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REVIEW ARTICLE

PANG Xiao-feng

Theory of bio-energy transport in protein molecules and its experimental evidences as well as applications (I)

Abstract A new theory of bio-energy transport along protein molecules, where energy is released by the hydrolysis of adenosine triphosphate (ATP), has recently been proposed for some physical and biological reasons. In this theory, Davydov's Hamiltonian and wave function of the systems are simultaneously improved and extended. A new interaction has been added into the original Hamiltonian. The original wave function of the excitation state of single particles has been replaced by a new wave function of the two-quanta quasi-coherent state. In such a case, bio-energy is carried and transported by the new soliton along protein molecular chains. The soliton is formed through the self-trapping of two excitons interacting with amino acid residues. The exciton is generated by the vibration of amide-I (C=O stretching) arising from the energy of the hydrolysis of ATP. The properties of the soliton are extensively studied by analytical methods and its lifetime for a wide range of parameter values relevant to protein molecules is calculated using the nonlinear quantum perturbation theory. The lifetime of the new soliton at the biological temperature of 300 K is large enough and belongs to the order of 10^{-10} s or $\tau/\tau_0 \geqslant 700$. The different properties of the new soliton are further studied. The results show that the new soliton in the new model is a better carrier of bio-energy transport and it can play an important role in biological processes. This model is a candidate of the bio-energy transport mechanism in protein molecules.

Keywords protein, biological energy, soliton, ATP hydrolysis, amide, exciton, life time, amino acid, quasi-coherent state, binding energy

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PANG Xiao-feng (✉)
Institute of Life Science and Technology, University of Electronic Science and Technology of Chengdu, Chengdu 610054, China
International Center for Material Physics, Chinese Academy of Sciences, Shenyang 110015, China
E-mail: pangxf@mail.sc.cninfo.net

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1 Constructed of the theory based on physical and biological backgrounds

In many biological processes of living systems, such as the muscle contraction, DNA reduplication, neuroelectric pulse transfer on the neurolemma, working of calcium pumps and sodium pumps, etc. are associated with bio-energy transport through protein molecules, where energy is released by the hydrolysis of adenosine triphosphate (ATP). Thus there here are always biological processes of energy transport from a production place to an absorption place in living systems. In general, bio-energy transport is carried out by means of protein molecules. Therefore, the study of bio-energy transport along protein molecules is a very interesting subject in biology and of important significance in life science. However, the understanding of the mechanism of bio-energy transport in biomacromolecular systems has been a long-standing problem that remains of great interest today. As an alternative to electronic mechanisms [1–3], it can be assumed that the energy is stored as vibrational energy in the C=O stretching mode (amide-I) of a protein molecular chain of polypeptide. Following Davydov's idea [4–12], the coupling between the amide-I vibrarional quantum (exciton) and the acoustic phonon (molecular displacements) in amino acid residues is taken into account; Through the coupling, nonlinear interaction appears in the motion of the vibrartional quanta, which could lead to a self-trapped state of the vibrational quantum. The latter plus the deformational lattice of amino acids together can travel over macroscopic distances along molecular chains, retaining the wave shape, energy, momentum and other properties of the quasiparticle.

In this way, the bio-energy can be transported as a localized "wave packet" or soliton. This is just Davydov's model of bio-energy transport in proteins, which was proposed in the 1970s [4–12].

Davydov's model of bio-energy transport work in α-helical proteins is shown in Fig. 1.

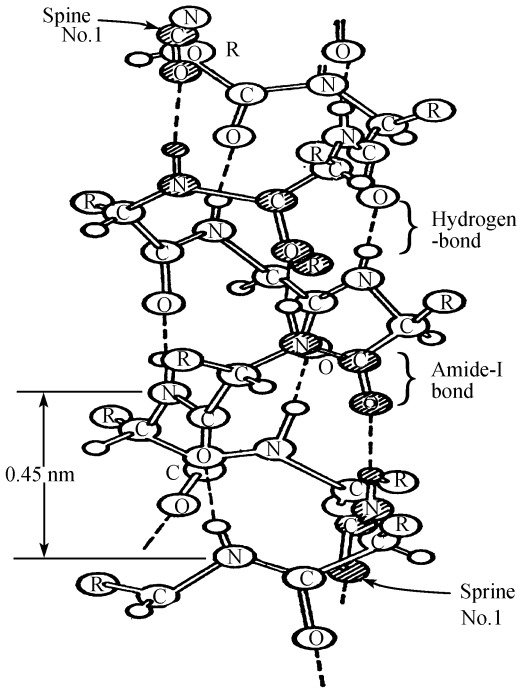

Fig. 1 Structure of α–helical protein.

