = \chi_1^2/(1-s^2)Jw, G_D = 4J\mu_D$ ,  $s^2 = v^2/v_0^2, v_0 = r_0 (w/M)^{1/2}$  is the sound speed in the protein molecular chains, v is the velocity of the soliton,  $r_0$  is the lattice constant. From the above result we know

that a positive  $\chi_1 = \chi$  means that when the hydrogen bond length decreases, the energy of the amide I vibration decreases, and vice versa. When  $\chi = 0$ , the amide I energy does not depend on the relative positions of the peptide groups and the amide I excitation propagates from one peptide group to the next due to the dipoledipole interactions J. In this case, an amide I excitation that is initially located at one peptide group will spread to other peptide groups, and the state will guickly cease to be localized. On the other hand, when  $\chi \neq 0$ , an excitation initially located at one peptide group will induce a distortion of the associated hydrogen bond (a compression for positive  $\chi$  and an expansion for negative  $\chi$  ), which, in turn, will decrease the energy of the corresponding amide I state. When the (negative) interaction energy is greater, in absolute terms, than the distortion energy, which is always positive, the state of the amide- I excitation together with the distortion has an energy that is lower than the state of the amide-I excitation in the absence of the distortion.

where the particle number operator  $\hat{N} = \sum_{n} B_{n}^{\dagger} B_{n}$ . This shows that the Davydov soliton is formed through self-trapping of one exciton with binding energy  $E_{BD} = -\chi_{1}^{4} / 3Jw^{2}$ .

# The Improved Models of Davydov's Theory

Davydov's idea yields a compelling picture for the mechanism of bio-energy

transport in protein molecules and consequently has been the subject of a large number of works including Takeno soliton model and Yomosa's model (T. Holstein 1959; S. Takeno 1983; S.Takeno 1984; S. Takeno 1985; S. Takeno 1986; V.K. Fedyamin et al. 1977; S. Yomosa 1983; S. Yomosa 1982; Gue Bai-lin and Pang Xiao-Feng 1987; A. C. Scott 1991; A. C. Scott 1982; A. C. Scott 1983; A. C. Scott 1982; A. C. Scott 1984; A.H. Rornero et al. 1999; D. W. Brown et al. 1986; D. W. Brown 1987; D. W. Brown 1988; D. W. Brown 1990; D. W. Brown 1986; D. W. Brown 1988; D. W. Brown and Z. lvic 1989; K. Lindenberg 1990; M. J. Skrinjar 1988; A. C. Scott 1987; A. C. Scott 1990; Pang Xiao-Feng 1986; Pang Xiao-Feng 1986; Pang Xiao-Feng 1987; P. L. Christiansen and A.C. Scott 1990; L J. Halding et al. 1988; L.Cruzeiro et al. 1988; L.Cruzeiro-Hansson 1993; L.Cruzeiro-Hansson 1992; A. C. Scott 1990; W. Forner 1991; W. Forner 1999; W. Forner 1991; W. Forner 1992: W. Forner 1993: Η. Motschman et al. 1989; P. S. Lomdahl and W. C. Kerr 1985; W. C. Kerr and P. S. Lomdahl 1989; X. Wang et al. 1989; X. Wang et al. 1989; J.P. Cottingham and J.W. Schweitzer 1989; J. W. Schweitzer 1992; J. M. Hyman et al. 1981; A. F. Lawrence 1986; B. Mechtly and P.B. Shaw 1988; L. MacNeil and A.C. Scott 1984; H. Bolterauer and M. Opper 1991; J. C. Eibeck et al. 1985; Pang Xiao-Feng 1990; Pang Xiao-Feng 1994; Pang Xiao-Feng 1999: Pang Xiao-Feng 1993; Pang Xiao-Feng 1994; Pang Xiao-Feng 1993; Pang Xiao-Feng 1996; Pang Xiao-Feng 1997; Pang Xiao-Feng 1993; Pang Xiao-Feng 1997; Pang Xiao-Feng 1987; Pang Xiao-Feng 1995; Pang Xiao-Feng 1996; Pang Xiao-Feng 1997; Pang Xiaofeng 1994; Pang Xiao-Feng 2000; Pang Xiao-Feng 1999; L Cruzeiro et al. 2009). A

lot of issues related to the Davydov model, including the foundation and accuracy of the theory, the quantum and classical properties and the thermal stability and lifetimes of the Davydov soliton have been extensively and critically examined by many scientists (A. C. Scott 1982; A. C. Scott 1983; A. C. Scott 1982; A. C. Scott 1984; A.H. Rornero et al. 1999; D. W. Brown et al. 1986; D. W. Brown 1987; D. W. Brown 1988; D. W. Brown 1990; D. W. Brown 1986; D. W. Brown 1988; D. W. Brown and Z. lvic 1989; K. Lindenberg 1990; M. J. Skrinjar 1988; A. C. Scott 1987; A. C. Scott 1990; Pang Xiao-Feng 1986; Pang Xiao-Feng 1986; Pang Xiao-Feng 1987; P. L. Christiansen and A.C. Scott 1990; L J. Halding et al. 1988; L.Cruzeiro et al. 1988; L.Cruzeiro-Hansson 1993; L.Cruzeiro-Hansson 1992; A. C. Scott 1990; W. Forner 1991; W. Forner 1999; W. Forner 1991; W. Forner 1992; W. Forner 1993; Η. Motschman et al. 1989; P. S. Lomdahl and W. C. Kerr 1985; W. C. Kerr and P. S. Lomdahl 1989: X. Wang et al. 1989: X. Wang et al. 1989; J.P. Cottingham and J.W. Schweitzer 1989; J. W. Schweitzer 1992; J. M. Hyman et al. 1981; A. F. Lawrence 1986; B. Mechtly and P.B. Shaw 1988; L. MacNeil and A.C. Scott 1984; H. Bolterauer and M. Opper 1991; J. C. Eibeck et al. 1985; Pang Xiao-Feng 1990; Pang Xiao-Feng 1994; Pang Xiao-Feng 1999; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993: Pang Xiao-Feng 1993: Pang Xiao-Feng 1994; Pang Xiao-Feng 1993; Pang Xiao-Feng 1996; Pang Xiao-Feng 1997; Pang Xiao-Feng 1993; Pang Xiao-Feng 1997; Pang Xiao-Feng 1987; Pang Xiao-Feng 1995; Pang Xiao-Feng 1996; Pang Xiao-Feng 1997; Pang Xiaofeng 1994; Pang Xiao-Feng 2000; Pang Xiao-Feng 1999; L Cruzeiro et al. 2009) and the following questions have been of particular concern. (1) What is the correct quantum mechanical description of

Davydov's soliton at low temperature? (2) How does the soliton get started on an alpha-helix proteins" ? (3) Is Davydov's soliton stable at the biological temperature 300K? If not, how long will it last ? (4) How may Davydov's theory be generalized to include charge transfer and more general protein structures? Therefore, considerable controversy has arisen in recent years concerning whether the Davydov soliton can provide a viable explanation for bio-energy transport. It is out of question that the fluctuations quantum 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 (L J. Halding et al. 1988; L.Cruzeiro et al. 1988; L.Cruzeiro-Hansson 1993; L.Cruzeiro-Hansson 1992; A. C. Scott 1990; W. Forner 1991; W. Forner 1999; W. Forner 1991; W. Forner 1992; W. Forner 1993; H. Motschman et al. 1989; P. S. Lomdahl and W. C. Kerr 1985; W. C. Kerr and P. S. Lomdahl 1989; X. Wang et al. 1989; X. Wang et al. 1989; J.P. Cottingham and J. W. Schweitzer 1989; J. W. Schweitzer 1992; J. M. Hyman et al. 1981; Pang Xiao-Feng 1994; Pang Xiao-Feng 1999; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993; Pang Xiao-Feng 1993). Other simulations showed that the Davydov soliton is stable at 300K (S. Yomosa 1982; Gue Bai-lin and Pang Xiao-Feng 1987; A. C. Scott 1991; A. C. Scott 1982; A. C. Scott 1983; A. C. Scott 1982; A. C. Scott 1984; A.H. Rornero et al. 1999), but they were based on classical equations of motion which are likely to yield unreliable estimates for the stability of the Davydov's soliton (A. S. Davydov 1973; A. S. Davydov 1991; A. S. Davydov 1979; A.S.Davydov 1983; A. S. Davydov 1982). The simulations based on the ID  $_2$  > state in Eq.(5a) generally show that the stability of the soliton decreases with increasing

temperatures and that the soliton is not sufficiently stable in the region of biological temperature. Since the dynamical equations used in the simulations are not equivalent to the Schrödinger equation, the stability of the soliton obtained bv these numerical simulations is unavailable or unreliable. The simulation (C.W.F. McClare 1974) based on the  $ID_1$  > state in Eq.(5b) with the thermal treatment of Davydov soliton (C.W.F. McClare 1974; Pang Xiao-Feng 1986), where the equations of motion are derived from a thermally averaged Hamiltonian. yields the wondering result that the stability of the soliton is enhanced with increasing temperature, predicting that  $ID_1 > -$  type soliton is stable in the region of biological temperature. Evidently, the conclusion is doubtful because the Davydov procedure in which one constructs an equation of motion for an average dynamical state from an average Hamiltonian, corresponding to the Hamiltonian averaged over a thermal distribution of phonons, is inconsistent with standard concepts of quantum-statistical mechanics in which a density matrix must be used to describe the system. Therefore, there exists not an exact fully quantummechanical treatment for the numerical simulation of the Davydov soliton. However, for the thermal equilibrium properties of the Davydov soliton, there is a quantum Monte Carlo simulation (P. S. Lomdahl 1985; W. C. Kerr and P. S. Lomdahl 1989). In the simulation, correlation characteristic of solitonlike quasiparticles occur only at low temperatures, about T<10K, for widely accepted parameter values. This is consistent at a qualitative level with the result of Cottingham et al. (X. Wang 1989; X. Wang 1989). The latter is a straightforward quantum-mechanical perturbation calculation. The lifetime of the Davydov soliton obtained by using this method is too small (about  $10^{-12} - 10^{-13}$  sec ) to be useful in biological processes. This shows clearly that the Davydov solution is not a true wave function of the systems. A through study in terms of parameter values, different types of disorder, different thermalization schemes, different wave functions, and different associated dynamics leads to a very complicated picture for the Davydov model (L. Cruzeiro-Hansson 1993; L.Cruzeiro-Hansson 1992; A. C. Scott 1990; W. Forner 1991; W. Forner 1999; W. Forner 1991; W. Forner 1992; W. Forner 1993; H. Motschman et al. 1989; P. S. Lomdahl and W. C. Kerr 1985; W. C. Kerr and P. S. Lomdahl 1989; X. Wang 1989). These results do not completely rule out the Davydov theory, however they do not eliminate the possibility of another wave function and а more sophisticated Hamiltonian of the system having a soliton with longer lifetimes and good thermal stability.

Indeed, the question of the lifetime of the soliton in protein molecules is twofold. In Langevin dynamics, the problem consists of uncontrolled effects arising from the semiclassical approxima- tion. In guantum 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 (D. W. Brown et al. 1986: D. W. Brown et al. 1987: D. W. Brown 1988; D. W. Brown 1990; D. W. Brown 1986; D. W. Brown 1988; D. W. Brown, Z. Ivic 1989; K. Lindenberg 1990; M. J. Skrinjar 1988; A. C. Scott 1987; A. C. Scott 1990). Although some of these wave functions lead to exact guantum states and exact quantum dynamics in the J=0 state, they also share a problem with the original Davydov wave function, namely that the degree of approximation included when  $J \neq 0$  is not known. Therefore, it is

necessary to reform Davydov's wave function.

Scientists had though that the soliton with a multiquantum (  $n \ge 2$  ), for example, the coherent state of Brown et al. (D. W. Brown 1986), the multi quantum state of Kerr et al. and Schweitzer, the two-quantum state of Cruzeiro -Hansson and Forner, and so on, would be thermally stable in the region of biological temperature and could provide a realistic mechanism for bio-energy transport in protein molecules. In the Brown et al's model (D. W. Brown 1986), the state of the excitons was denoted by a coherent state vector  $|A(t)\rangle$ , which is defined by

$$|A(t)\rangle = |a_1(t)\rangle \otimes |a_2(t)\rangle \otimes ... \otimes |a_N(t)\rangle$$

wherein  $\left|a_{n}(t)\right\rangle$  is a pure coherent state defined by

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

where the complex scalar  $\alpha_n(t)$  is the coherent-state amplitude, which may take on all values in the complex plane, The product state  $|A(t)\rangle$  may be defined by the property that  $a_n |A(t)\rangle = a_n(t) |A(t)\rangle$  for all of the  $a_n$ . The expectation value of a Hamiltonian operator of the system  $H[a, a^+]$  in the state  $|A(t)\rangle$  is therefore a real scalar function  $H[a(t), a^*(t)]$  for all the  $\alpha_n(t)$  and their complex conjugates. Thus we can presume that the starting Hamiltonian operator is in normal ordered form so that there is no ambiguity in the

 $H[a,a^+]$ relationship between and  $H[a(t), a^{*}(t)]$ . Then we can obtain the properties of the exciton-soliton in the system by general method. However, the assumption of the standard coherent state is unsuitable or impossible for biological protein molecules because there are innumerable particles in this state and one could not retain conservation of the number of particles of the system and is also inconsistent with the fact that the bioenergy released in ATP hydrolysis can excite only two guanta of amide-I vibration.

In the Schweitzer's model (J. M. Hyman 1981) of the multiquantum state the state of the excitons was denoted by

$$\begin{aligned} \left|\varphi(t)\right\rangle &= \sum_{m} \alpha(m,t) \left|0\right\rangle_{ex} \\ &= \frac{1}{\sqrt{m!}} \sum_{nm} \varphi_{nm}(t) (B_{n}^{+})^{m} \left|0\right\rangle_{ex} \end{aligned}$$

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

In Forner 's model of two-quanta (W. Forner 1992),he represented the state of the exciton by

$$\left|\varphi(t)\right\rangle == \frac{1}{\sqrt{2!}} \left(\sum_{n} \varphi_{n}(t) B_{n}^{+}\right)^{2} \left|0\right\rangle_{ex}$$

Forner's numerical results (W. Forner 1991; W. Forner 1999; W. Forner 1991; W. Forner 1992; W. Forner 1993; H. Motschman et al. 1989; P. S. Lomdahl and W. C. Kerr 1985) shows that the soliton of two-quantum state is more stable than that with a one-quantum state.

Cruzeiro-Hansson (A. C. Scott 1990) 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 (A. C. Scott 1990):

$$|\phi(t)\rangle = \sum_{n,m=l}^{N} \varphi_{nm} (\{u_{l}\},\{P_{l}\},t) B_{n}^{+} B_{m}^{+} |0\rangle_{ex},$$
(13)

where  $B_n(B_n^+)$  is the annihilation (creation) operator for an amide-I vibration quantum (exciton),  $u_i$  is the displacement of the lattice molecules,  $P_l$  is its conjugate momentum, and  $\left|0>_{\mathrm{ex}}\right|$  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  $v = JW/\chi_1^2$  and  $Ln\beta(\beta = 1/K_BT)$  in the so-called two-quantum state, Eq.(13), 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 that of the onequantum state. From the results of above thermal averages, he drew the conclusion that the wave function with a two-guantum state can lead to more stable soliton solutions than the wave function with a onequantum 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.(13) (A. C. Scott 1990), we can find that the Cruzeiro-Hansson wave function does not represent exactly the two-quantum state. To find out how many quanta the state Eq.(13) indeed contains, we have to compute the expectation value of the exciton number operator.

 $N = \sum_{n} B_{n}^{+} B_{n}$ , in this state, Eq.(13), and sum over the sites, i.e., the exciton numbers N are

$$N = \langle \varphi | \sum_{n} B_{n}^{+} B_{n} | \varphi \rangle = \sum_{ijlmn} \varphi_{im}^{*} \varphi_{jlex} \langle 0 | B_{i} B_{m} B_{n}^{+} B_{n} B_{j}^{+} B_{l}^{+} | 0 \rangle_{ex}$$
(14)  
$$= \sum_{nj} (\varphi_{nj}^{*} \varphi_{jn} + \varphi_{jn}^{*} \varphi_{jn}) + \sum_{nl} (\varphi_{nl}^{*} \varphi_{nl} + \varphi_{ln}^{*} \varphi_{nl}) = 4$$

where we use the relations

$$[B_{n}, B_{j}^{+}] = \sigma_{nj}, \sum_{nl} |\varphi_{nl}|^{2} = 1$$
  

$$_{ex} < 0 |B_{n}^{+}|_{0} >_{ex} = _{ex} < 0 |B_{n}^{+}B_{n}|_{0} >_{ex}$$
  

$$=_{ex} < 0 |B_{n}^{+}B_{m}B_{1}|_{0} >_{ex} = ... = 0$$

Therefore, the state, Eq.(13), as it is put forward (A. S. Davydov, and A.D.Suprun 1973) in Eq.(13) deals, in contradiction to the author's statements, with four excitons (quanta), instead of two excitons. Obviously it is not possible to create the four excitons by the energy released in the ATP hydrolysis (about 0.43 eV). Thus the author's wave function is still not relevant for protein and his discussion molecules. and conclusion are all unreliable and implausible in that paper (A. C. Scott 1990).

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

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

Subsequently, Cruzeiro L.et al (D.A. Baylor and A.L. Hodgkin 2003; A.F. Huxley, R. Nidergerke 1954; A. S. Davydov 1975; A. S. Davydov 1976) and Pouthier et al (A. S. Davydov and A.A. Eremko 1977; A. S. Davydov et al. 1978) proposed a dynamical model of nonconserving Davydov monomer nonconserving involvina Davvdov а Hamiltonian for the energy transport, in which they thought that the Davydov's model cannot describe the conversion of that energy into work, because it conserves the number of excitations. With the aim of describing conformational changes, they considered a nonconserving generalization of the model, which is found to describe

essentially a contraction of the hydrogen bond adjacent to the site where an excitation is present. Unlike the one-site Davydov model, that contraction is time dependent because the number of excitations is not conserved. However, considering the time average of the dynamical variables, the results reported here tend to the known results of the Davydov model.

Meanwhile, K.Moritsugu et.al (A. S. Davydov and N.I. Kislukha 1976) and H.Fujisaki et al. considered the anharmonic coupling between the amide-I mode and intramolecular normal modes. These models are helpful for solving the problem of bioenergy transport in protein molecules.

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

## Pang's theory of bio-energy and its properties in protein molecues

The results obtained by many scientists over the years show that the Davydov model, whether it be the wave function or the Hamiltonian, is indeed too simple, i.e.., it does not denoted elementary properties of the collective excitations occurring in protein molecules, and many improvements to it have been unsuccessful, as mentioned above. What is the source of this problem? It is well known that the Davydov theory on bioenergy transport was introduced into protein molecules from an exciton-soliton model in generally one-dimensional molecular chains (Davydov and A.A.Serikov 1972; L. S. Brizhik and A. S.Davydov 1984; H. Fohlich 1952). Although the molecular structure of the alpha-helix protein is analogous to some molecular crystals, for example acetanilide (ACN) (in fact, both are polypeptides: the alpha-helix protein molecule is the structure of three peptide channels, ACN is the structure of two peptide channels. If comparing the structure of alpha helix protein with ACN, we find that the hydrogen-boned peptide channels with the atomic structure along the longitudinal direction are the same except for the side group), a lot of properties and functions of the protein molecules are completely different from that of the latter. The protein molecules are both a kinds of soft condensed matter and bio-self -organization with action functions, for instance, selfassembling and self-renovating. The physical concepts of coherence. .collective order effects. and mutual correlation are very important in bio-selforganization, including the protein molecules, when compared with generally molecular systems (H. Fohlich 1983; K. H. Spatschek and F. G. Mertens 1994; F. A. Popp, K. H. Li and Q. Gu, 1993; Mae Wan Ho, F. A. Popp, U. 1994; Pang Xiao-Feng 2000). Therefore, it is worth studying how we can physically describe these properties. We note that Davydov operation also is not strictly correct. Therefore, we think that a basic reason for the failure of the Davydov model is just that it ignores completely the above important properties of the protein molecules.

Let us consider the Davydov model with the present viewpoint. First, as far as the Davydov wave functions. both  $|D_1 > and |D_2 >$ , are concerned, they are not true solutions of the protein molecules. On the one hand, there is obviously asymmetry in the Davydov wave function since the phononic parts is a coherent state, while the excitonic part is only an excitation state of a single particle. It is not reasonable that the same nonlinear interaction generated by the coupling between the excitons and phonons produces different states for the phonon and exciton. Thus, Davydov's wave function should be modified, i.e., the excitonic part in it should also be coherent or quasicoherent to represent the coherent feature of collective excitation in protein molecules. However, the standard coherent (D. W. Brown 1986) and large-n excitation states (X. Wang et al. 1989) are not appropriate for the protein molecules due to the above reasons. 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 two-quanta protein quasi-coherent state for the molecular systems (Pang Xiao-Feng 2001; Pang Xiao-Feng, and Y.P. Feng Yuan-Ping 2005; Pang Xiao-Feng, Zhang Huai-Wu, Yu Jia-Feng, Feng Yuan-Ping 2005; Pang Xiao-Feng, Yu Jia-Fengand Liu Mei-Jie 2010;

Pang Xiao-feng, Feng Yuan Ping, Zhang Huai-wu and S. M. Assad 2006; Pang Xiao-Feng 2001; Pang Xiao-Feng 2001; Pang Xiao-Feng 2002; Pang Xiao-Feng 2001; Pang Xiao-feng 2001; Pang Xiao-Feng and Chen Xiang-Rong 2002; Pang Xiao-feng and Chen Xiang-Rong, 2002; Pang Xiao-Feng and Chen Xiang-Rong, 2001; Pang Xiao-Feng 2001; Pang Xiao-feng 2001; Pang Xiao-Feng 2001; Pang Xiao-Feng, Luo Yu-Hui, 2004; Pang Xiao-feng, Yu Jia-feng and Luo Yu-hui, 2005; Pang Xiao-Feng, Zhang Huai-Wu, and Yu Jia-feng and Luo Yu-hui 2005; Pang Xiao-feng, and Y.H. Luo, 2005; Pang Xiao-feng and Zhang Huai-wu, 2005; Pang Xiao-feng, 2008; Pang Xiaofeng, 2008; Pang Xiao-feng 2010; Pang Xiao-Feng1,2 and LIU Mei-Jie, 2009; Pang Xiao-feng 2009; Pang Xiao-feng and Lui mei-jie, 2009; Pang Xiao-feng, 2008; Pang Xiao-feng, Yu Jia-feng and Lao Yu-hui. 2007; Pang Xiao-feng, 2007; Pang Xiaofeng, Yu Jia-feng and Lao Yu-hui. 2007; Pang Xiao-feng and Liu Mei-jie, 2007; Pang Xiao-feng, Zhang Huai-Wu ,Yu Jia-feng and Luo yu-hui, 2006; Pang Xiao-feng, Zhang Huai-Wu, 2006; Pang Xiao-feng, Chen Xianron, 2006; Pang Xiao-feng, Zhang Huaiwu, 2006; Pang Xiao-feng, 2003; Pang Xiao feng, 2012; Pang Xiao-Feng, 2007).

$$\left|\Phi\left(t\right)\right\rangle = \left|\varphi\left(t\right)\right\rangle \left|\beta\left(t\right)\right\rangle = \frac{1}{\lambda} \left[I + \sum_{n} \varphi_{n}\left(t\right)B_{n}^{+} + \frac{1}{2!}\left(\sum_{n} \varphi_{n}\left(t\right)B_{n}^{+}\right)^{2}\right]\right| 0 >_{ex}$$
(15)  
$$\times \exp\left\{-\frac{i}{h}\sum_{n} \left[\beta_{n}\left(t\right)P_{n} - \pi_{n}\left(t\right)u_{n}\right]\right\} \left|0 >_{ph}\right\}$$

where  $B_n^+$  (B<sub>n</sub>) is boson creation (annihilation) operator for the exciton,  $|0>_{ex} and |0>_{ph}$  are the ground states of the exciton and phonon, respectively,  $u_n$  and P<sub>n</sub> are the displacement and momentum operators of the lattice oscillator at site n, respectively.  $\lambda$  is a normalization constant, we assume hereafter that  $\lambda = 1$  for convenience of calculation, except when explicitly mentioned. The  $\varphi_n(t)$ ,

 $\beta_n(t) = \langle \Phi(t) | u_n | \Phi(t) \rangle$  and

 $\pi_n(t) = \langle \Phi(t) | P_n | \Phi(t) \rangle$  are there sets of unknown functions.

A second problem arises for the Davydov Hamiltonian (A. S. Davydov, 1973; A. S. Davydov, 1991; A. S. Davydov, 1979; A.S.Davydov, 1983; A. S. Davydov, 1982). The Davydov Hamiltonian takes into account the resonant or dipole-dipole interaction of the neighboring amide-I vibrational quanta in neighboring peptide groups with an electrical moment of about 3.5D, but why do we not consider the changes of relative displacement of the neighboring peptide groups arising from this interaction? Thus, it is reasonable to add the new interaction term,  $\chi_2(u_{n+1}-u_n)(B_{n+1}^+B_n+B_m^+B_{n+1})$  , into the Davydov Hamiltonian to represent correlations of the collective excitations and collective motions in the protein molecules, as mentioned above (A. S. Davydov, 1973; A. S. Davydov, 1991; A. S. Davydov, 1979; A.S.Davydov, 1983; A. S. Davydov, 1982). Although the dipole-dipole interac- tion 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, we replace Davydov's Hamiltonian (Pang Xiaofeng, (2000); [Pang Xiao-feng (2001a); Pang Xiao-feng, and Y.P.Feng Yuan-ping (2005); Pang Xiao-feng et al. (2005); Pang Xiaofeng, et al. (2010a); Pang Xiao-feng, et al. (2006a); Pang Xiao-feng, (2001b); Pang Xiao-feng, (2001c); Pang Xiao-feng, (2002); Pang Xiao-feng, (2001d); Pang Xiao-feng, (2001e); Pang Xiao-feng and Chen Xiangrong (2002a); Pang Xiao-feng and Chen Xiang-rong, (2002b); Pang Xiao-feng and Chen Xiang-rong (2001); Pang Xiao-feng (2001f); Pang Xiao-feng, (2001g); Pang Xiao-feng (2001h); Pang Xiao-Feng and Luo Yu-Hui (2004); Pang Xiao-feng, et al. (2005a); (2005b); Pang Xiao-feng, and Y.H.Luo, (2005); Pang Xiao-feng and Zhang Huai-wu, (2005); Pang Xiao-feng, , (2008a); (2008b); Pang Xiao-feng (2010b); Pang Xiao-Feng and LIU Mei-Jie, (2009); Pang Xiao-feng, (2009); Pang Xiao-feng and Lui mei-jie,Int. (2009); Pang Xiao-feng, (2008c); Pang Xiao-feng et al. (2007a); Pang Xiaofeng, (2007a); Pang Xiao-fenget al. (2007b); Pang Xiao-feng and Liu Mei-jie, (2007); Pang Xiao-feng, et al. (2006b); Pang Xiaofeng and Zhang Huai-Wu, (2006a); Pang Xiao-feng and Chen Xianron, (2006); Pang Xiao-feng and Zhang Huai-wu, (2006b); Pang Xiao-feng, (2003); Pang Xiao feng, (2012)) by

$$H = H_{ex} + H_{ph} + H_{int} = \sum_{n} \left[ \varepsilon_0 B_n^+ B_n - J \left( B_n^+ B_{n+1} + B_n B_{n+1}^+ \right) \right] + \sum_{n} \left( \frac{P_n^2}{2M} + \frac{1}{2} w \left( u_n - u_{n-1} \right)^2 \right) + \sum_{n} \left[ \chi_1 \left( u_{n+1} - u_{n-1} \right) B_n^+ B_n + \chi_2 \left( u_{n+1} - u_n \right) \left( B_{n+1}^+ B_n + B_n^+ B_{n+1} \right) \right]$$
(16)

where  $\varepsilon_0 = 0.205 \text{ev}$  is the energy of the exciton (C=0 stretching mode). The present nonlinear coupling constants are  $\chi_1 \text{and} \chi_2$ . They represent the modulations of the onsite energy and resonant (or dipole-dipole) interaction energy of excitons caused by the molecules displacements, respectively .M is

the mass of a amino acid molecule and w is the elasticity constant of the protein molecular chains. J is the dipole-dipole interaction energy between neighboring sites. The physical meaning of the other quantities in Eq.(16) are the same as those in the above explanations.

The Hamiltonian and wave function shown in Eqs.(31)-(32) are different from Davydov's. We added a new interaction term,  $\sum_{n} \chi_2 (u_{n+1} - u_n) (B_{n+1}^+ B_n + B_n^+ B_{n+1})$ , into the original Davydov Hamiltonian. Thus the Hamiltonian now has an one-by-one correspondence on the interactions and can represent the features of mutual correlations of the collective excitations and of collective motions in the protein molecules. We here should point out that the different coupling between the relevant modes was also considered by Takeno et al. (L.Cruzeiro et al. (1988);L.Cruzeiro-Hansson, (1993);L.Cruzeiro-Hansson, (1992); A. C. Scott, (1990) W. Förner , (1991a); W. Förner (1991b)) and Pang [Pang Xiao-feng, (1990); Pang Xiao-feng, (1994); Pang Xiao-feng, (1999a); Pang Xiao-feng, (1993a); Pang Xiao-feng, (1993b); Pang Xiao-feng, (1993c); Pang Xiao-feng, (1993d); Pang Xiao-feng, (1993e); Pang Xiao-feng, (1993f); Pang Xiao-feng, (1994); Pang Xiao-feng, (1993g); Pang Xiao-feng, (1996); Pang Xiao-feng, (1993h); Pang Xiao-feng, (1993i); Pang Xiao-feng, (1997a); Pang Xiao-feng, 1997b); Pang Xiao-feng, (1987); Pang Xiao-feng, (1995); Pang Xiao-feng, , (1996); Pang Xiao-feng, (1997c); Pang Xiao-feng, 1994; Pang Xiao-feng et al. (2000); Pang Xiaofeng, (1999b) 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.(15)-(16).

Obviously, the new wave function of the exciton in Eq.(15) is not an excitation state of a single particle, but rather a coherent state, or accurately, a quasicoherent state because it is just an effective truncation of a standard coherent state, retains only fore three terms of expansion of a standard coherent state, at the same time, when the

 $arphi_n(t)$  is small, for example,  $\left|arphi_n(t)
ight|$  << 1, it approximately also represent can mathematically as a standard coherent state[(K. H. Spatschek and F. G. 1994; F. A. Popp et al. 1993; Mae Wan Ho, et al. 1994; Pang Xiao-feng, (2000); [Pang Xiao-feng (2001a); Pang Xiao-feng, and Y.P.Feng Yuan-ping (2005); Pang Xiao-feng et al. (2005); Pang Xiao-feng, et al. (2010a); Pang Xiao-feng, et al. (2006a); Pang Xiao-feng, (2001b); Pang Xiao-feng, (2001c); Pang Xiao-feng, (2002); Pang Xiao-feng, (2001d); Pang Xiao-feng, (2001e); Pang Xiao-feng and Chen Xiang-rong (2002a); Pang Xiaofeng and Chen Xiang-rong, (2002b); Pang Xiao-feng and Chen Xiang-rong (2001); Pang Xiao-feng (2001f); Pang Xiao-feng, (2001g); Pang Xiao-feng (2001h); Pang Xiao-Feng and Luo Yu-Hui (2004); Pang Xiao-feng, et al. (2005a); (2005b); Pang Xiao-feng, and Y.H.Luo, (2005); Pang Xiaofeng and Zhang Huai-wu, (2005); Pang Xiao-feng, , (2008a); (2008b); Pang Xiaofeng (2010b); Pang Xiao-Feng and LIU Mei-Jie, (2009); Pang Xiao-feng, (2009); Pang Xiao-feng and Lui mei-jie, Int. (2009); Pang Xiao-feng, (2008c); Pang Xiao-feng et al. (2007a); Pang Xiao-feng, (2007); Pang Xiao-fenget al. (2007b); Pang Xiao-feng and Liu Mei-jie, (2007); Pang Xiao-feng, et al. (2006b); Pang Xiao-feng and Zhang Huai-Wu, (2006a); Pang Xiao-feng and Chen Xianron, (2006);

$$|\varphi(t)\rangle \sim \exp\left[-\frac{1}{2}\sum_{n} |\varphi_{n}(t)|^{2}\right]$$

$$\exp\left\{\sum_{n} \varphi_{n}(t)B_{n}^{+}\right\} |0\rangle_{ex} =$$

$$\exp\left\{\sum_{n} [\varphi_{n}(t)B_{n}^{+} - \varphi_{n}^{*}B_{n}]\right\} |0\rangle_{ex}$$
(17)

where  $\sum_{n} |\varphi_{n}(t)|^{2} = 1$ , n denotes the sites of amino acids. Therefore we refer to it

as quasi- coherent state due to these characteristics. Thus Eq.(15) can represent simultaneously the coherent features of collective excitations, phonons and excitons, in the proteins. The condition of  $|\varphi_n(t)| \ll 1$ is also quite correct and resonable for the proteins consisting of amino acids of several hundreds or thousands because of  $\sum_{n} |\varphi_{n}(t)|^{2} = 1$ . Therefore, Eq.(17) is justified and a correct representation. It is well known that the coherent state is certainly normalized, then it is natural that the  $|\varphi_{n}(t)\rangle$  in Eq.(31) or  $|\Phi(t)\rangle$  in Eq.(15) should be also normalized. Thus we should choose  $\lambda=1$  in Eq.(15). This means that we cannot choose other values of  $\lambda \neq 1$  in Eq. (15), or else,  $|\varphi_{i}(t)\rangle$  cannot represent as a standard coherent state in Eq.(17). With that, in this case of  $\lambda \neq 1$ ,  $|\varphi_{r}(t)\rangle$  is neither a quasi-coherent state nor a excited state of single particle, that is, it has not any

biological and physical meanings in this case. This shows clearly that choice of  $\lambda$ =1 in Eq.(15) is correct and reasonable. In such a case it is not an eigenstate of number operator because of

$$\begin{split} \hat{N} | \phi(t) \rangle &= \sum_{n} B_{n}^{\prime} B_{n} \left| \phi(t) \rangle = \left\{ \sum_{n} \phi_{n}(t) B_{n}^{\prime} + \left( \sum_{n} \phi_{n} \phi_{n}(t) B_{n}^{\prime} \right)^{2} \right\} | 0 \rangle_{ex} \\ &= 2 | \phi(t) - \left( 2 + \sum_{n} \phi_{n}(t) B_{n}^{\prime} \right) | 0 \rangle_{ex} \end{split}$$

Therefore, the  $\left| \phi(t) \right>$  represents indeed

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

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$$N = \langle \varphi(t) | \hat{N} | \varphi(t) \rangle = \sum_{n} \langle \varphi(t) | B_{n}^{t} B_{n} | \varphi(t) \rangle = \left\{ \sum_{n} |\varphi_{n}(t)|^{2} + \left( \sum_{n} |\varphi_{n}(t)|^{2} \right) \left( \sum_{m} |\varphi_{m}(t)|^{2} \right) \right\}$$
$$= \left( \sum_{n} |\varphi_{n}(t)|^{2} \right) \left( 1 + \sum_{m} |\varphi_{m}(t)|^{2} \right) = 2$$

where we utilize Eq.(8) and the following relations [S.Takeno, 1985]:

$$\sum_{n} |\phi_{n}(t)|^{2} = 1, \sum_{m} |\phi_{m}(t)|^{2} = 1, [B_{n}.B_{m}^{t}] = \delta_{nm}$$
  

$$e_{x} < 0 | B_{n}^{+} | 0 >_{ex} =_{ex} < 0 | B_{n}^{+}B_{n} | 0 >_{ex} =_{ex} < 0 | B_{n}^{+}B_{m} | 0 >_{ex}$$
  

$$=_{ex} < 0 | B_{n}^{+}B_{m}B_{1} | 0 >_{ex} =_{ex} < 0 | B_{n}^{+}B_{m}B_{1}^{+}B_{n} | 0 >_{ex}$$
  

$$=_{ex} < 0 | B_{n}^{+}B_{m}B_{1}^{+}B_{1}B_{1} | 0 >_{ex} =_{ex} < 0 | B_{n}^{+}B_{m}B_{1}^{+}B_{1}B_{1}B_{1} | 0 >_{ex} .... = 0$$

Therefore, the new wave function in Eq.(31) is a quasi-coherent state containing only two quanta, it 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. In the meanwhile, as far as the form of new wave function in Eq.(31) is concerned, it is either two- quanta states proposed by Forner [W. Förner, (1991); W. Förner (1991); W. Förner , (1999); W. Förner W. Förner , (1992); W. Förner (1991); (1993): H. Motschman, W. Förner and J. (1989). and Cruzeiro-Hansson Ladik [L.Cruzeiro, et al. (1988); L.Cruzeiro-(1993); L.Cruzeiro-Hansson, Hansson. (1992); A. C. Scott, (1990) ] or a standard coherent state proposed by Brown et al .[ A.H. Rornero, et al. (1999); D. W. Brown, et al. (1986); D. W. Brown et al. (1987); D. W. Brown, et al. (1988); D. W. Brown, et al. 1990; D. W. Brown, et al. (1986); D. W. Brown (1988); D. W. Brown and Z. Ivic, (1989); K. Lindenberg et al. (1990) and Kerr et al's (P. S. Lomdahl and W. C. Kerr, (1985); W. C. Kerr and P. S. Lomdahl, (1989) and Schweitzer et al's multiquanta states[W. C. Kerr and P. S. Lomdahl, (1989); X. Wang, et al. (1989). Therefore, the wave function, Eq.(31), is new for the protein molecular systems. It not only exhibits the basic features of collective excitation of the excitons and phonons caused by the nonlinear interaction generated in the system but also agrees with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) may only create two amide-I vibrational guanta, thus, it can also make the numbers of excitons maintain conservation in the Hamiltonian, Eq.(16). 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.(15) and (16), but cannot be obtained by the wave function of state of the system in other models, including the one-quanta state (A. S. Davydov, 1982; C.W.F. McClare, (1974); A. S. Davydov and A.D.Suprun, 1973; A. S. Davydov, (1973); A. S. Davydov, 1991) and the two-quanta state (L.Cruzeiro, et al. (1993): (1988);L.Cruzeiro-Hansson, L.Cruzeiro-Hansson, (1992); A. C. Scott (1990); W. Förner, (1991); W. Förner, (1991); W. Förner (1999); W. Förner (1991); W. Förner , (1992); W. Förner (1993); H. Motschman, et al. (1989) Therefore ,the above Hamiltonian and wave function, Eqs.(15) and (16), are reasonable and appropriate to the protein molecules.