Following Davydov's idea, the Hamiltonian describes such a system in the form of

$$\begin{aligned} H_{\mathrm{D}} &= \sum_n \left[\varepsilon_0 B_n^+ B_n - J(B_n^+ B_{n-1} + B_n B_{n+1}^+)\right] \\ &+ \sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2} w(u_n - u_{n-1})^2\right] \\ &+ \sum_n \left[\chi_1 (u_{n+1} - u_{n-1}) B_n^+ B_n\right] \\ &= H_{\mathrm{ex}} + H_{\mathrm{ph}} + H_{\mathrm{int}} \end{aligned} \tag{1}$$

where $\varepsilon_0 = 0.205$ eV is the amide-I quantum energy, J is the dipole-dipole interaction energy between neighboring sites, $B_n^+(B_n)$ is the creation (annihilation) operator for an amide-I quantum excitation (exciton) in site n, u_n is the displacement operator of a lattice oscillator at site n, P_n is its conjugate momentum operator, M is the mass of an amino acid molecule, w is the elasticity constant of the protein molecular chains, and χ_1 is a nonlinear coupling parameter and represents the coupling size of the exciton-phonon interaction. The wave function of the systems proposed by Davydov is in the form of

$$\begin{aligned} |D_2(t)\rangle &= |\varphi_{\mathrm{D}}(t)\rangle\, |\beta(t)\rangle = \sum_n \varphi_n(t) B_n^+ \\ &\cdot \exp\left(-\frac{\mathrm{i}}{\hbar}\sum_n [\beta_n(t) P_n - \pi_n(t) u_n]\right) |0\rangle \end{aligned} \tag{2}$$

or

$$|D_1(t)\rangle = \sum_n \left\{\varphi_n(t) B_n^+ \exp\left(\sum_q \left[\alpha_{nq}(t) a_q^+ - \alpha_{nq}^*(t) a_n\right]\right)\right\} |0\rangle \tag{3}$$

where $|0\rangle = |0\rangle_{\mathrm{ex}} |0\rangle_{\mathrm{ph}}, |0\rangle_{\mathrm{ex}}|$ and $|0\rangle_{\mathrm{ph}}$ are the ground states of the exciton and phonon, respectively, $a_q(a_q^+)$ is the annihilation (creation) operator of the phonon with ware vector q, $\varphi_n(t)$ and $\beta_n(t) = \langle \Phi | u_n | \Phi \rangle$ and $\pi_n(t) = \langle | \Phi | P_n | \Phi \rangle$ and $\alpha_{nq}(t) = \langle D_1(t) | a_q | D_1(t) \rangle$ are some undetermined functions of time.

Obviously, $|\varphi_{\mathrm{D}}(t)\rangle = \sum_n \varphi_n(t) B_n^+ |0\rangle_{\mathrm{ex}}$ in Eq. (2) is an eigenstate of the number operator, $\hat{N} = \sum_n B_n^+ B_n$, corresponding to a single excitation, i.e., $\hat{N} |\varphi_{\mathrm{D}}(t)\rangle = |\varphi_{\mathrm{D}}(t)\rangle$.