We now derive the equations of motion of the exciton and phonon in Pang's model. In this case we first give the interpretation of  $\beta_n(t)$  and  $\pi_n(t)$  in Eq.(15).

As it is known, the phonon part in the new wave function in Eq.(15) depending on the displacement and momentum operators is a coherent state of the normal model of creation and annihilation operators, then we can obtain the equation of motion for the  $\beta_n(t)$  utilizing the above results and following formulas of the expectation values of the Heisenberg equations of operators,  $u_n$  and  $P_n$ , in the state  $|\Phi(t)\rangle$ ,

$$i\hbar\frac{\partial}{\partial t}\left\langle \boldsymbol{\Phi}(t)\big|\boldsymbol{u}_{n}\big|\boldsymbol{\Phi}(t)\right\rangle = \left\langle \boldsymbol{\Phi}(t)\big|\big[\boldsymbol{u}_{n},H\big]\big|\boldsymbol{\Phi}(t)\right\rangle, \ i\hbar\frac{\partial}{\partial t}\left\langle \boldsymbol{\Phi}(t)\big|\boldsymbol{P}_{n}\big|\boldsymbol{\Phi}(t)\right\rangle = \left\langle \boldsymbol{\Phi}(t)\big|\big[\boldsymbol{u}_{n},H\big]\big|\boldsymbol{\Phi}(t)\right\rangle$$

At the ame time, we can obtain the dynamic equation of  $\varphi_n(t)$  using a, basic assumption in the derivation, which is that

 $|\Phi(t)\rangle$  in Eq.(31) is a solution of the timedependent Shrödinger equation [A. S. Davydov, 1982; V.K.Fedyamin, 1977; [Pang

Xiao-feng (2001a); Pang Xiao-feng, and Y.P.Feng Yuan-ping (2005); Pang Xiao-feng et al. (2005); Pang Xiao-feng, et al. (2010a); Pang Xiao-feng, et al. (2006a); Pang Xiaofeng, (2001b); Pang Xiao-feng, (2001c); Pang Xiao-feng, (2002); Pang Xiao-feng, (2001d); Pang Xiao-feng, (2001e); Pang Xiao-feng and Chen Xiang-rong, (2002b); Pang Xiao-feng and Chen Xiang-rong, (2002b); Pang Xiao-feng and Chen Xiangrong (2001); Pang Xiao-feng (2001f); Pang Xiao-feng , (2001g); Pang Xiao-feng (2001h); Pang Xiao-Feng and Luo Yu-Hui (2004); Pang Xiao-feng, et al. (2005a); (2005b); Pang Xiao-feng, and Y.H.Luo, (2005); Pang Xiao-feng and Zhang Huai-wu, (2005); Pang Xiao-feng, , (2008a); (2008b); Pang Xiao-feng (2010b); Pang Xiao-Feng and LIU Mei-Jie, (2009); Pang Xiao-feng, (2009); Pang Xiao-feng and Lui mei-jie,Int. (2009); Pang Xiao-feng, (2008c); Pang Xiao-feng et al. (2007a); Pang Xiao-feng, (2007); Pang Xiao-fenget al. (2007b); Pang Xiao-feng and Liu Mei-jie, (2007); Pang Xiao-feng, et al. (2006b); Pang Xiao-feng and Zhang Huai-Wu, (2006a); Pang Xiao-feng and Zhang Huai-wu, (2006b); Pang Xiao-feng, (2003); Pang Xiao feng, (2012))]:

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = H |\Phi(t)\rangle \quad . \tag{18}$$

In this case the left-hand side of Eq.(15) is denoted by

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = \left\{ i\hbar \left\{ \sum_{n} \dot{\varphi}_{n}(t)B_{n}^{+} + \sum_{n} \dot{\varphi}_{n}(t)\varphi_{n}(t)B_{n}^{+}B_{n}^{+}|0\rangle_{ex} \right\} \right\} |\beta(t)\rangle$$
$$+ \left|\varphi(t)\rangle \left\{ \sum_{n} \left\{ \beta_{n}(t)P_{n} - \pi_{n}(t)u_{n} + \frac{1}{2} \left[ \beta_{n}(t)\dot{\pi}_{n}(t) - \dot{\beta}_{n}(t)\pi_{n}(t) \right] \right\} |\beta(t)\rangle \right\}$$
(19)

Now again left-multiplying the both sides of Eq.(18)-(19) by  $\langle \Phi(t) |$ , we yield left-hand side of Eq.(18)-(19) to be

$$i\hbar \langle \Phi(t) | u_n | \Phi(t) \rangle = i\hbar \sum_n \varphi_n^*(t) \varphi_n(t) \left( \sum_m \varphi_m^*(t) \varphi_m(t) + I \right)$$
$$= \frac{5}{4} \sum_n \left[ \dot{\beta}_n(t) \pi_n(t) - \dot{\pi}_n(t) \beta_n(t) \right] \sum_n \left| \varphi_n(t) \right|^2$$

Similarly, for the right-hand side of Eq.(34) we can have

$$\left\langle \Phi(t) \middle| \left( H_{ex} + H_{ph} + H_{int} \right) \middle| \Phi(t) \right\rangle = \left\{ \sum_{n} \left\{ \varepsilon_{0} \middle| \varphi_{n}(t)^{2} \middle| - J \varphi_{n}^{*}(t) \left[ \varphi_{n+l}(t) - \varphi_{n-l}(t) \right] \right\} \\ \times \left( 1 + \sum_{m} \left| \varphi_{m}(t) \right|^{2} \right)$$

$$+ \left\{ \sum_{n} \left\{ \chi_{1} \left[ \beta_{n+1}(t) - \beta_{n-1}(t) \right] \varphi_{n}(t) \right|^{2} + \chi_{2} \left[ \beta_{n+1}(t) - \beta_{n-1}(t) \right] \right\} \\ \times \varphi^{*}(t) \left[ \varphi_{n+1}(t) - \varphi_{n-1}(t) \right] \right\} \left\{ 1 + \sum_{m} \left| \varphi_{m}(t) \right|^{2} \right\} + \frac{5}{2} W(t) \sum_{n} \left| \varphi_{n}(t) \right|^{2} \\ \text{where } W(t) = \left\langle \beta(t) \left| H_{ph} \right| \beta(t) \right\rangle = \sum_{n} \left( \frac{1}{2M} \pi_{n}^{2}(t) + \frac{1}{2} w \left[ \beta_{n}(t) - \beta_{n-1}(t) \right]^{2} \right) + \sum_{q} \frac{1}{2} \hbar \omega_{q}$$

and utilizing the above equations and the relations

$$\begin{split} &\sum_{n} \left[ \beta_{m+1}(t) - 2\beta_{m}(t) + \beta_{m-1}(t) \right] \beta_{m}(t) = -\sum_{n} \left[ \beta_{m+1}(t) - \beta_{m-1}(t) \right]^{2}, \\ &\left\langle \Phi(t) \left| \sum_{n} \left( B_{n}^{+} B_{n-1} + B_{n} B_{n-1}^{+} \right) \right| \Phi(t) \right\rangle = \sum_{n} \left[ \varphi_{n}^{*}(t) \varphi_{n+1}(t) + \varphi_{n-1}^{*}(t) \varphi(t) \left[ 1 + \sum_{m} \left| \varphi_{m}(t) \right|^{2} \right], \\ &\left\langle \Phi(t) \left| \sum_{n} \left( u_{n+1} - u_{n-1} \right) \left( B_{n}^{+} B_{n} \right) \right| \Phi(t) \right\rangle = \sum_{n} \left\{ \beta_{m+1}(t) - \beta_{m-1}(t) \right] \varphi_{n}(t) \right|^{2} \left\{ 1 + \sum_{m} \left| \varphi_{m}(t) \right|^{2} \right\}, \\ &\left\langle \Phi(t) \left| \sum_{n} \left( u_{n-1} - u_{n} \right) \left( B_{n}^{+} B_{n-1} + B_{n} B_{n-1}^{+} \right) \right| \Phi(t) \right\rangle = \sum_{n} \left\{ \beta_{m+1}(t) - \beta_{m-1}(t) \right] \left[ \varphi_{n}^{*}(t) \varphi_{n+1}(t) + \varphi_{n-1}^{*}(t) \varphi(t) \right] \right\} \\ &\times \left( 1 + \sum_{m} \left| \varphi_{m}(t) \right|^{2} \right) \end{split}$$

From the above equations we can obtain

$$i\hbar \frac{\partial}{\partial t} \varphi_{n}(t) = \varepsilon_{0} \varphi_{n}(t) - J [\varphi_{n+1}(t) + \varphi_{n-1}(t)] + \chi_{1} [\beta_{n+1}(t) + \beta_{n-1}(t)] \varphi_{n}(t) - \chi_{2} [\beta_{n+1}(t) + \beta_{n}(t)] \times [\varphi_{n+1}(t) + \varphi_{n-1}(t)] + \frac{5}{2} \bigg[ W(t) - \frac{1}{2} \sum_{m} \left[ \dot{\beta}_{m}(t) \pi_{m}(t) - \dot{\pi}_{m}(t) \beta(t) \right] \bigg] \varphi_{n}(t)$$

Then the dynamic equation can also be obtained, which is represented by

$$M\ddot{\beta}_{n}(t) = w \Big[ \beta_{n+1}(t) - 2\beta_{n}(t) + \beta_{n-1}(t) \Big] + 2\chi_{1} \Big[ \big| \phi_{n+1}(t) \big|^{2} - \big| \phi_{n-1}(t) \big|^{2} \Big] + 2\chi_{2} \Big\{ \varphi_{n}^{*}(t) \big[ \varphi_{n+1}(t) - \varphi_{n-1}(t) \big] + \varphi_{n}(t) \Big[ \varphi_{n+1}^{*}(t) - \varphi_{n-1}^{*}(t) \big] \Big\}$$
(20)

From Eq.(20) we see that the presence of two quanta for the oscillators increases the driving force on the phonon field by that factor when compared with the Davydov theory.

A basic assumption in the derivation is that  $|\Phi(t)\rangle$  in Eq.(18) is a solution of the time- dependent Shrödinger equation [V.K.Fedyamin,1977; (K. H. Spatschek and F. G. 1994; F. A. Popp et al. 1993; Mae Wan Ho, et al. 1994; Pang Xiao-feng, (2000); [Pang Xiao-feng (2001a); Pang Xiao-feng, and Y.P.Feng Yuan-ping (2005); Pang Xiaofeng et al. (2005); Pang Xiao-feng, et al. (2006a); Pang Xiao-feng, (2001b); Pang Xiao-feng, (2001c); Pang Xiao-feng, (2002); Pang Xiaofeng , (2001d); Pang Xiao-feng, (2001e); Pang Xiao-feng and Chen Xiang-rong (2002a); Pang Xiao-feng and Chen Xiangrong, (2002b); Pang Xiao-feng and Chen Xiang-rong (2001); Pang Xiao-feng (2001f); Pang Xiao-feng , (2001g); Pang Xiao-feng (2001h); Pang Xiao-Feng and Luo Yu-Hui (2004); Pang Xiao-feng, et al. (2005a); (2005b); Pang Xiao-feng, and Y.H.Luo, (2005); Pang Xiao-feng and Zhang Huai-wu, (2005); Pang Xiao-feng, , (2008a); (2008b); Pang Xiao-feng (2010b); Pang Xiao-Feng and LIU Mei-Jie, (2009); Pang Xiao-feng, (2009); Pang Xiao-feng and Lui mei-jie,Int. (2009); Pang Xiao-feng, (2008c); Pang Xiaofeng et al. (2007a); Pang Xiao-feng, (2007); Pang Xiao-fenget al. (2007b); Pang Xiaofeng and Liu Mei-jie, (2007); Pang Xiaofeng, et al. (2006b); Pang Xiao-feng and Zhang Huai-Wu, (2006a); Pang Xiao-feng and Chen Xianron, (2006);

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = H |\Phi(t)\rangle, \text{ we can obtain}$$

$$i\hbar \frac{\partial}{\partial t} \varphi_n(t) = \varepsilon_0 \varphi_n(t) - J [\varphi_{n+1}(t) + \varphi_{n-1}(t)] + \chi_1 [\beta_{n+1}(t) + \beta_{n-1}(t)] \varphi_n(t)$$

$$- \chi_2 [\beta_{n+1}(t) + \beta_n(t)] \times [\varphi_{n+1}(t) + \varphi_{n-1}(t)]$$

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

In the continuum approximation and from the above equation we get

$$i\hbar\frac{\partial}{\partial t}\varphi(x,t) = R(t)\varphi(x,t) - Jr_0^2 \frac{\partial^2}{\partial x^2}\varphi(x,t) - G_p |\varphi(x,t)|^2 \varphi(x,t)$$
(21)

And

$$\frac{\partial \beta(x,t)}{\partial \xi} = \frac{\partial \beta(x,t)}{\partial x} = -\frac{4\left(\chi_1 + \chi_1\right)}{w\left(1 - s^2\right)r_0} \left|\phi(x,t)\right|^2$$
(22)

where  $\xi = x - x_0 - vt$   $R(t) = \varepsilon_0 - 2J + \frac{5}{2} \left\{ W(t) - \frac{1}{2} \sum_m \left[ \dot{\beta}_m(t) \pi_m(t) - \dot{\pi}_m(t) \beta(t) \right] \right\}$ and  $s = v/v_0$ . Then the soliton solution of Eq.(22) is obtained, it is  $\phi(x,t) = \left(\frac{\mu_p}{2}\right)^{1/2} \sec h \left[ \left( \mu_p / r_0 \right) (x - x_0 - vt) \right] \times \exp \left\{ i \left[ \frac{\hbar v}{2Jr_0^2} (x - x_0) - E_v \frac{t}{\hbar} \right] \right\}$  (23)

with 
$$\mu_{P} = \frac{2(\chi_{1} + \chi_{2})^{2}}{w(1 - s^{2})J}$$
,  $G_{P} = \frac{8(\chi_{1} + \chi_{2})^{2}}{w(1 - s^{2})}$  (24)

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

On the other hand, in order to investigate the influences of guantum 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 wave function 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 wave function is a reasonable choice for the protein molecules because it not only can exhibit the coherent features of collective excitations arising from the nonlinear interaction between the excitons and phonons, but also retain the conservation of number of particles and fulfill the fact that the energy released by the hydrolysis reaction of ATP molecules can only excite two quanta. In such a case , using a standard calculating method ( J P.Cottingham and J. W. Schweitzer, (1989); J. W. Schweitzer, (1992) Pang Xiao-feng, (2000); Pang Xiao-feng (2001a); Pang Xiaofeng, and Y.P.Feng Yuan-ping 2005; Pang Xiao-feng Zhang Huai-wu, Yu Jia-feng Feng Yuan-ping, (2005) and widely accepted parameters we found out the region encompassed of the excitation or the linear

extent of the new soliton,  $\Delta X = 2\pi r_0 / \mu_p$ , which is greater than the lattice constant  $r_0$  i.e.,  $\Delta X > r_0$  as shown in table 1. Otherwise, we calculated the amplitude squared of the new soliton using Eq.(23) in its rest frame, which is  $|\phi(X)|^2 = \frac{\mu_p}{2} \sec h^2(\frac{\mu_p X}{r_0})$ . Thus

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

## The Lifetimes of Pang's Soliton Transporting the Bio-energy in Protein Molecules at Biological Temperature

## Partially diagonalized form of the model Hamiltonian in Pang's theory

The lifetime of the soliton in the protein molecules is an centre or key problem in the process of bioenergy transport because it can determine that whether the soliton possess certain biological meanings and can play an important role in the biological process, or speaking, only if the soliton has enough long lifetimes, then it is really used in the biological processes.

However, this question of lifetime of the soliton is twofold. In the Langevin dynamics unpredictable effects arise from the semiclassical approximation. In the quantum treatment there is the problem that an exact wave function is lacking. In the Davydov model in Eqs.(1) - (4), both the wave function and the Hamiltonian of the systems, is too simple. A first problem of the model concerns the Davydov wave functions, both  $ID_1$  > and  $ID_2$  >. These are asymmetric since the phononic part is a coherent state, while, the excitonic part is an excitation state of a single-particle. It is not reasonable that the nonlinear interaction generated by the coupling between the excitons and phonons produces different states for the phonon and the exciton. Thus, the Davydov's wavefunction should be modified (V.K.Fedyamin, 1977), i.e., the excitonic part in it should also be coherent or quasi-coherent (S.Yomosa, (1982); Gue Bai-lin and Pang Xiao-feng, (1987). However, the standard coherent state (G..E.Schulz and R.H.Schirmar, 1979) and large-`n excitation state are not appropriate to the protein molecules due to the reasons mentioned above. Similarly, Förner's and Cruzeiro-Hansson's two-quanta states do not fulfill the above criteria.

For convenience of calculation, we here represent the wave function of the system in Eq.(31) by (S.Yomosa, 1983)

$$|\Phi(t) \ge = |\phi(t) \ge |\beta(t) \ge = U_1 10 \ge_{ex} U_2 10 \ge_{ph},$$
(40)

$$\frac{1}{\lambda} \left[ 1 + \sum_{n} \phi_{n}(t) B_{n}^{+} + \frac{1}{2!} (\sum_{n} \phi_{n}(t) B_{n}^{+})^{2} \right], \quad (40a)$$

$$U_{2} = \exp\left\{-\frac{i}{\hbar}\sum_{n} [\beta_{n}(t)P_{n} - \pi_{n}(t)u_{n}]\right\}$$
(40b)

$$= \exp\left\{\frac{1}{\sqrt{N}}\sum_{q}\alpha_{q}(t)a_{q}^{+} - \alpha_{q}^{*}(t)a_{q}\right\}.$$
 (40c)

Where we assume  $\sum\limits_{i} {|\, \boldsymbol{\phi}_i \, |}^2 = n$  , 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 guanta, instead of multiquanta (n>2). Therefore. the Hamiltonian and wave function of the systems. Eas. (31)-(32),or (40) are reasonable and appropriate to the protein molecules. Using standard the transformation where in Eq.(32), Eq.(32)  $\omega_{q} = 2(w/M)^{1/2} \sin((\frac{r_{0}q}{2}))$ 

becomes

$$H = \sum_{n} \left[ \epsilon_{0} B_{n}^{+} B_{n} - J (B_{n}^{+} B_{n+1} + B_{n+1}^{+} B_{n}) \right] + \sum_{q} \hbar \omega_{q} (a_{q}^{+} a_{q} + \frac{1}{2})$$

$$+ \frac{1}{\sqrt{N}} \sum_{q,n} [g_{1}(q) B_{n}^{+} B_{n} + g_{2}(q) (B_{n}^{+} B_{n+1} + B_{n}^{+} B_{n+1})] (a_{q} + a_{-q}^{+}) e^{inr_{0}q}$$
(41)

where 
$$g_1(q) = 2\chi_1 i \left[\frac{\hbar}{2M\omega_q}\right]^{1/2} \sin r_0 q; \quad g_2(q) = \chi_2 \left[\frac{\hbar}{2M\omega_q}\right]^{1/2} (e^{ir_0 q} - 1)$$
 (42)

In a semiclassical and continuum approximations, from Eq.(36) we can obtain the envelope soliton solution Eq.(38) in the Pang's model, we now represent Eq.(38) by (J. P.Cottingham and J. W. Schweitzer, (1989); J. W. Schweitzer, (1992))

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

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

The energy of the new soliton is

$$\mathsf{E}_{\mathsf{S01}} = 2\left[ (\varepsilon_0 - 2\mathbf{J}) + \frac{\hbar^2 v^2}{4 J r_0^2} - \frac{2\mu_p^2}{3} \mathbf{J} \right] \tag{45}$$

Thus we can also find out that

$$\alpha_{q}(t) = \frac{i\pi(\chi_{1} + \chi_{2})}{w\mu_{p}(1 - v^{2}/v_{0}^{2})} \left[\frac{M}{2\hbar\omega_{q}}\right]^{\frac{1}{2}} (\omega_{q} + qv) \csc h(\pi qr_{0}/2\mu_{p})e^{iqvt} = \alpha_{q}e^{iqvt}$$
(46)

This treatment yields a localized coherent structure with size of order  $2\pi r_0/\mu_p$ that propagates with velocity v and can transfer energy  $E_{S01} < 2\epsilon_0$ . Unlike bare excitons that are scattered by the interactions with the phonons, but this soliton state describes a quasi-particle consisting of the two excitons plus a lattice deformation and hence a priori includes interaction with the acoustic phonons. So the soliton is not scattered and spread by this interaction of lattice vibration, and can maintain its form, energy, momentum and other guasiparticle 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 Pang's soliton. In addition the energy of the soliton state is below the bottom of the bare exciton bands, the energy gap being  $4\mu_{\rm p}^2 J/3$  for small velocity of propagation. Hence there is an associated with energy penalty 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, 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.

We now diagonalize partially the model Hamiltonian in order to calculate the lifetime of the soliton in Eq.(43), using the quantum perturbation method (W. C. Kerr and P. S. Lomdahl, (1989); X. Wang, et al. (1989). Since one is interested in investigating the case where there is initially a soliton moving with a velocity v on the chains, it is conveniently to do the analysis in a frame of reference where the soliton is at rest. In this case we should consider the Hamiltonian in this rest frame of the soliton,  $\widetilde{H}$ -vP, where P is the total momentum, and P=  $\sum_q \hbar q (a_q^+ a_q - B_q^+ B_q)$ , where

 $B_q^+ = \frac{1}{\sqrt{N}} \sum\limits_n e^{iqnr_0} B_n^+.$  Also, in order to have

simple analytical expressions we make the usual continuum approximation. Thus it gave

$$\begin{split} \widetilde{H} &= \int_{0}^{L} dx 2 \Biggl[ (\varepsilon_{0} - 2J) \phi^{+}(x) \phi(x) + Jr_{0}^{2} \frac{\partial \phi^{+}}{\partial x} \frac{\partial \phi}{\partial x} - \frac{i\hbar v}{2} \Biggl( \frac{\partial \phi^{+}}{\partial x} \phi(x) - \phi^{+}(x) \frac{\partial \phi}{\partial x} \Biggr) \Biggr] \\ &+ \sum_{q} \hbar(\omega_{q} - qv) a_{q}^{+} a_{q} + \frac{1}{\sqrt{N}} \sum_{q} 2[g_{1}(q) + 2g_{2}(q)] (a_{-q}^{+} + a_{q}) \int_{0}^{L} dx e^{ikx} \phi^{+}(x) \phi(x) \end{split}$$
(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  $\varpi_q \approx (w/M)^{1/2} r_0 |q|$ ,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 (A. C. Scott, 1983)

$$\mathbf{b}_{q} = \mathbf{a}_{p} - \frac{1}{\sqrt{N}} \, \boldsymbol{\alpha}_{q}, \ \mathbf{b}_{q}^{+} = \mathbf{a}_{q}^{+} - \frac{1}{\sqrt{N}} \, \boldsymbol{\alpha}_{q}^{*}, \tag{48}$$

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

$$|\widetilde{0}\rangle_{ph} = \exp\left[\frac{1}{\sqrt{N}}\sum_{q} (\alpha_{q}(t)a_{q}^{+} - \alpha_{q}^{*}(t))a_{q}\right]|0\rangle_{ph}$$
(49)

which is a coherent phonon state (A. C. Scott, 1991), i.e. , b<sub>q</sub>  $|\tilde{0}\rangle_{ph} = 0$ . The Hamiltonian

H in Eq.(48) can now be rewritten as

$$\widetilde{H} = \int_{0}^{L} 2dx \,\varphi(x) [\varepsilon_{0} - 2J + V(x) - Jr_{0}^{2} \frac{\partial^{2}}{\partial x^{2}} + i\hbar \frac{\partial}{\partial x}] \varphi(x) + \\ \sum_{q} \hbar(\omega_{q} - qv) [b_{q}^{+}b_{q} + \frac{1}{\sqrt{N}} (\alpha_{q}b_{q}^{+} + \alpha_{q}^{*}b_{q}^{+})] + W + \\ \frac{1}{\sqrt{N}} \sum 2[g_{1}(q) + 2g_{2}(q)] (b_{-q}^{+} + b_{q}) \int_{0}^{L} dx e^{iqx} \varphi^{+}(x) \varphi(x)$$
(50)

where 
$$W = \frac{1}{N} \sum_{q} \hbar(\omega_{q} - qv) |\alpha_{q}|^{2}$$
,  $V(x) = \frac{1}{N} \sum_{q} [g_{1}(q) + 2g_{2}(q)](\alpha_{-q}^{*} + \alpha_{-q})e^{iqx}$  (51)

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

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

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

$$V(x) = -2J\mu_{p}^{2} \sec h^{2}(\mu_{p}x/r_{0})$$
(52)

In order to partially diagonalize the Hamiltonian Eq.(50) we introduce the following canonical transformation[L. D.Landau,1933; V.K.Fedyamin, 1977]

$$\varphi(x) = \sum_{j} A_{j} C_{j}(x), \ \varphi^{+}(x) = \sum_{j} C_{j}^{*}(x) A_{j}^{+}$$
(53)

where 
$$\int C_1^*(x)C_j(x)dx = \delta_{lj}, \sum_j C_j^*(x')C_j(x) = \delta(x - x'), \int dx |C_j(x)|^2 = 1$$
 (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 Appenix A. Obtained partially diagonalized Hamiltonian is as follows

$$\widetilde{H} = W + E_{s}A_{s}^{+}A_{s} + \sum_{k} E_{k}A_{k}^{+}A_{k} + \sum_{q}\hbar(\omega_{q} - qv)b_{q}^{+}b_{q} + \frac{1}{\sqrt{N}}\sum_{q}\hbar(\omega_{q} - qv)(b_{q}^{+}\alpha_{q} + \alpha_{q}^{*}b_{q})(1 - A_{s}^{+}A_{s}) + \frac{1}{\sqrt{N}}\sum_{kk'q}F(k,k',q)(b_{-q}^{+} + b_{q})A_{k'}^{+}A_{k} - \frac{1}{\sqrt{N}}\sum_{kq}\widetilde{F}(k,q)(b_{-q}^{+} + b_{q})(A_{s}^{+}A_{-k} - A_{k}^{+}A_{s})$$
(55)

$$C_{s}(x) = \left(\frac{\mu_{p}}{2r_{0}}\right)^{1/2} \sec h(\mu_{p}x/r_{0}) \exp[i\hbar xv/2Jr_{0}^{2}], \quad \text{with } E_{s} = 2\left[\epsilon_{0} - 2J - \frac{\hbar^{2}V^{2}}{2Jr_{0}^{2}} - \mu_{p}J\right]$$
(56a)

$$C_{k}(x) = \frac{\mu_{p} \tanh(\mu_{p} x / r_{0}) - ikr_{0}}{\sqrt{Nr_{0}} [\mu_{p} - ikr_{0}]} \exp[ikx + \frac{i\hbar vx}{2Jr_{0}^{2}}],$$
(56b)

with  $E_k = 2 \left[ \epsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - J(kr_0)^2 \right]$ 

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

$$\approx 2[g_1(q) + 2g_2(q)] \left\{ 1 - \frac{i\mu_p q r_0}{[\mu_p + i(k+q)r_0][\mu_p - ikr_0]} \right\} \approx F[k, (k+q), q] \delta_{k'k+q}$$
(57)

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

$$\alpha_{q} = \frac{i\pi(\chi_{1} + \chi_{2})}{w\mu_{p}(1 - s^{2})} \left[ \frac{M}{2\hbar\omega_{q}} \right]^{1/2} (\omega_{q} + qv) \csc h(\pi qr_{0}/2\mu_{p})$$

$$W = \frac{2}{3}\mu_{p}^{2}J$$
(59)

and

For this  $\alpha_q$ ,  $|\,0>_{ph}$  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 Pang's 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 H in Eq.(55) is

$$\langle \psi | \tilde{H} | \psi \rangle = 2(\varepsilon_0 - 2J - \frac{\hbar^2 v^2}{4Jr_0^2}) - \frac{4}{3}J\mu_p^2$$
  
(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<sub>sol</sub>, or the sum of the energy of the bound state in Eq.(56a), E<sub>s</sub>, and the deformation energy of the lattice,

W, i.e.,  $\langle \psi | H | \psi \rangle = E_{sol} = E_s + W$ . This is an interesting result, which shows clearly that the soliton formed by the above quasi-coherent state by virtue of this mechanism is just a self-trapping state of the two excitons

plus the corresponding deformation of the lattice. However, it should be noted that  $|\psi\rangle$  is not an exact eigenstate of  $\widetilde{H}$  owing to the presence of the terms in  $\widetilde{H}$  with  $A_k^+$   $A_s$  and  $A_s^+A_{-k}$ .

### Transition probability and decay rate of Pang's soliton as well its lifetimes in protein molcules

We now calculate the transition probability and decay rate of the quasicoherent soliton arising from the perturbed potential by using the first-order quantum perturbation theory developed by Cottingham, et al. (J.P.Cottingham and J. W. Schweitzer, (1989); J. W. Schweitzer, (1992), 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 H in Eq.(55) into  $H_0 {+} V_1 {+} V_2$  , where

$$H_{0} = W + E_{s}A_{s}^{+}A_{s} + \sum_{k}E_{k}A_{k}^{+}A_{K} + \sum_{q}\hbar(\omega_{q} - vq)b_{q}^{+}b_{q} + \frac{1}{\sqrt{N}}\sum_{q}\hbar(\omega_{q} - vq)(\alpha_{q}b_{q}^{+} + \alpha_{q}^{*}b_{q})(1 - A_{s}^{+}A_{s})$$
(61)

$$V_{1} = \frac{1}{\sqrt{N}} \sum_{kk'q} F(k, k+q, q) (b_{-q}^{+} + b_{q}) A_{k'}^{+} A_{k}$$
(62)

$$V_{2} = \frac{1}{N} \sum_{kq} \tilde{F}(k,q) (b_{-q}^{+} + b_{q}) (A_{s}^{+}A_{k} - A_{s}^{+}A_{-k}), \quad V = V_{1} + V_{2}$$
(63)

where H<sub>0</sub> describes the relevant quasi-particle excitations in the protein. This is a soliton together with phonons relative to the distorted lattice. The resulting delocalized excitations belongs to an exciton-like band with phonons relative to a uniform lattice. The bottom of the band of the latter is at the energy  $4J\mu_p^2/3$  relative to the soliton, in which the topological stability associated with removing the lattice distortion is included.

We now calculate the decay rate of the new soliton along the following lines by using Eq.(61) and V<sub>2</sub> 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.(31) is replaced by (n+1) terms of the expression of a coherent state  $\frac{1}{\lambda} exp[\sum_{n} \phi_n(t)B_n^+]10 >_{ex}$ . Finally we find out the decay rate of the new soliton with two-quanta from it. In such a case H<sub>0</sub> is chosen such the ground state, |n> has energy W+n  $E'_s$  in the subspace of excitation number equal to n, i.e.,  $< n \mid \sum_i B_i^+ B_i \mid n >=< nl(A_s^+ A_s + \sum_k A_k^+ A_k)ln >= n$ . In this subspace the eigenstates have the simple form  $|n-m,k_1k_2...k_m, \{n_q\} >$ 

$$=\frac{1}{\sqrt{(n-m)!}}(A_{S}^{+})^{n-m}A_{k_{1}}^{+}A_{k_{2}}^{+}\cdots A_{k_{m}}^{+}|0>_{ex}\Pi\frac{(d_{q}^{+})^{n_{q}}}{\sqrt{n_{q}!}}1\widetilde{0}>_{ph}^{n-m}$$
(64)

where 
$$d_q = b_q + \frac{m}{n} \frac{1}{\sqrt{N}} \alpha_q = a_q - \frac{n-m}{n} \frac{1}{\sqrt{N}} \alpha_q$$
 (m≤n, n and m are all intgers )  
(65)

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

$$E_{n-m;k_1...k_{m_1};\{n_q\}}^{(0)} = (1 - (m/n)^2)W + (n-m)E'_s + \sum_{j=1}^m E'_{k_1} + \sum_q \hbar(\omega_q - vq)n_q$$
(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:

$$|n\rangle = \frac{1}{\sqrt{n!}} \prod_{q} \frac{(b_{q}^{+})^{n_{q}}}{(n_{q}!)^{1/2}} (A_{s}^{+})^{n} |0\rangle_{es} |\tilde{0}\rangle_{ph}$$
(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:

$$|\alpha k\rangle = \prod_{q} \frac{(a_{q}^{+})^{n_{q}}}{\sqrt{n_{q}!}} |0\rangle_{ph} (A_{k}^{+})^{n} |0\rangle_{ex}$$
(68)

with corresponding energy E\_k{n\_q}=n E\_k^{'} + \sum\_q \hbar(\omega\_q - vq) n\_q caused by the part, V\_2, in the

perturbation interaction V. In this case, the initial phonon distribution will be taken to be at thermal equilibrium. The probability of the above transitions in lowest order perturbation theory is given by

$$\overline{W} = \frac{1}{\hbar^2} \int_0^t dt' \int_0^t dt'' \left\{ \sum_{\alpha k' = 1} P_1^{(ph)} < n | \exp\left(\frac{iH_0 t''}{\hbar}\right) V_2 \exp\left(\frac{-iH_0 t''}{\hbar}\right) | \alpha k' > \cdot \right. \\ \left. < \alpha k' | \exp\left(\frac{iH_0 t'}{\hbar}\right) V_2 \exp\left(\frac{-iH_0 t'}{h}\right) | n > \right\}$$
(69)

We should calculate the transition probability of the soliton resulting from the perturbed potential,(V1+V2), at first-order in perturbation theory. Following Cottingham and Schweitzer (A.S.Davydov, 1983)'s method, we estimate only the transition from the soliton state to delocalized exciton states caused by the potential V2, 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<sub>1</sub> term in the Hamiltonian is an interaction between the delocalized excitons and the phonons. The main effect of  $V_1$  is to modify the spectrum of the delocalized excitatons in the weak coupling limit  $(J\mu_p/K_BT_0 <<1$ , the definition of  $T_0$  is given below). As a result the delocalized excitons and phonons will have their energies shifted and also have finite lifetimes. These effects are ignored in our calculation since they are only of second order in  $V_1$ .

The sum over / in Eq.(69) indicates a sum over an initial set of occupation numbers for phonons relative to the distorted lattice with probability distribution  $P_{\rm l}^{\rm ph}$ , which is taken to be the thermal equilibrium distribution for a given temperature T. Since

$$e^{-iH_0t} | n, \{n_q\} \ge exp\{-i(W + nE'_q)t/\hbar - i\sum_q (\omega_q - qv)b_q^+b_qt\} | n, \{n_q\} > nd$$

and

$$e^{iH_0t} | n-1, \{n'_q\} \ge exp\left\{-i[(1-\frac{1}{n^2})W + (n-1)E'_s + E'_k]t/\hbar - i\sum_q (\omega_q - qv)d^+_q d_q t\right\} | n-1, \{n'_q\} > 0$$

where  $d_q=b_q+\frac{1}{n}\frac{1}{\sqrt{N}}\alpha_q$ , using the explicit form for V<sub>2</sub> and the fact that the sum over states |

 $k'\alpha, \{n_q'\}$  > contains a complete set of phonons for each values of k', one can rewrite  $~\overline{W}~$  as

$$\overline{W} = \frac{1}{\hbar^{2}} \frac{\pi^{2}}{2n\mu_{1}N^{2}} \sum_{k} \sum_{k'} \sum_{k'} [g_{1}^{*}(k) + 2g_{2}^{*}(k)] [g_{1}(k'') + 2g_{2}(k'')] \frac{(kr_{0})(k''r_{0})}{(n\mu_{1})^{2} + (k'r_{0})^{2}} \operatorname{Sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}} (k - k') \right] \cdot \operatorname{Sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}} (k'' - k') \right] \int_{0}^{t} dt' \int_{0}^{t} dt' \left[ \exp \left[ \frac{-i}{\hbar} \left( n(n^{2} - \frac{2}{3}n)\mu_{1}^{2}J + nJ(k'r_{0})^{2} \right)(t' - t'') \right] \right] \cdot \operatorname{Sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}} (\omega_{q} - qv)b_{q}^{+}b_{q}(t' - t'') \right] (b_{k}^{+} + b_{-k}) \exp \left[ i\sum_{q} (\omega_{q} - qv)a_{q}^{+}a_{q}(t' - t'')(b_{-k'}^{+} + b_{k'}) \right] \right] \right]$$

$$(70)$$

where 
$$g_1(k) + 2g_2(k) = 2\chi_1 (\frac{\hbar}{2M\omega_k})^{1/2} [A(\cos t_0 k) - 1) + i(A+1)\sin(t_0 k)] \approx 2i(A+1)(t_0 k)\chi_1 (\frac{\hbar}{2M\omega_k})^{1/2},$$
  
 $\mu_1 = \frac{\chi_1^2 (1+A^2)}{\omega(1-s^2)J}, A = \chi_2 / \chi_1$ 
(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  $\frac{d\overline{w}}{dt}$ . By straightforward calculation, the average transition probability or decay rate of the soliton is given by

$$\begin{split} &\Gamma_{n} = \lim_{t \to \infty} \frac{d\overline{W}}{dt} = \frac{4}{\hbar} \left[ \frac{\pi^{2}}{2n\mu_{1}N^{2}} \right]_{kkk''} \left[ \left[ g_{1}^{*}(k) + 2g_{2}^{*}(k) Ig_{1}(k'') + 2g_{2}(k'') \right] \frac{(kr_{0})(k''r_{0})}{(n\mu_{1})^{2} + (k'r_{0})^{2}} \cdot \operatorname{sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}}(k-k') \right] \right] \cdot \\ &\operatorname{sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}}(k''-k') \right] \operatorname{Re} \left\{ \int_{0}^{\infty} dt \exp \left[ -\frac{i}{\hbar} \left( n(n^{2} - \frac{2}{3}n)\mu_{1}^{2}J + nJ(k'r_{0})^{2} \right) t \right] \right] \cdot \\ &< \exp \left[ i\sum_{q} (\omega_{q} - qv)b_{q}^{+}b_{q}t \right] (b_{k}^{+} + b_{-k}) \exp \left[ -i\sum_{q} (\omega_{q} - qv)a_{q}^{+}a_{q}t \right] (b_{-k'}^{+} + b_{k'}) > \right\} \right\} \\ &= \frac{4}{\hbar^{2}} \frac{\pi^{2}}{2n\mu_{1}N^{2}} \sum_{kk'k''} \left\{ \left[ g_{1}^{*}(k) + 2g_{2}^{*}(k) Ig_{1}(k'') + 2g_{2}(k'') \right] \frac{(kr_{0})(k''r_{0})}{(n\mu_{1})^{2} + (k'r_{0})^{2}} \operatorname{sech} \left[ \frac{\pi r_{0}(k-k')}{2n\mu_{1}} \right] \cdot \\ &\operatorname{sech} \left[ \frac{\pi r_{0}}{2n\mu_{1}} (k''-k') \right] \operatorname{Re} \int_{0}^{\infty} dt U(k, k''t) \exp \left[ -\frac{i}{\hbar} \left( n(n^{2} - \frac{2}{3}n)\mu_{1}^{2}J + nJ(k'r_{0})^{2} \right) t \right] \right\}$$
(72)

where the thermal average is

$$\begin{split} U(k,k'',t) = &< \exp[i\sum_{q}(\omega_{q} - qv)b_{q}^{+}b_{q}t](b_{k}^{+} + b_{-k})\exp[-i\sum_{q}(\omega_{q} - qv)a_{q}^{+}a_{q}t](b_{-k'}^{+} + b_{k'}) >> \\ \text{with} \\ << A >> = Tr\{A\exp[-\beta\sum_{q}\hbar(\omega_{q} - qv)b_{q}^{+}b_{q}]\}/Tr\{\exp[-\beta\sum_{q}\hbar(\omega_{q} - qv)b_{q}^{+}b_{q}]\} \\ = Tr\{A\exp[-\beta\sum_{q}\hbar(\omega_{q} - qv)b_{q}^{+}b_{q}]\}/Z_{ph} \end{split}$$
(73)  
and  $Z_{ph} = \prod_{q}(1 - \exp[-\beta\hbar(\omega_{q} - qv)]\}^{-1}, \ (\beta = \frac{1}{K_{B}T})$ 

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 U(k,k'',t), which is described in Appendix B. The decay rate obtained finally is

$$\Gamma_{n} = \lim_{t \to \infty} \frac{d\overline{W}}{dt} = \frac{2}{n\mu_{1}\hbar^{2}} \frac{\pi^{2}}{N^{2}} \sum_{kk'} \left[ |g_{1}(k) + 2g_{2}(k)|^{2} \frac{(r_{0}k)^{2} \operatorname{sech}^{2}[\pi(k-k')r_{0}/2n\mu_{1}]}{(n\mu_{1})^{2} + (k'r_{0})^{2}} \operatorname{Re}\int_{0}^{\infty} dt \cdot \left\{ \exp[-i(nJ(k'r_{0})^{2} + n(n^{2} - \frac{2}{3}n)\mu_{1}^{2}Jt/\hbar + R_{n}(t) + \xi_{n}(t)] \frac{\exp[i(\omega_{k} - kv)t]}{\exp[\beta\hbar(\omega_{k} - kv)] - 1} \right\} \right]$$
(74)

Where\

$$R_{n}(t) = -\frac{1}{n^{2}N} \sum_{k} |\alpha_{k}|^{2} \{i - \exp[-i(\omega_{k} - kv)t]\}, \quad \xi_{n}(t) = -\frac{4}{n^{2}N} \sum_{k} \frac{|\alpha_{k}|^{2} \sin^{2}[\frac{1}{2}(\omega_{k} - kv)t]}{\exp[\beta\hbar(\omega_{k} - kv)] - 1}$$
(75)

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 sech<sup>2</sup>[ $\pi$ (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 in our calculation because the phonons in the initial and final states are defined relative to different deformations.

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

We should point out that the

(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 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<sub>2</sub>(t) and  $\xi_2(t)$  are

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

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

i.e.,

$$\lim_{t\to\infty}\xi_2(t) = -\eta t , \ \eta = \pi R_0 / \beta \hbar = \pi R_0 k_B T / \hbar$$
 (78)

Where

$$R_{0} = \frac{4(\chi_{1} + \chi_{2})^{2}}{\pi \hbar w} (M / w)^{1/2} = \frac{2J \mu_{p} r_{0}}{\pi \hbar v_{0}},$$

$$\omega_{\alpha} = \frac{2\mu_{p}}{\pi} (\frac{w}{M})^{1/2}, \quad T_{0} = \hbar \omega_{\alpha} / K_{B}$$
(79)

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

$$\frac{1}{\pi\hbar} \operatorname{Re} \int_{0}^{\infty} dt \exp \left\{ -i[2J(k'r_{0})^{2} + \frac{4}{3}J\mu_{p}^{2} - \hbar\omega_{k}]t/\hbar + R_{2}(t) + \xi_{2}(t) \right\}$$

$$\approx \frac{1}{\pi\hbar} (2.43\omega_{a})^{-R_{0}} \Gamma(1-R_{0})[\eta^{2} + (\delta(k,k')/\hbar)^{2}]^{-(1-R_{0})/2} \left[ 1 - \frac{1}{2} \left[ \frac{\pi R_{0}}{2} + (1-R_{0}) \left( \frac{\delta(k,k')}{\eta\hbar} \right) \right]^{2} \right] (80)$$

(76)

Where  $\delta(k,k') = 2J(k'r_0)^2 + \frac{4}{3}\mu_p^2 J - \hbar\omega_k, \Phi_1 = \frac{R_0\pi}{2}, \Phi_2 = [(1 - R_0)\tan^{-1}\left(\frac{\delta(k,k')}{\eta\hbar}\right)]$  (81)

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

$$\Gamma_{2} = \lim_{t \to \infty} \frac{d\overline{W}}{dt} = \frac{2}{\mu_{p}} \left(\frac{\pi}{N}\right)^{2} \sum_{kk'} \left[ \frac{(kr_{0})^{2} |g_{1}(k) + 2g_{2}(k)|^{2} \operatorname{sec} h^{2}[(\pi r_{0}/2\mu_{p})(k-k')]}{[\mu_{p}^{2} + (k'r_{0})^{2}][\exp(\beta\hbar\omega_{k}) - 1]} (2.43\omega_{\alpha})^{-R_{0}} \right] \left\{ \frac{\left(\eta^{2} + \frac{1}{\hbar^{2}} [\frac{4}{3}\mu_{p}^{2}J + 2(k'r_{0})^{2}J - \hbar\omega_{k}]^{2}\right)^{(1+R_{0})/2}}{\hbar^{2}\eta^{2} + [\frac{4}{3}\mu_{p}^{2}J + 2(k'r_{0})^{2}J - \hbar\omega_{k}]^{2}} \right\} \left\{ 1 - \frac{1}{2} \left[ \frac{R_{0}\pi}{2} + (1-R_{0}) \left[ \frac{\frac{4}{3}\mu_{p}^{2}J + 2(k'r_{0})^{2}J - \hbar\omega_{k}}{\hbar\eta} \right] \right]^{2} \right\}$$

$$(82)$$

This is the final analytical expression for the decay rate of the quasi-coherent solition with two-quanta. Evidently, it is different from that in the Davydov model (L. D.Landau, 1933). To emphasis the difference of the decay rate between the two models, the corresponding quantity for the Davydov soliton is rewritten as [L. D.Landau,1933)

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

where

$$\eta_{\rm D} = \pi R_0^{\rm D} K_{\rm B} T / \hbar , \ R_0^{\rm D} = \frac{2\chi_1^2}{\pi \hbar w} (\frac{M}{w})^{1/2} , \ \omega_{\alpha}^{\rm D} = \frac{2\mu_{\rm D}}{\pi} (\frac{M}{w})^{1/2}$$
(84)

Equation (83) can also be found out from Eq.(74) at n=1 by using the Cottingham et al's approximation ( $J \cdot P$ .Cottingham and J. W. Schweitzer, 1989).

The two above formulaes in 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,  $\left\{1 - \frac{1}{2} \left[\frac{R_0 \pi}{2} + (1 - R_0) \left[(\frac{4}{3} \mu_p^2 J + 2(\dot{k'r_0})^2 J - \hbar \omega_k) / \hbar \eta\right]\right]^2\right\}$  is added, while in Eq.(83) the factor,  $\left(\frac{\omega_\alpha}{\eta_D}\right)^{-R_0^D} \eta_D \quad \text{replaces} \quad \text{the term}$  $(2.43\omega_d)^{-R_0} \cdot (\eta^2 + \frac{1}{\hbar^2} [\frac{4}{3} \mu_p^2 J + 2(\dot{k'r_0})^2 J - \hbar \omega_k]^2)^{(\frac{1+R_0}{2})})$ 

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 the parameter values of alpha helix protein molecules, which are

We first calculate the solution of Eqs.(15)-(19) numerically in the uniform and periodic proteins with single chain utilizing the above average values for these parameters in alpha helix protein molecules in Fig.1, which are

$$J = 1.55 \times 10^{-22} J, w = (13 - 19.5) N/m, M = (1.17 - 1.91) \times 10^{-25} kg = 114m_p,$$
  

$$\chi_1 = 62 \times 10^{-12} N, \quad \chi_2 = (10 - 18) \times 10^{-12} N, r_0 = 4.5 \times 10^{-10} m.,$$
(85)

we find out the values of  $\eta$ ,  $R_0$  and To at T=300K in both models, which are listed in table 2. From this table we see that the  $\eta$ ,  $R_o$  and  $T_o$  for Pang's model are about 3 times larger than those in the Davydov model due to the increases of  $\mu_p$  and the non-linear interaction coefficient  $G_p$ . Thus

the approximations used in the Davydov model by Cottingham, et.al ( J . P.Cottingham and J. W. Schweitzer, 1989) can not be applied in our calculation for the lifetime of Pang's soliton, although we utilized the same quantum-perturbation scheme. Hence we can audaciously suppose that the lifetimes of Pang's soliton are greatly changed.

## The lifetime of Pang's soliton and its features

The above expression, Eq.(78), allows us to compute and study numerically the decay rate,  $\Gamma_{\rm 2},$  and the lifetimes of Pang's soliton,  $\tau = 1/\Gamma_2$ , for above values of the physical parameters of the  $\alpha$ -helical protein molecules in Eq.(85). Using the above parameter values and the above Eq.(83) and at  $v=0.2v_0$  and assuming the wavevectors are in the Brillouin zone then we can obtain the values of  $\Gamma_{\!_2}$  is between 1.54×10<sup>10</sup>S<sup>-1</sup>-1.89×10<sup>10</sup>S<sup>-1</sup>. This corresponds to the soliton lifetimes, T, is between 0.53×10 <sup>10</sup>S—0.65×10<sup>-10</sup>S at T=300K, or speaking,  $\tau/\tau_0{=}510{-}630,$  where  $\tau_0{=}r_0/v_0$  is the time for travelling one lattice spacing at the speed of sound, which is  $(M/w)^{1/2}$ =0.96×10<sup>-13</sup>S. In this amount of time the new soliton, travelling at two tenths of the speed of sound in the chain, would travel several hundreds of lattice spacings, that is several hundred times more than the time of Davydov soliton, which is  $\tau/\tau_0 < 10$  at 300K (S.Takeno, 1985)i.e. when Davydov soliton is transported at a half of the sound speed, it can only cover less than 10 lattice spacing in its lifetime... The lifetime for Pang's soliton is enough long for bio-energy transport. Therefore the guasi-coherent Pang's soliton is a viable mechanism for the bio-energy transport along the protein molecules at biological temperature.

We are very interested in the relation between the lifetime of the quasi-coherent soliton and temperature. Fig. 2 shows the relative lifetimes  $\tau/\tau_0$  of Pang's soliton versus temperature T for a set of widely accepted parameter values mentioned above. Since one assumes that v<v<sub>0</sub>, the soliton will not travel the length of the chain unless  $\tau/\tau_0$  is large compared with L/r<sub>0</sub>, where L=Nr<sub>0</sub> is the typical length of the protein molecular chains. Hence for L/r<sub>0</sub>≈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 changes of lifetime of Pang's soliton with the temperature are shown in Fig.3, which exhibits that the lifetime of Pang's soliton is decreased rapidly as temperature increases, but below T=310K it is still large enough to fulfill the criterion. Thus, Pang's soliton can play an important roles in biological processes.

For comparison we plotted log  $(\tau / \tau_0)$  versus simultaneously the temperature relations for the Davydov soliton and Pang's soliton is showed in Fig.3. 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 is really too small, in which it can only travel fewer than the lattice spacings in half the speed of sound in the protein chain (S.Takeno, 1985; 1986). Hence it is true that the Davydov soliton is ineffective for the biological processes (S.Takeno, 1985; 1986).

We can also study the dependence of the lifetime of Pang's soliton on some special parameters by using Eqs.(8)and (Pang Xiao-feng, 1993i). In this case we still chose and used the parameter values mentioned above. In Pang's model we know from Eq. (82) that the lifetime of the soliton depends mainly on these parameters of coupling constants ( $\chi_1+\chi_2$ ), M, w, J, phonon energy  $\hbar \omega_k$ , as well as on the composite parameters  $\mu(\mu=\mu_p)$ , R<sub>0</sub> and T/T<sub>0</sub>. At a given temperature,  $\tau/\tau_0$  increases with increasing  $\mu$  and T<sub>0</sub>. The dependences of

the lifetime  $\tau/\tau_0$ , on  $(\chi_1+\chi_2)$  and  $\mu$  at 300K are shown in Figs. 4 and 5, respectively. Since  $\mu$  is inversely proportional to the size of the soliton, and can determine the binding energy of Pang's soliton in Pang's model, therefore it is an important parameter. We may think it be an independent variable. In such a case the other parameters in Eq. (82) used still the

above values in Eq.(85). It is clear from Figs. 4 and 5 that the lifetime of Pang's soliton,  $\tau/\tau_0$ , increases rapidly with increasingµand ( $\chi_1+\chi_2$ ). Furthermore, when µ≥5.8 and ( $\chi_1+\chi_2$ )≥7.5×10<sup>-11</sup>N, which are values appropriate to Pang's model, we find  $\tau/\tau_0 > 500$ .



Fig. 2. Soliton lifetime  $\tau$  relatively to  $\tau_0$  as a function of the temperature T for parameters appropriate to the  $\alpha$ -helical molecules in Pang' model in Eq.(82).





Fig. 3.  $log(\tau/\tau_0)$  versus the temperature T for the soliton. The solid line is result of Pang' model inEq.(8), the dashed line is the result of Davydov model in Eq.(83).



Fig. 4.  $\tau/\tau_0$  versus ( $\chi_1+\chi_2$ ) relation in Eq.(82)

For a comparison we showed also the corresponding result obtained using Eq.(83) in Fig. 5, where the values of original Davydov model are shown in a dashed line in this Figure. We can see from this figure 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 dependence on the parameter ( $\chi_1+\chi_2$ ), but the result for the Davydov soliton is not drawn in Fig. 4.

These results verified again that the quasi-coherent soliton in Pang's model is a likely candidate for the mechanism of bioenergy transport in the protein molecules.

In addition, Fig. 5 shows clearly that a basic mechanism and ways for increasing the lifetime of the soliton in protein molecules is to enhance the strength of the exciton-phonon interaction.

In Fig.6 we plot  $\tau/\tau_0$  versus  $\eta$ . Since  $-\eta$ 

(184)

designates the influence of the thermal phonons on the soliton, thus it is also an important quantity. We here may regard it also is an independent variable. In this case, other parameters in Eq.(82) are the values mentioned above. From this figure we see that  $\tau/\tau_0$  increases with increasing  $\eta$ . Therefore, to enhance  $\eta$  can also increase the value of  $\tau/\tau_0$ .

In order to understand clearly the behavior of the lifetime of quasi-coherent soliton with varying parameter values in a wide range,we study further the variation of  $\tau/\tau_0$  in the limit  $\varpi_a t \rightarrow 0$  in Eq.(75) , i.e., this

is in the initial case, in which we can evaluate analytically the values of R<sub>2</sub>(t) and  $\xi_2(t)$ . In fact, for  $\omega_a t < 1$  both R<sub>2</sub>(t) and  $\xi_2(t)$  have power-series expansions.

To lowest order as  ${}^{\omega_a t} {\rightarrow} 0,$  one finds from Eq.(75):

$$\xi_{2}(t) \approx -\frac{R_{0}K_{B}^{2}TT_{0}\pi^{2}}{3\hbar^{2}}t^{2},$$
(87)



Fig. 5.  $\tau/\tau_0$  versus  $\mu$  relation. The solid and dashed lines are results of Eq.(82) and Eq.(83),respectively

using 
$$\operatorname{coth}(\pi\omega_{\alpha} t) \approx [(\pi\omega_{\alpha} t)^{-1} + \frac{\pi}{3}\omega_{\alpha} t]$$
 we has  

$$\frac{1}{\pi\hbar}\operatorname{Re}\int_{0}^{\infty} dt \exp\left\{-i\left[2J(k'r_{0})^{2} + \frac{4J\mu_{p}^{2}}{3} - \hbar\omega_{k}\right]t/\hbar + R_{2}(t) + \xi_{2}(t)\right\} \approx \left[4\pi(3\zeta(3)R_{0}K_{B}^{2}T_{0}^{2} + R_{0}\pi^{2}K_{B}^{2}T_{0}^{2}) + R_{0}\pi^{2}K_{B}^{2}T_{0}^{2} + R_{0}\pi^{2}K_{B}^{2}T_{0}^{2}$$



Fig. 6.  $\tau/\tau_0$  versus  $\eta$  relation in Eq.(82)

when  $T/T_0 > 1$  and  $\pi^4 R_0 T/2\mu T_0 > 1$ . The above integral is the generalization of the usual  $\delta$ -function for energy conservation in zero- temperature perturbation theory. Thus we can obtain from Eqs.(74) and (88) at n=2 the decay rate of the soliton as

$$\Gamma_{2} = \frac{2\pi^{3}}{\mu_{p}\hbar N^{2}K_{B}} \left( \frac{\pi}{R_{0}T_{0}[3\zeta(3)T_{0} + \pi^{2}T/3]} \right)^{-\frac{1}{2}} \sum_{kk'} \frac{(kr_{0})^{2} |g_{1}(k) + 2g_{2}(k)|^{2}}{\mu_{p}^{2} + (k'r_{0})^{2}} \sec h^{2} \left[ \left( \frac{\pi r_{0}}{2\mu_{p}} \right)(k-k') \right]$$

$$\left\{ \exp \left[ \frac{\left[ 2J(k'r_{0})^{2} + \frac{4}{3}\mu_{p}^{2}J - \hbar\omega_{k} + \frac{1}{6}R_{0}\pi^{2}K_{B}T_{0}\right]^{2}}{4\left[ 3\zeta(3)R_{0}K_{B}^{2}T_{0}^{2} + R_{0}K_{B}^{2}TT_{0}\pi^{2}/3\right]} \right] \left[ \exp(\beta\hbar\omega_{k}) - 1 \right] \right\}^{-1}$$

$$\left\{ \exp \left[ \frac{\left[ 2J(k'r_{0})^{2} + \frac{4}{3}\mu_{p}^{2}J - \hbar\omega_{k} + \frac{1}{6}R_{0}\pi^{2}K_{B}T_{0}\right]^{2}}{4\left[ 3\zeta(3)R_{0}K_{B}^{2}T_{0}^{2} + R_{0}K_{B}^{2}TT_{0}\pi^{2}/3\right]} \right] \left[ \exp(\beta\hbar\omega_{k}) - 1 \right] \right\}^{-1}$$

$$\left\{ \exp \left[ \frac{\left[ 2J(k'r_{0})^{2} + \frac{4}{3}\mu_{p}^{2}J - \hbar\omega_{k} + \frac{1}{6}R_{0}\pi^{2}K_{B}T_{0}\right]^{2}}{4\left[ 3\zeta(3)R_{0}K_{B}^{2}T_{0}^{2} + R_{0}K_{B}^{2}TT_{0}\pi^{2}/3\right]} \right] \left[ \exp(\beta\hbar\omega_{k}) - 1 \right] \right\}^{-1}$$

The expression of the decay rate of Pang's s oliton in this limit is different from Eq.(82). Therefore, studying properties of the lifetime of Pang's soliton in such a case are helpful in understanding the behavior of the soliton. A summary of the results obtained from Eq.(89) are given in Figs.7-10.

The dependence of lifetime on temperature T is shown in Fig.7, which has been obtained from the numerical evaluation of Eq.(89). In Figs.8 and 9 we plot  $\tau/\tau_0$  versus ( $\chi_1+\chi_2$ ) and versus  $\mu$ , respectively, at T=300K. From Figs.7-9 we see that  $\tau/\tau_0$ 

increases as T decreases and with increasing  $\mu$  and  $(\chi_1 + \chi_2)$ . Furthermore, it is clear from this Gaussian expression in Eq (84) that the lifetime of Pang's soliton will be large if  $\mu$  and  $(\chi_1 + \chi_2)$  are larger, but the Gaussian expression is very small for k and k' between  $-\pi/r_0$  and  $+\pi/r_0$ , i.e., in the Brillouin zero. Obviously, the temperature dependence of the lifetime of Pang's soliton mainly due to the temperature is dependence of the width of the Gaussian, which decreases with decreasing temperature. The dashed line in Fig.9 is the result for the Davydov soliton under the

same conditions. It is clear that the lifetime of the Davydov soliton is lower than that of Pang's soliton, especially at large  $\mu$ , although at low  $\mu$  the difference between them is small. Taking Fig.5 also into account we find that the lifetime of the Davydov soliton is indeed very low. However this is not the case for Pang's soliton.

In Fig. 10 we plot  $\tau/\tau_0$  as a function of  $T_0$  at T=300K.  $T_0$  is related to the Debye temperature of the systems, therefore it is also an important quantity. We here regard it as an independent variable and calculate and evaluate that the changes of  $\tau/\tau_0$  w ith varying  $T_0$  using Eq.(89). From this figure in Fig.10 we see that the lifetime of Pang's soliton is large if  $T_0$  is either large or small,

because the Gaussian expression in Eq.(89) is very small for k and k' between  $-\pi/r_0$  and  $+\pi/r_0$ . As a point of reference, note that these parameters have the values T/T<sub>0</sub>~1.03 ----1.06,  $JT/K_BT_0^2$  =4.10 at 300K and µ=5.81-5.96 depending on whether the widely accepted or the"three-channel"parameter values for the alpha-helical protein are assumed. From these results it is clear that using widely accepted, realistic parameter values, then Pang's model can satisfy the relation  $\tau/\tau_0 \ge 500$  at 300K for large  $\mu$  and T<sub>0</sub>. HencePang's soliton model large provides a viable candidate for the bioenergy transport processes in the protein molecules.



Fig. 7.  $\tau/\tau_0$  versus T relation in the new model in Eq.(87)



Fig. 8.  $\tau/\tau_0$  versus ( $\chi_1+\chi_2$ ), relations in the new model in Eq.(87)



Fig. 9 .  $\tau/\tau_0$  versus  $\mu$  relation in the new model in Eq.(87), the dashed line is Davydov model's data



Fig. 10.  $\tau/\tau_0$  versus  $T_0$  relation

The above results indicated clearly that Pang's soliton, which is responsible for the bio-energy transport along the protein molecules is thermal stability and has at least,  $\tau/\tau_0=515$ , or  $0.55\times10^{-10}$ S at T=300K. In this time Pang's soliton can transport over several hundreds of amino acid residues, which is larger about 300 times than that of Davydov's soliton, no matter how changes of molecular structure of the protein molecules because the latter are closely related to

these parameters mentioned above, such as  $(\chi_1+\chi_2)\;,\eta,\mu$  and  $T_0\;.$ 

The above calculations and results are helpful to resolve the controversies on the lifetime of Davydov's soliton, which is too small in the region of biological temperature. Pang's model containing the quasi-coherent wavefunction of the two-quanta nature and an added interaction in the Hamiltonian produced a stable soliton at biological temperatures. Pang's soliton has a long enough lifetime. Therefore, the distinction of the natures and features of the two kinds of solitons in Pang's and Davydov's models [A. S. Davydov, (1973); A. S. Davydov, 1991; A. S. Davydov, (1979); A.S.Davydov, (1983); A. S. Davydov, (1982), ); [Pang Xiao-feng (2001a); Pang Xiao-feng, and Y.P.Feng Yuan-ping (2005); Pang Xiao-feng et al. (2005); Pang Xiao-feng.et al. (2010a); Pang Xiao-feng, et al. (2006a); Pang Xiao-feng, (2001b); Pang Xiao-feng, (2001c); Pang Xiao-feng, (2002); Pang Xiao-feng, (2001d); Pang Xiao-feng, (2001e); Pang Xiao-feng and Chen Xiang-rong (2002a); Pang Xiaofeng and Chen Xiang-rong, (2002b); Pang Xiao-feng and Chen Xiang-rong (2001); Pang Xiao-feng (2001f); Pang Xiao-feng , (2001g); Pang Xiao-feng (2001h); Pang Xiao-Feng and Luo Yu-Hui (2004); Pang Xiao-feng, et al. (2005a); (2005b); Pang Xiao-feng, and Y.H.Luo, (2005); Pang Xiaofeng and Zhang Huai-wu. (2005): Pang Xiao-feng, , (2008a); (2008b); Pang Xiaofeng (2010b); Pang Xiao-Feng and LIU Mei-Jie, (2009); Pang Xiao-feng, (2009); Pang Xiao-feng and Lui mei-jie, Int. (2009); Pang Xiao-feng, (2008c); Pang Xiao-feng et al. (2007a); Pang Xiao-feng, (2007); Pang Xiao-fenget al. (2007b); Pang Xiao-feng and Liu Mei-jie, (2007); Pang Xiao-feng, et al. (2006b); Pang Xiao-feng and Zhang Huai-Wu, (2006a); Pang Xiao-feng and Chen Xianron, (2006); Pang Xiao-feng and Zhang Huai-wu, (2006b); Pang Xiao-feng, (2003); Pang Xiao feng, (2012)) are shown in Table 2. From this table we know that Pang's repulsed and refused model the shortcomings of the Davydov model (A. S. Davydov, (1973); A. S. Davydov, 1991; A. S. Davydov, (1979); A.S.Davydov, (1983); A. S. Davydov, (1982)., the new soliton in Pang's model is thermal stable, and has a long enough lifetime at biological temperature 300K, thus it can play an important role in the biological processes. Thus, Pang's theory is correct, it can resolve the controversy on the thermal stability and lifetime of the soliton excited in protein molecules, Pang's soliton is a real carrier of bio-energy transport in the protein molecules in the living systems.

In one word, we here proposed a new theory of bio-energy transport in the protein molecules in living systems based on some physical and biological reasons, where the energy is released from the reaction of hydrolysis of ATP molecules. In this new theory, Davydov's Hamiltonian and wave function of the systems are simultaneously improved and extended.A new interaction has been added to the original Hamiltonian, the original Davydov wave function of the excitation state of single particles for the excitons in the Davydov model have been replaced by a new wave function of twoquanta quasi-coherent state in Pang's model, in which the bio-energy is carried and transported by Pang's soliton along protein molecular chains, which are formed through the still self- trapping of two excitons, interacting amino acid residues, where the exciton is generated by vibrations of amide-I (C = O stretching) arising from the energy of hydrolysis of ATP. We gave the soliton solutions of dynamic equation and studied further their properties by analytical method in Pang's model. The results obtained indicate that Pang's model gave high nonlinear interaction energy for Pang's soliton. which can cancel and suppress the linear disperseve energy, thus Pang's soliton transporting the bio-energy has quite high binding energy and stability. Therefore, Pang's model for the bio-energy transport differs completely from the Davydov model.

We here calculated also the lifetime of Pang's soliton at the biological temperature 300K using the non-linear quantum perturbation theory in a wide range of

parameter values of  $\alpha$ -helical protein molecules. The investigated results show that the lifetime of Pang's soliton at 300K is large enough and belongs to the order of  $10^{-10}$  second, or  $\tau/\tau 0 \ge 700$ , in which the soliton can transport over several hundred amino acid molecules.

features of Pang's soliton through comparing with those of Davydov's soliton, in which we elucidated that Pang's soliton can play an important role in biological processes with respect to the models of Davydov and others.. Thus we can judge that Pang's model is a candidate of the bio-energy transport mechanism in protein molecules.

Therefore, we here exhibited the

Table 2.	Comparison of	f the Nature o	of the Solitons	between Pang	g's Model	and Davy	dov'sModel
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Parameters Model	Lifetime at 300K(S)	Critical temperature(K)	Number of amino acid traveled by soliton in lifetime
Pang's model	10-9-10-10	320	Several handreds
Davydov model	10-12-10-13	<200	Less than 10



## Fig. 11. The pump-probe response of the anomalous (1650 cm<sup>-1</sup>, *filled circles*) as well as of the normal band (1666 cm<sup>-1</sup>, *open circles*) of ACN after selectively exciting the former (D. W. Brown, et al. 1986).

Hamm et al. (D. W. Brown, 1986; D. W. Brown, (1987); [D. W. Brown, (1988); D. W. Brown, 1990; D. W. Brown, et al. (1986); D. W. Brown, (1988); D. W. Brown and Z. Ivic, (1989). measured the lifetimes of the solitons by pump-probe spectroscopy in acetanilide and proteins. Fig. 11 shows the pump-probe response of both the anomalous (1650 cm<sup>-1</sup>, filled circles) as well as of the "normal" band (1666 cm<sup>-1</sup>, open circles) of ACN after selectively exciting the former (D. W. Brown; 1986). At early times, a bleach of only the anomalous band occurs, which recovers on a fast 2-ps timescale. However, this relaxation is not complete, and a small negative signal remains. This indicates that the system does not relax back into the initial ground state,

but into а state that is either spectroscopically dark or outside of spectral window. On a somewhat longer timescale (35 ps), the energy still present in the crystal thermalizes. That is, the anomalous band loses intensity (a negative signal in the difference spectroscopy of Fig. 11 and the 1666 cm<sup>-1</sup> band gains intensity, exactly as in the stationary spectra of Fig. 8 when we increase the temperature. Hence, after vibrational relaxation of the initially pumped state, energy relaxes through a unknown pathway, but then reappears as heat after 35 ps. A very similar relaxation behavior was also found for the N-H band (D. W. Brown, 1986). Therefore, we can determined from this experiment that the lifetime of the soliton excitation in ACN is 35ps.

Hamm et al provided also a compelling evidence for vibrational self-trapping in NMA, which is similar with that in crystalline ACN because the former's molecular structure resemble ACN's. In particular, both crystals, ACN and NMA, have an orthorhombic structure and consist of quasi-1D chains of hydrogen-bonded peptide units (-CO-NH-) with structural properties that are similar to those of  $\alpha$ -helices. Thus they are often regarded to be the model compound for peptides and proteins. However, the mechanism is expected to be generic and should occur in this crystal. Nevertheless, no convincing experimental evidence for selftrapping in NMA had been found so far. However, they carefully measured infrared spectra of NMA (A. C. Scott, 1990) by pumpprobe experiment and compared the infrared

absorption spectra and the pump-probe spectra of the amide-I and NH modes of acetanilide (ACN) and N-methylacetamide as well as their deuterated derivatives. The amide-I bands of NMA shows а temperature-dependent sideband, but it is less distinct than in ACN in Fig. 12. On the other hand, the N-H band of NMA is accompanied by a sequence of satellite peaks, the spacings between which are larger than in ACN (which could be since NMA is lighter, and hence since lattice tentatively phonons are at higher frequencies). Comparing the pump-probe responses of these spectral anomalies in both crystals gave very similar results, providing evidence that vibrational selftrapping is indeed a common effect in hydrogen-bonded crystals. \

The generation of nerve impulse in nerve fiber arising from the bio-energy released by ATP hydrolyses reaction and its features of transport along the nerve fibers in living systems

## The basic structure of nerve fibers in life systems

The unit of the nervous system in animals is the nerve cell or the neuron. It is the unit of structure and function of nervous system, its main function is to accept, process and transfer the nerve information, to complete the functions of the nervous system. It consists of nerve cells having different sizes and forms, which is shown in Fig.12.



Fig.12. The structure of the neuron. (Pang Xiao-feng, 2007b; W.L.Liu, 1994)

In addition to general structure of cell, which contains the membrane, cytoplasm and nuclear, the neuron or nerve cell is also composed of the membrane, cytoplasm and nuclear, but their sizes and shapes are different those of general cell. In particle, the neuron is a fiber cell and contains the cellbody and many bumps, such as one axon and many dendrite, which are issued from the cell-body, in the cytoplasm there are an austenite (or Nissl substances), which is a active part and the position of syntheses of protein molecules. At the same time, the neurons involve also the large number of micro-tube and micro-trabecular, which is formed through accumulated by a plenty of large number of polarized protein molecules, which resembles with a polymer formed by many dipoles in accordance with the style of order arrangement, it is also an acted sites of the narcotics of central nervous. In fact, the size and shape of different neurons are very distinct, but their structures are almost same, they can all be represented by Fig.12 (Pang Xiao-feng, 2007b; W.L.Liu, 1994).

The branch of the axon is called the lateral branch. The lengths of axon and lateral branch are not same, their differences are also very large, some are very short, which are about several micrometers, but the lengths of most of bumps in the neurons are very great, such as their lengths may reach 1m in the persons and animals. When the axons are contacted with other cell bodies, some structures of myelin sheathes may occur in the neurons for the persons and animals. However, the neurons without myelin sheathes exist also in some organisms. Experiments verified that thirty six carbon olefine acid (DHA) promotes the forms of the myelin sheathes in the processes of extension and metabolism of the neural axons.

The axon endings in Fig. 12 can both output electric-information and release the neurotransmitter to affect another neurons or non-nerve cells. This means that the axons and lateral brarches can all link with other -nerve cells by virtue of the synapseses and another cell bodies. Thus a completely neural signal transmission system is formed in this case.

The dendrites and most axons vertebrates neurons and membranous organelles, which can synthesis cell-bodies and extra telecom and neurotransmitter release, in order to affect the close contact with it another, the axons and all collateral can be a nerve cell through the synapse and another cell precursors, and form a neural signal transmission system. The dendrites and axons of most neurons in vertebrates are issued from their cell bodies ocated in the center of the cells. The cellbody contains the nuclear and organelles feature of membranous having to responsible for synthesizing and processing protein molecules. At the same time, the synapses of the neuron are often located between the dendrites and cell-body, this means that the cell-body participate also the information integration and collection. The experimental results showed that the dendritic structure of a special nerve cells can enhance the calculation functions of nerve cells in the (W.L.Liu, 1994).

## The form of the synaptic structures and its properties in nerve cell membrane

The synaptic structures have very important roles in the nerve activities, its structure and features are worth to study seriously. Its form is described as follows.

The axons at the grown position in the

neuron are grown and extended some larger cones, in this case their cone end of the protuberance or bumps can contact or combine to form a function wide organ with the bottom of axons or dendrites or cell-body of neighboring neuron. The organ between two neurons is referred to as the synaptic as shown in Fig.13 ((Pang Xiao Feng, (2011); Pang Xiao-feng, (2011); W. X. Zhu and L Li, 2000; M. Peyrard, et al., 1992). Synaptic is a contact area and small gap having exceptional function, which can transport and transfer the neural signals from one neuron to other neuron. However, they are not continuous in the protoplasm. The synaptic is, in essence, the association origin of function between two nerve cells and the position of contact of structures. Through the associations and their works, the neurons and receptor cells as well as the effect or cells are associated together to form a complete system of transmission of There signals. are not neural the transmission and transport of neural signals without the synaptic. Therefore the synaptic is a key origin in neurobiology.

It is estimated that the human brain has about  $10^{14} \sim 10^{15}$  synapses. Single synaptic is a complex of incoming - outgoing unit of signs, which is just a basic feature of the neurons. All neurons are all linked together through them. The related linkage between two neurons or seaking, the synaptic contains three parts: the before-part of synaptic of active cells or their protuberance given out, after-part of synaptic of cells accepted activation or their protuberance and the part or gap etween them. Therefore, the correct forms of linkage of the synapses require not only the right guidance of growth of the protuberances along the surface of cells and extracellular pathways, but also the specific identification between the presynaptic and postsynaptic cells. At the same time, it demands also stability of synapses in the activation in the motion of



Fig. 13. synaptic structure in the neuron (Pang Xiao-feng, 2007b; W.L.Liu, 1994).

In biology, the synaptic connections, or speaking shape or form of e synaptic are various. If an axon or a lateral branch are terminated in another neurons, then it is called the axis - body synapse, but the synaphic between the axons and dendrites is called the axon-dendrite synaphtic, the synaptic between two axons is the axonaxon synaptic. If one axon is terminated on the skeletal muscle fibers, then it is referred to as the neuromuscular endplate.

time and space.

A basic feature of the synaptic transmission are the valve and one single direction of the transfer, its information of transfer can be integrated and has a plasticity, i.e., its efficiency and functions are variable, the capacity of transferred information are higher and have the multipurposes. These features are the foundation of orderly neural activity and learning and memory of animals and persons ((Pang Xiao-feng, 2007b; W.L.Liu, 1994).

In the central nervous system, the typical presynaptic and postsynaptic compositions are closely associated on the membrane each other, which will lead to the alienation of contacted membrane, thus the two layer membranes should be separated by a narrow synaptic gap. The synaptic gap is an analogue matter of basement membrane. which is derived from the before- and aftermembranes. The materials in the synaptic gap are all the protein molecules, which involved the alkaline amino acid with high concentrations, its interstitial matter has the sialic acid and glycoprotein, etc. In the side of pre-synaptic there are the synaptic corpuscles of swollen and tapered protuberance, in which many vesicles with a lot of neurotransmitter of high concentration

are contained.

The synaptic has three types of chemical synaptic and electric synaptic and their hybrid. The chemical synaptic and electric synaptic, specially, the former exist widely in all animals and Human beings, but the latter exists only in the invertebrate and lower vertebrate animals, their nerveinformations are transferred by means of the variations of electric potentials among the gap junctions of synapses, in which the circuit impedance between two neurons is very larger, but their electric-potentialare lower. The chemical synaptic is widely existent in the nervous systems in the breastfeeding animals, its transport of the nerveinformations are carried out by virtue of the release and transport of chemical materials, which are called as the neurotransmitters. or messenger, such as the endocrine hormone, neural hormone of cells, etc. Chemical synapses is the most complicated synapses in the nervous system, their connections possess a specificity, such as its transport of nerveinformation has a exact direction from one neurons to another neurons and polarity. Its polarity is mainly determined by a group vesicles and paralleling of synaptic membranes. There is a gap with the size of 20nm between the membranes of two neurons in the parallel membrane, its density of material is larger, specially for the pair-side membrane involving the protuberance of synaptic vesicles.

The comparison of properties of chemic and electric synapses is shown in Table 3.

The structure of the chemical synapses is shown in Fig.14. It contains the submicrostructures of the synaptic endplate, synaptic vesicles, front membrane of synaptic, aftermembrane of synaptic,synaptic vesicles and postsynaptic membrane. The synapsin 1 in the front membrane is a protein molecule and a heterodimer constructed by the protein molecules with the molecular weigh of 166kDa and are related to the synaptic vesicles. After the synapsin 1 is in phosphorylation state, it is separated from the vesicles membranes and combination with the cytoplasmic membrane through cell skeleton, thus some neurotransmitters are released in this case. The phosphorylation is agan catalyzed by the calcium/calcium modulin dependent protein kinase 1, which can activated by the internal flow Ca2 +, when a nerve impulse occurs. The determined compositions in the postsynaptic membrane are the membrane receptor, thickening of postsynaptic (PSD) and the enzymes. which can make PSD phosphorylation and dephosphorylation. The thickening of postsynaptic is mostly formed by the cytoskeleton of the membrane, which contains the many microtubules, nerve filaments, and combines many proteins and proteolytic enzymes. The main composition of PSD is the peptides of 50kDa or proteins. The above components are all shown in Fig.14, in which the calcium/calmodulin protein kinase  $\Box \Box$  (CaM  $\Box$ ) is a major biochemical components of synapses and exists mainly in the presynaptic endings and PSD, and it is also one of the homologous kinase family. It is consisted of 12 subsites with weighs of 50  $\sim$  60 kDa , which is a larger polymer of proteins, its basical function is itself phosphorylation of subunits. So-called itself phosphorylation is just make the kinases have a function of switch, then the kinas can still maintain itself bio-activity after short calcium-information signals are accepted. This feature is very advantageous to the long-time activity of the postsynaptic and their variations. Otherwise, there are another some scaffolding proteins in the postsynaptic, which contains the actins and the protein of 43kDa (Pang Xiao-feng, 2007b; W.L.Liu, 1994), Pang Xiao feng, 2006].

## Table 3. The comparisons of properties of chemic and electric synapses (Pang Xiaofeng, 2007b; W.L.Liu, 1994); Pang Xiao feng, 2006)

The chemic synapses	The electric synapses
the affection of action potential of the presynaptic on electric potential of after membranes is small	the action potential of presynaptic is a direct factor of the transport
presynaptic potential caused a large number of synchronous releasing of neurotransmitters by the small bubble under action of cooperation of Ca <sup>2+</sup>	without this effect
the releses of eurotransmitter produce the appearing of local and different potentials of postsynaptic membrane, its sizes can be integrated, the postsynaptic potential can be inverted when it is varied	the postsynaptic potential has not been inverted, when it is varied
there is synaptic vesicles in this case	without synaptic vesicle
it can be both excited and nhibited	it can only be excited
it is easily influenced in chemicalfactors	it is not influenced
its effect can be sux(0.1)mmarized in the space and time, it has also a integrated effect	1: 1, few integration



Fig. 14. The configuration and biochemical properties of chemical synapses, where mp denotes the corpuscles in the membrane, PSD denotes the thickening of postsynapses (Pang Xiao-feng, 2007b; W.L.Liu, 1994); Pang Xiao feng, 2006)

The Nerve Excitation and form of Nerve Impulse under Influence of Bio-energy Released from Hydrogetic Reaction of ATP Molecules

Forms of action electric-potential and nerve impulse on nerve mechanisms

What is nerve excitement? It is that the nervous tissues give out a strong reaction, when its strength reaches or exceeds the certain threshold. This phenomenon appears also in the muscle tissue. Its main feature and performance are that the electricpotential across the cytoplasmic membranes generated a fast variation. In this case the strength of variation of electric-potential is used to characterize and mark the state and intensity of the nerve-excitation. We here will discuss the excitation states of the nerve and its features and representations in the nerve system.

As it is known, the molecular structure of the neurons is also same with those of general cells, although their configurations have some differences, such as the distributions of the ions of Na<sup>+</sup>, K<sup>+</sup> and Cl<sup>-</sup> on the membrane of the neurons are same with those of other cells, i.e., they are all nonuniformly distributed in the side and outside of the cell membrane , in which the number of Na<sup>+</sup> ions in its outside are more than those in its inside, but the distributions of K<sup>+</sup> and Cl are just inverse, namely he numbers of K<sup>+</sup> and Cl<sup>-</sup> ions in the inside of cell membrane are more than those in its outside. This means that an electric potential formed and appeared on the cell is membrane due to the non-uniform of distribution of the charges or ions in the inside and outside of cell membrane, this is necessary to results in the differences of permeability of ions to the cell membrane. Thus the electric-potential is formed, which is called the resting potential of cell or the potential of numbers, its size is about -40 --70mV, i.e., the electric-potential in inside of cell membrane is lower than that in its outside, which was verified by the experiments and theory of biophysical theory. These results manifested clearly there are many ions in inside and outside of cell membrane, but the numbers for different

ions are different. These phenomena indicated that there are also some channels of the ions on the cell membranes, which are formed by membrane -spanning proteins molecules, but their electric resistances of different ions are different. The above resting potential of cell membrane can be determined and obtained using the above results.

In particle, in the nervous tissues the compositions of the inside and outside electrolytes are also different, such as the concentrations of Na<sup>+</sup> and Cl<sup>-</sup> are more many in the outside of the axons of activesquid, but much less in its , but the distribution of K<sup>+</sup> is just opposite. In the resting state, the charge distributions in the inside and outside of the cell membrane in the nerve fibers is still negative in the interior and position in the exterior, thus its electric potential is about ~70mV , its membrane resistance is  $10^3~\Omega/cm^3,$  its membrane capacitance is 1 mf/cm ((Pang Xiao feng, 2006; Chen vi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, I.R. (2007); W. Fann, et al. (1990); P. Hamm and G.P. Tsironis, (2007))

The huge differences of permeabilities and resistances of these ions on the cell membrane in the squid animal lead on to distinctions their large of electricpotentials. The researches indicated the differences of the potentials can be represented by  $P_{K}{:}\ P_{Na}{:}\ P_{cI}$  = 1: 0.04: 0.45, where  $P_{K^{n}}$   $P_{Na}$  and  $P_{CI}$  are the electricpotentials of K<sup>+</sup>, Na<sup>+</sup> and Cl<sup>-</sup> ion on the membrane. This result exhibited that  $K^+$ plays important part in the form of resting electric potential of huge axons in the squid. In this case, most of the K<sup>+</sup> ions are in free states, but half of Na<sup>+</sup> ions either are in the combined states or form some products in the cells, otherwise, Ca2+ ions are almost completely in the combined states with

some negative ions or in organelles (mitochondria, etc.) in the cells. Therefore the permeability of Na<sup>+</sup> on the membrane is small in resting states of cells.

The above properties of permeability of ions can be checked by some experiments. for example, the variations of permeability of ions on the membrane was measured, when some specific inhibitors are added in it. For instance, the water-soluble paralytic poison tetrodotoxin (TTX), which are extracted from some fishes and newts in California, are added in the gaps between their axons, the experiments found that the channels and corresponding movements of Na + ions in the nerve and muscle fibers are stopped completely. If the TTXs are injected in the axons, the permeability of Na<sup>+</sup> ions is not changed. However, if the frog toxin (BTX), which is a kind of steroid alkaloids, is injected in the above animals, it will result in the depression of resting electric-potential and increases of the permeability of Na<sup>+</sup> ions. If the inhibitors of four procedures (TEA) are injected in the axon, then the permeability of Na<sup>+</sup> ions have been not varied, but it can stop completely the movement of K<sup>+</sup> across the membrane. These experimental results not only conform the validity of the above exhibited that results but also the movements of K<sup>+</sup> across the membrane are completely independent relative to that of Na<sup>+</sup> ions. This represented also that the penetration abilities of different ions on the membranes have a strong specificity. The identified effects of the inhibitors of TTX and TEA on the permeability of Na<sup>+</sup> and K<sup>+</sup> make that we can assume that the transport of the ions across the membranes are carried out by virtue of protein - lipid compounds or ion channels. Thus each ion has itself special channel of ions. The tetrodotoxins stopped the transport of Na+ because they have closed the channels of sodium ions in the area of one square

micron. The experimental measures indicated that there are 100 channels of Na<sup>+</sup> in the area of one square microns. In the resting or inactivity state, it is estimated experimentally that the conductivity of Na<sup>+</sup> in a sodium channel is about  $4 \times 10^{-12} \Omega^{-1}$ . but about  $12 \times 10^{-12} \Omega^{-1}$  for K<sup>+</sup> in the potassium channe ((Pang Xiao-feng, 2007b; W.L.Liu, 1994; (Pang Xiao feng, 2006; Chen yi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, I.R. (2007); W. Fann, et al. (1990); P. Hamm and G.P. Tsironis, (2007); R.H. Austin, 2003; Pang XF, 2007)

On the other hand, in resting state the permeability of potassium ions across the excited membrane of cell is larger than that sodium ions. In addition. some of macromolecules or ions with negative charges inside cell membrane cannot penetrate the membrane, based on these results we can establish the relationship of these ions between the inside and outside cell membranes. In this case, we mark these different ions in inside and outside cell membrane by the subscript 1, 2. Because again there are also some ions with negative charge of monovalence as mebtioned above. which is denoted by P<sup>-</sup>, Thus we can represented the relationship of the chemical potentials of these ions in outside and inside cell membrane in the equilibrium state on the basis of the conditions of equality of the chemical potentials and charges in the inside and outside the cell membrane of the ions of  $K^+$  and  $CI^-$ , which is denoted (Pang Xiao-feng, 2007b) by

$$\mu_{k_1}^+ = \mu_{k_2}^+, \ \mu_{cl_1}^- = \mu_{cl_2}^-$$
 (25)

where  $\mu_i$  is the chemical potential of the ion. In the ideal solution, the chemical potentials can be represented by

$$\mu_{i} = \mu_{i}^{(0)} + RT \ln C_{i} + Z_{i}F\phi$$
(26)

where  $\mu_i^{(0)}$  is the chemical potential in the standard state, C<sub>i</sub> is the concentration of the ion in the solution, Z<sub>i</sub> is chemical valence of the ion,  $\phi$  is the resting electric potential of corresponding element, F is Faraday constant.

From Eqs. (25-26) we can obtain

$$\mu_{K_{1}^{+}}^{(0)} + RT \ln[K^{+}]_{1} + F\phi_{1} = \mu_{K_{2+}}^{(0)} + RT \ln[K^{+}]_{2} + F\phi_{2}$$
(27)

$$\mu_{Cl_1}^{(0)} + RT \ln[C\Gamma]_1 - F\phi_1 = \mu_{Cl_2}^{(0)} + RT \ln[C\Gamma]_2 - F\phi_2$$
(28)

The following results can be obtained from Eqs.(27)-(28)

$$\frac{[K^+]_1}{[K^+]_2} = \frac{[Cl^-]_2}{[Cl^-]_1} = V$$
(29)

Equation (29) is called as Gibbs-Dsnnan condition , v is Donnan proportional constant.

From Eqs. (27) -(28) we can gain the potential of the ion across the membrane

$$\phi = \phi_1 - \phi_2 = -\frac{RT}{F} \ln \frac{[K^+]_1}{[K^+]_2} = \frac{RT}{F} \ln \frac{[C\Gamma]_1}{[C\Gamma]_2} = \frac{RT}{F} \ln \nu (30)$$

Because the resting potential is mainly caused by the permeability of K<sup>+</sup> ions, if the concentration y of potassium ions  $[K^+]_2 = 20$  mmol and  $[K^+]_1 = 100$ mmol are inserted in Eq.(27) –(28)we can easily obtain  $\phi_k = -75$ mV, this is basically consistent with the experimental value of resting electric potential value of -70mV measured. This

verified clearly that the distribution of the ions on the cell membrane described mentioned above are correct. This conformed strongly that the resting electricpotential of the membrane is produced by the permeability of K<sup>+</sup> ions (Pang Xiao-feng, 2007b; W.L.Liu, 1994; Pang Xiao feng, 2006; Chen yi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, (2007); W. Fann, et al. (1990).

If second condition:

$$[K^+]_1 = [Cl^-]_1 + [P^-] \text{ and }$$
 
$$[K^+]_2 = [Cl^-]_2 = C_2$$
 (31)

is used we can find out the following relationship

$$v = \frac{[P^{-}]}{2C_2} + \sqrt{\left(\frac{[P^{-}]}{2C_2}\right)^2 + 1}$$

## The theorem of work of sodium pump and potassium pump and their as well use of bio-energy on the nerve membranes

As it is known from the above results. the ions of Na+, K<sup>+</sup> and Cl<sup>-</sup> can be displaced and flowed along the ionic channels on the cell membranes due to their nonuniformities of distribution, which promote the fluxes of Na<sup>+,</sup> K<sup>+</sup> and Cl<sup>-</sup> along their directions of decrease of electric chemical potentials. Thus some ion-currents are occurred on the membrane. This results in just occurring of the electric signs in the cells. Obviously, the electric signs are, in essence, generated due to the open and close of the ionic channels. In the normal state Na<sup>+</sup> ions are shifted from the outside cell membrane to its interior, but t the displacement of K<sup>+</sup> and Cl<sup>-</sup> are just inverse and to the outside membrane from its interior. Very clearly,

these fluids will induce the variations of distribution of these ions from the nonuniform state to the uniform state, thus the electric-signs of the cells will decreased, which are not advantageous for the growth of the cell or life. In this case it is guite necessary to maintain the ion concentration gradient on both sides of the cell membrane mentioned above. In order to gain this purpose, its basic method to construct and grow some ion pumps, such as the sodium pump and potassium pump, which can hand and carry Na<sup>+</sup> ions to the outside membrane from inside membrane, and can hand and carry also K<sup>+</sup> ions to the inside membrane from outside membrane, respectively. Thus the nonuniform distribution of Na<sup>+</sup> ions and K<sup>+</sup> ions or their gradients of concentration on the cell membrane can be always maintained or restored also in active life bodies using these ionic pumps . In other words these ion pumps can provide the bioenergies to carry away these ions to specifying positions to maintain the gradients of concentration of these ions in both sides of the cell membrane to a certain level, then all life activities can remain and continue, if the bio-energy is supplied enough . Or else, the life activities will be completely stopped. Therefore we can say that the Na<sup>+</sup> and K<sup>+</sup> pumps and the supply of bio-energy play very important roles in the life activities [(Pang Xiao-feng, 2007b; W.L.Liu, 1994); Pang Xiao feng, 2006, Chen vi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, (2007); W. Fann, (1990).

However, how can these ion pumps be constituted and grown? Very clearly, the work can be carried out and finished by some special protein molecules or enzymes, which can also bring away and carry away these ions to specifying positions. These proteins or enzymes are some rotary motor –proteins or ATP synthases, such as the rotary motor –protein as shown in Fig. 15, DNA helicase motor and **RNA** polysaccharide enzymes motor. We here will elucidate the structures and functions of the ion pump in the ATP s synthase in Fig. 15, which can shoulder the work of syntheses of ATP and can provide the bio-energy. The enzyme is composed of the part of proton conduction, F0 , and its part of promotion, F1. When the protons traverse the F0, ATP molecules will be synthesized in F1, thus the bio-eneraies generate immediately by means of the hydrolyses reaction of ATP molecules. This reaction is reversible. In this case, the bio-energy can promote the protons to move along the inverse directions, if the hydrolyses reaction of ATP molecules occurs in F1. Because F1 can catalyze the hydrolysis of ATP molecules, then it is called as F<sub>1</sub>-ATP enzyme. The ATP synthesized enzymes exist also in the inner membrane of the mitochondrial and the serosa in the bacteria as well as capsule membrane in the chloroplasts.

In the process of syntheses of ATP molecules, the chemical potential of the protons must be consumed and expended, but the chemical potential can be complemented by the biological membrane including the light-chemical systems. When ATP enzymes rotate the protons along the inverse direction, the hydrolyses of ATP molecules occur, thus the electric-chemical potential of the protons is also formed in this case.

However, the transmission mechanism of the protons in the reverse reaction is always related to the hydrolysis of ATP molecules. As it is known, the syntheses and hydrolyses of ATP molecules are carried out by the  $F_1$ -ATP enzymes on the enzyme membrane.  $F_1$ -ATP enzyme has a strong activity of hydrolyses of ATP molecules, but  $F_0$  part of the enzyme can also cause the shift of the protons and promote further their movements of across the membranes. The distance between the part of F<sub>1</sub>-ATP enzyme in the hydrolytic enzymes and the proton transmission area is about 8nm, they are linked by  $\gamma$  sub-base. Therefore, the syntheses and hydrolyses of ATP molecules and proton transmission are completed through the mutual combination among them using the  $\gamma$  sub-base, in which the increment of rotation is about 120<sup>0</sup>, but the direction of  $\gamma$  base will be rotated about 120<sup>0</sup>, when one hydrolysis reaction of ATP molecules is appeared , thus its efficiency is close to 100%.

Obviously, the structure features of rotary motor- ATP synthase and its functions can use to explain and elucidate the mechanism of sodium pump and potassium pump in nerve systems mentioned above, in which the sodium pump carry and bring the Na<sup>+</sup> from the inside cell membrane to outside cell membrane, but the potassium pump carry and bring the K<sup>+</sup> from the outside cell membrane to inside cell membrane to maintain the gradients of concentration of these ions in both sides of the cell membrane. These functions are carried out in virtue of its special identification abilities to the sodium and potassium ions through their rotation features and special atomic weighs and moved stats as well as the sizes of combination positions such as  $F_0$  and  $F_1$ of the motor ATP synthase.

Certainly, the motions and states of the motor ATP synthase are very complicated, if they are in detail investigated. These problems are worth to study deeply and completely.

At present, we again elucidated in detail the essences and properties of work of sodium pump and potassium pump in the nerve systems.

In practice, the Na+ ions and K+ ions

with water flow together along their channels, if these ions move along their ionic channels across the cell membranes. Once they are flowed over the cell membranes, then water will be taken off from these ions. In this case these ions in the dehydrations can be absorbed by other polar groups in these ionic channels. In order to maintain the ion concentration difference between the inside and outside membrane of the nerve fiber cells at the required level, the sodium pump must work constantly and make the hydrolysis of ATP molecules release continuously the bio- energy in the entire life period.

In the nerves systems of the crab, about 50% of metabolic energy were used in the sodium pump in the nerve fibers in the resting state. In the crab the hydrolysis of ATP molecules is together finished by ATP-enzyme, K<sup>+</sup>, Na<sup>+</sup> and mg<sup>2+</sup>, where ATP-enzyme is a part of the membrane, its other part is in outside cell membrane. In this case there are an interaction between the enzymes in the outside membrane and K+ in the outside cells .

Generally speaking, when  $K^+$  exists, the work of potassium pump will be stopped, the sodium channels are opened duo to the excitation of Na<sup>+</sup> in this case, then the sodium pump start its work to make or to forces Na<sup>+</sup> ions up- shift along the direction of increase of its concentration. In this time, Na<sup>+</sup> ions are displaced and transferred into the inside membrane by virtue of its ionic motions in channels and their interactions with some moved carriers, which guarantees the the gradient of its concentration between both sides of cell membrane and the transport of Na<sup>+</sup> ions in plasma.

On the other hand,  $K^+$  ions will be also shifted to the inner of cells under action of the difference of electric- potential generated by the active transport in Na <sup>+</sup> ions. Therefore, the flowing of the Na <sup>+</sup> don't depend on the difference of electric potential in the cell membrane (which is right in the case of below the interval of threshold values), but the flowing of K <sup>+</sup> ions in inside cell is increased with the increase of the difference of electric-potential between both sides of cell membrane. This is just so-called the effect of the electric coupling between Na <sup>+</sup> and K <sup>+</sup> ion transport in the nerve systems. These results were confirmed in the researched results of the giant axons in the Grape snail obtained by F. Coase autumn, et al [(Pang Xiao-feng, 2007b; W.L.Liu, 1994); Pang Xiao feng, 2006, Chen yi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, (2007); W. Fann, (1990); P.Hamm and G.P.

Tsironis, 2007; R.H. Austin, 2003; Pang XF; 2007)

From the above investigations we can conclude that we must use bio-energy to maintain the nonuniformal distribution of Na<sup>+</sup> ions and K<sup>+</sup> ions and their gradients of concentration on the cell membrane using the sodium pump and potassium pump as well as the bio-energy released by hydrolysis reaction of ATP molecules. It is very interesting that these processes can go on and be finished simultaneously in these ionic pumps under action of the bio-energy. Therefore we concluded that there are not works of the sodium pump and potassium pump as well as life activity of cell without the bio-energy.



Fig. 15. The structure of rotary motor – synthase (Pang Xiao feng, 2006, Chen yi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, (2007); W. Fann, (1990); P.Hamm and G.P. Tsironis, 2007; R.H. Austin, 2003; Pang XF; 2007))

## Forms of Action Electric-potential and Nerve Impulse under Action of Bioenergy in the Nerve Systems

We know from the above investigations that the ions of Na<sup>+</sup>, K<sup>+</sup> and Cl<sup>-</sup> are not the uniform distribution in the inside and outside cell membrane and their permeabilities across the membrane are also different, thus

there is a resting electric- penitential of -40 --70mV in cell membrane, which arise from the motion of K<sup>+</sup> ions. This means that the distribution of electric-potential of the membrane is the positive in outside membrane and negative in inside membrane, respectively, namely, the membrane is in the polar state in the resting state, which is just the state of polarization of cell membrane.

However, when the cells are stimulated by a small electric signs, then its states and features will be changed. If a glass capillary electrode is inserted in the inside of the cells, then the depressions of the absolute value of negative differences of electric-potential between the inside and outside membrane e in a short period of time are inspected and observed. The values of decreases of the differences of electric-potential are further depressed with the increasing distance between measured and stimulated electrodes. This indicated that the electricpotential is localized. In general, when the stimuli are small, the changes of the negative potential in the inside membrane are small, which does not exceed a threshold. However, if the stimulated intensity is increased to exceed the threshold, then the electric-potentials of many excitable cells will be varied greatly and fast to become the positive values in inside membrane and negative in outside membrane from the above state at the time of 0.5ms. Subsequently, the change will increase continuously with increasing time, and makes the positive electric-potential reaches a maximum value (about 50 mV) at a determined time, which is called the depolarization of the membrane. After this , the electric-potential will gradually decrease to original value at about 1ms, which is called stored polarization of the membrane. However, the depressed state of the electricpotential cannot sopped and is depressed continuously to a minimum, which is referred to as superpolarization. This changes of the electric-potential is referred to as an action electric-potential, which is represented in Fig. 16.

The action electric-potential indicated clearly the changed features and rules of the electric- potential on cell membrane and ionic permeability across the cell membranes with varying time under action of external electric sign and influences of bio-energy. The variations can be described as follows. In the resting state the cell membrane is in the polarization state, its electric - potential is about -40 - -60 mV, which is caused by the motions and the increases of permeability of K+ ions. However, the depolarization is caused by the increases of permeability of Na<sup>+</sup> ions across the membrane under the influence of sodium pump and bio-energy released in the hydrolyses reaction of ATP molecules, which carry away Na<sup>+</sup> ions from the inside membrane into the outside membrane, thus the electric-potential in the outside membrane is increased, its strength is larger than that in inside membrane, thus the cell membrane is in the depolarization state, in which the electric- potential is lifted as shown in Fig. 16. However, once the electric-potential reach a maximum, the potassium pump is started to work, it carries K<sup>+</sup> ions into the inside membrane from the outside membrane, thus the electricpotential is depressed and the cell membrane is in restored polarization state. the membrane is further in the superpolarization state with increasing time due to the inertial motion of K<sup>+</sup> ions, which are shown in Fig.16. Therefore, the electricpotential across the membrane of the neurons are determined and controlled by the relative permeabilities of ions of Na<sup>+</sup>, K<sup>+</sup> and Cl<sup>-</sup>, and their concentration gradient across membrane, but the bio-energy, which cause the concentration gradient of the ions in both sides of membranes, are carried out by the above ionic pumps, but their energies are obtained from the hydrolyses reaction of ATP molecules. The ionic pumps can not only pump initiatively out some ions but also bring these ions into the cells to maintain always the concentration gradient across membrane at a solid level. In this case the sodium pump can pump out three Na<sup>+</sup> in the

outside of cell membrane to inside membrane , but the potassium pump can pump out two  $K^+$  to inner membrane from outside membrane to change the electric potential on the cell membrane. When the variation of electric-potential of the axon membrane exceeds its threshold, then the action electric-potential is triggered, thus the excitement of the neurons occurs in the nervous system.

The action electric-potential is an electric signs, or speaking, it is essentially a nerve electric-impulse having certain electric-signs, its signs is great, rapid change and has a solid shape. It is exhibited and represented in the electricpotential having the constancies of size and form, its change of whole shape can be controlled in several milliseconds and depend not on the types and possess of the stimulation, and possess the nature of the "all or nothing". The action electricalpotential has not the distinction of size, but it can transport the nervous -biological information the fiber along nerve membranes in a stable wave form with certain frequency i, the higher of its frequency, the fast of its speed.



time

Fig. 16. The action electric-potential of cell membrane I[(Pang Xiao-feng, 2007b;
W.L.Liu, 1994)., Pang Xiao feng, 2006, Chen yi zhang, 1995; Han Jie shen, 1993; Cheng, Jie Ji and Ling Ke chun, 1981; P. Hamm, (2007); W. Fann, (1990); P.Hamm and G.P. Tsironis, 2007; R.H. Austin, 2003; Pang XF; 2007)].

Once the action electric- potential reached the nerve terminal, then it will trigger and release some nerve neurotransmitters, in this case its secretion rate are also very higher. Obviously, this kind of action electric-potential is generated under synergistic action of Na<sup>+</sup> and K<sup>+</sup> ions in their channels. Because the open and close of two ion channels go on very accurately, then the contrary variation of the depolarization of following membrane and its difference of electrical -potential are quickly completed, if the action electrical- potential occurs, this means that the electricalpotential in inside cell is higher than that in outside cell. Subsequently, they back to the level of resting electrical- potential. In the change case of the action electrical-potential, it will be propagated along the axons from one neurons to other in the speed of 120m/s through the synapses up to the central nervous systems and the brain to cause nerve excitement.

Quite clearly, the action electricalpotential is determined by the motions and distributions of ions of Na+, K+ and Cl-. Thus the electrical-potential across cell membrane under action of constant electricfield across membrane e is represented I[158-160, W. Fann, (1990); P.Hamm, G.P. Tsironis, (2007); R.H. Austin, et al. (2003); Pang XF. (2007) by

$$V = \phi = -\frac{K_B T}{F} \ln \left\{ \frac{P_K [K^+]_i + P_{Na} [Na^+]_i + P_{Cl} [Cl^-]_0}{P_K [K^+]_0 + P_{Na} [Na^+]_0 + P_{Cl} [Cl^-]_i} \right\}$$
(32)

where  $P_{K}$ ,  $P_{Na}$  and  $P_{CI}$  denote the permeabilities of Na, K and Cl ions across the cell membrane, respectively,  $[]_o$  and  $[]_i$ are the concentrations of ions in inside and outside membranes, respectively. Evidently, the electrical-potential across cell membrane in Eq.(32) are related only to Na, K and Cl ions, but only if the electric-potential in the is lifted inside membrane and the permeability of Na ions across the membrane from outside to inside is increased, then the values of the electricpotential across membrane will be changed to the positive from negative in the inner membrane. Subsequently, Na ions will infiltrate in the inner nerve fiber membrane, thus the electrical-potential will be lifted, which will lead to increases of osmotic quantity and speed of Na ions. However, when the electrical-potential in the inner membrane is lifted to certain value, a hysteresis effect occurs. In this case the permeability of K ions across the membrane is also increased. Because the concentration of Na ions in the inner fiber membrane are higher, then they can outwardly osmoses to the exterior of membrane. When the action electricalpotential is formed, the permeability of K ions will be increased and is faster than that of Na ions after 0.33ms, then the electricalpotential will return to original value (-70eV) from the maximum (+50mV). This effect

cannot be varied although the influence of ion movement of penetration exist because it depend only the speed of motion of K ions to the outside of membrane.

The Na ions in the nerve-fiber membrane, which are in the rising period of action electrical- potential in Fig. 16, can pump out from the inner membrane by the sodium pump. This phenomenon can be verified in the following experiments.

- (A). Its maximum is increased, if the concentration of Na ions in the solution in outside membrane is lifted. On the contrary, if the concentration of Na<sup>+</sup> ions in outside membrane is depressed, then its maximum is decreased.
- (B). The maximum is decreased, when the concentration of Na ions in the solution in inside membrane is lifted.
- (C). The experiment found that the aeneration of action electricalpotential is accompanied always with the increases of shifted speed of Na ions along the direction of increase of the gradient of electrical -chemical potential. In the great nerve fibers in the squid, one time of the action electrical- potential will result the Na ions of 3.1nmol./cm<sup>2</sup> to come in the fiber cell. The experimental results can explain qualitatively the increases of permeability of Na ions across the membrane, if the action electrical- potential appears . This can be verified by the experimental values of the permeability of the ions of Na<sup>+</sup>, K<sup>+</sup> and Cl<sup>-</sup> across the membrane, for Na<sup>+</sup>, K<sup>+</sup> and Cl<sup>-</sup> their proportions are from 1:0.04:0.45 in resting case to 1:20:0.45 in the depolarization state and appearing of action electrical- potential. This experimental results affirm that the

rising period of action electricalpotential or occurring of its depolarization effect in Fig.16 arises from the lifting of concentration or penetration of Na ions across membrane. Thus this verified that the analyses and results mentioned above are correct.

In practice, the experiment of the radioactive tracer of sodium atomic motion in the squid indicated that the flowed guantities of movements of Na and K ions are small in its generated period, such as in the giant axon of the squid, about (3-4) x 10<sup>-</sup> <sup>12</sup> mol/cm<sup>2</sup> of Na<sup>+</sup> are shifted and absorbed only, the same number of K<sup>+</sup> ions are lost and moved during the action electricalpotential or the period of electric-impulse. This indicated that the variation of concentration of Na or K ions are very small, are only one over one hundred thousand of the total numbers during one period of impulse of action electrical-potential. This is due to the inertia effect of depolarization functions of the membrane, which results in the depolarization effect of the membrane. In this case the nerve fiber membrane cannot occur second reaction of stimulus, only if the permeability of these ions are restored to original state, these ions can react to external stimulus after the time of 0.5-2 ms. Otherwise, the temperature can also greatly influence the above changes. If the temperature is varied from 6 to 7, then the permeability of K ions increases, but the loss of Na ions is increased, thus the amplitude of the action electrical-potential will be decreased more.

The above results manifest clearly that the bio-energy released in the hydrolysis reaction of ATP molecules plays key and important parts in works of sodium pump and potassium pump as well as the generation of action electrical-potential, there are not works of sodium pump and potassium pump as well as the generation of action electrical-potential without the bioenergy.

## The Transport of Nerve Impulse on the Nerve Membranes the Sodium Pump and Potassium Pump

The above investigations manifested that the energy released from hydrolytic reaction of ATP molecules are imported to trigger the work of sodium pump and potassium pump, let the sodium ions and potassium ions move along their channels to form the excitement of nerve membrane and to further produce and launch some nerve impulses. Fig. 17 indicated the excitation of an impulse. If the bio-energy is imported and provided continuously to the sodium pump and potassium pump, then the transport of the nerve impulse can be formed, then the impulse will be transported along the nerve fiber membranes, which can be represented in Fig.17. Concretely speaking, in the front before part of the excited area or first end the cell membrane is in the restored polarization state, which is denoted in "static membrane " in this figure. Subsequently, the cell membrane is in a polarization state due the stimulus of externally applied to electrical-signs, such as electric current or field, in which the sodium current is formed due to the action of sodium pump and the bio-energy, meanwhile, where the electricpotential of the membrane is also varied to the negation in the outside membrane from the positive in the inside membrane. In the linkage region between the excited area and non-excited area there are the lifting of the electrical-potential of membrane and its depolarization due to that the sodium current flow over the membrane from inner to exterior in the non-excited area. When the electrical-potential of membrane reach the threshold value in this region, then the action electrical-potential and an impulse occur in new excited area.

In the subsequent part of the excited area the potassium current will also occurs due to form of the potassium pump and influence of the bio-energy, which makes the membrane restore to the polarize state. In this case the current, which is started from original excited area, makes the cell membrane reach the threshold in new region, thus one new excitation and corresponding action electricalnew potential are formed, its formed process can be denoted in the excitation - depolarization - restored polarization, which is shown in Fig.17. This process is gone repeatedly on, then the transfer of action electricalpotential along the nerve membranes is appeared and carried out. In this case. This is just the mechanism of the transfer of action electrical-potential.

## The Confirmation of Feature of Terahertz Wave of Transport of Nerve imPulse along the Neve Fibers arlsing from the Bio-energy

At present, a key problem is to confirm the features of the above action electric – potential or nerve electric-impulse. However, how can we determine this feature of the nerve electric-impulse ? What are its features? what are the methods determining the features of the nerve electric-impulse? These problems have been not studied up to now, but they are quite worth to investigate deeply and carefully in this case.



Fig. 17. Form of nerve excitement in the nerve system (W. Fann, (1990); P.Hamm, G.P. Tsironis, (2007); R.H. Austin, et al. (2003); Pang XF. (2007))

We know from above investigations that the nerve impulse, or the action electricpotential shown in Fig.16, is formed and produced in virtue of periodic, hard and fast rule changes of distribution of the sodium and potassium ions in the inner and surface of nerve membranes as well as periodic works of sodium pump and potassium pump arising from the bio-energy released from the hydrolyses reaction of ATP molecules as mentioned and described above. We can say that there is not the nerve impulse without the works of sodium pump and potassium pump, or the bio-energy. Therefore the works of sodium pump and potassium pump, or the bio-energy play a key and important role in the form of the nerve impulse. Very clearly, the bio-energy, which results in works of sodium pump and potassium pump. However, the bio-energy released from the hydrolyses reaction of ATP molecules must be carried and transported to the sodium pump and potassium pump by Pang's soliton from the reaction position to the positions of work of sodium pump and potassium pump, respectively. Hence there are not also the works of sodium pump and potassium pump without the transport and transmission of Pang's soliton. This implies that the form and features of the nerve impulse are related directly and closely with the properties of Pang's soliton, or speaking, the properties of the nerve impulse.

As it is well known, Pang's soliton has always a certain or limited lifetime. So called the lifetime is just the times of existence and life of Pang's soliton or the delayed and maintained times of bio-energy transport in the life systems. If Pang's soliton is more than and exceed this lifetime, then Pang's soliton and transport of bio-energy as well as the works of the sodium pump and potassium pump will be disappeared and eliminated all and immediately, namely, the sodium pump and potassium pump can only work in the lifetime, the nerve impulse also can only occur in this lifetime of Pang's soliton, rather than in any or all times because the bio-energy or Pang's soliton exists only in its lifetimes. Therefore, the features of the nerve impulse are closely related to the lifetimes of Pang's soliton, or peaking, the lifetimes of Pang's soliton can determine the features of the nerve impulse. namely, only if the times forming the nerve impulse are exactly in the lifetime of Pang' soliton, then a stable nerve impulse can be produced, or else, it cannot be formed. This showed clearly that the nerve impulse formed in this case should have certainly special features and properties, i.e., it is demanded necessarily that the time forming the nerve impulse must be limited and controlled by the lifetime of Pang's soliton, namely it must be shorter than he lifetime of Pang's soliton transporting the bio-energy because the nerve impulse can obtain and absorb the sufficient and enough bio-energy supplied Pang's soliton for its form in this case. Then the nerve impulse formed in this case is affirmatively stable. Or else, the nerve impulse cannot be formed, or, formed nerve impulse it is also not stable because the nerve impulse can obtain and absorb not the sufficient and enough bio-energy supplied from Pang's soliton in its formed process.

As it is known from the above result, the lifetime of Pang's soliton transporting the bio-energy is  $0.53 \times 10^{-10}$ S- $0.65 \times 10^{-10}$ S in the protein molecules. Otherwise, Hamm et al (P. Hamm, I.R. (2007); W. Fann, (1990); P.Hamm, (2007); R.H. Austin,. (2003); Pang XF. (2007) measured the lifetimes of the solitons by pump-probe spectroscopy in acetanilide and protein molecules, its result is  $35Ps=35 \times 10^{-12}$ S, which approaches quite the above lifetimes of Pang's soliton .

In accordance with this request and the above values of the lifetimes of Pang's soliton and the experimental result of the soliton we can decide and determine that the feature and frequencies of the nerve impulse. In this case we judged that the nerve impulse is not a millimeter wave, but the terahertz wave. Its reasons are described as follows.

As it is well known that the wavelengths of millimeter wave is 1-10 millimeter, then its frequency is  $3\times10^{10}$  Hz  $-3\times10^{11}$  Hz. This means that the times forming one impulse with millimeter wave are about  $(1/3)\times(10^{-10} - 10^{-11})$  second. Obviously, the times are longer than or approach the lifetime of  $0.53\times10^{-10}$ S  $-0.65\times10^{-10}$ S for Pang's soliton and  $35\times10^{-12}$ S of experimental value of the soliton transporting the bio-energy released from the hydrolyses reaction of ATP

molecules. Thus we can affirm that the nerve impulse arising from the bio-energy is not absolutely the millimeter wave in accordance with the above rules and standards.

Inversely, we can conform and affirm that the nerve impulse is a real terahertz wave because the latter possess the frequencies of 10<sup>11</sup>-10<sup>12</sup> Hz. Thus the times forming and producing one nerve impulse with terahertz wave are about  $(10^{-11} - 10^{-12})$  second. Very clearly the times are all shorter than the lifetimes of Pang's soliton and the experimental value of the soliton transporting the bio-energy . This means that the terahertz wave can be easily formed and is also very stable in the nerve systems in this case according to the above rules and standards. Thus we can affirm that the nerve impulse arising from the bio-energy is absolutely a real terahertz wave in accordance with the above rules and standards.

### CONCLUSION

Thus the above investigations affirmed and conformed that the nerve impulse arising from the bio-energy released from hydrolyses reaction of ATP molecules is a real terahertz wave. This s first time to verify and demonstrate that the nerve impulse occurred in nerve system is a kind of terahertz wave. This conclusion has very important significance in biology and nerve science.

## **COMPETING INTERESTS**

Author has declared that no competing interests exist.

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