The Davydov soliton obtained from Eqs. (1), (2) in the semiclassical limit by use of the continuum approximation has the from

$$\begin{aligned} \varphi_{\mathrm{D}}(x,t) &= \left(\frac{\mu_{\mathrm{D}}}{2}\right)^{1/2} \mathrm{sech}\left[\frac{\mu_{\mathrm{D}}}{r_0}(x - x_0 - vt)\right] \\ &\cdot \exp\left\{\mathrm{i}\left[\frac{\hbar v}{2 J r_0^2}(x - x_0) - E_v t/\hbar\right]\right\} \end{aligned} \tag{4}$$

corresponding to an excitation localized over a scale r_0/μ_{D}, where $\mu_{\mathrm{D}} = \frac{\chi_1^2}{(1-s^2)wJ}, G_{\mathrm{D}} = 4J\mu_{\mathrm{D}}, s^2 = \frac{v^2}{v_0^2}, v_0 = r_0(w/M)^{1/2}$ is the sound speed in the protein molecular chains, v is the velocity of the soliton, r_0 is the lattice constant. Evidently, the soliton contains only one exciton, i.e., $N = \langle \varphi_{\mathrm{D}}(t) | \hat{N} | \varphi_{\mathrm{D}}(t) \rangle = 1$. This indicates that the Davydov soliton is formed through the self-trapping of one exciton with binding energy E_{BD} [2], $E_{\mathrm{BD}} = \frac{-\chi_1^4}{3Jw^2}$.

Davydov's idea yields a compelling picture for the mechanism of bio-energy transport in protein molecules and consequently it has been the subject of a large number of works [13–80]. A lot of issues related to Davydov's model, including the foundation and accuracy of the theory, the quantum and classical properties and the thermal stability and lifetime of the Davydov soliton have extensively been studied by many scientists [13–80]. However, considerable

controversy has arisen in recent years concerning whether the Davydov soliton is sufficiently stable in the region of biological temperature to provide a viable explanation for bio-energy transport. It is out of question that quantum fluctuations and thermal perturbations are expected to cause the Davydov soliton to decay into a delocalized state. Some numerical simulations indicated that the Davydov soliton is not stable at the biological temperature of 300 K [30–51, 62–80]. Other simulations indicated that the Davydov soliton was stable at 300 K [30–39], but they were based on the classical equations of motion which were likely to yield unreliable estimates of the stability of the soliton [13–18]. The simulations based on the $|D_2\rangle$ state in Eq. (2) generally indicate that the stability of the soliton decreases with the increase in temperature and that the soliton is not sufficiently stable in the region of biological temperature. Since the dynamical equations used in the simulations are not equivalent to the Schrödinger equation, the stability of the soliton obtained by these numerical simulations is unavailable or unreliable. The simulation [34] based on the $|D_1\rangle$ state in Eq. (3) with the thermal treatment of Davydov [31–33], where the equations of motion are derived from a thermally averaged Hamiltonian, yields the confusing result that the stability of the soliton is enhanced with the increase in temperature, predicting that the $|D_1\rangle$-type soliton is stable in the region of biological temperature. Evidently, the conclusion is doubtful because the Davydov procedure in which an equation of motion for an average dynamical state is constructed from an average Hamiltonian, corresponding to the Hamiltonian averaged over a thermal distribution of phonons, is inconsistent with the standard concepts of quantum-statistical mechanics in which a density matrix must be used to describe the system. Therefore, any exact fully quantum-mechanical treatment for the numerical simulation of the Davydov soliton does not exist. However, for the thermal equilibrium properties of the Davydov soliton, there is a quantum Monte Carlo simulation [48, 49]. In the simulation, correlation characteristics of solitonlike quasiparticles occur only at low temperatures, about $T < 10$ K, for widely accepted parameter values. This is consistent at a qualitative level with the result of Cottingham *et al*. [50–51]. The latter is a straightforward quantum- mechanical perturbation calculation. The lifetime of the Davydov soliton obtained by using this method is too short (about 10^{-12}–10^{-13} s) to be useful in biological processes. This indicates clearly that the Davydov solution is not a true wave function of the systems. A thorough study in terms of parameter values, different types of disorder, different thermalization schemes, different wave functions, and different associated dynamics leads to a very complicated picture for Davydov's model [35–47]. These results do not completely rule out the Davydov theory; however, they do not eliminate the possibility of another wave function and a more sophisticated Hamiltonian of the system having a soliton with longer lifetime and better thermal stability.

Indeed, the question of the lifetime of the soliton in protein molecules is twofold. In Langevin dynamics, the problem consists of uncontrolled effects arising from the semiclassical approximation. In quantum treatments, the problem has been the lack of an exact wave function for the soliton. The exact wave function of the fully quantum Davydov model has not been known up to now. Different wave functions have been used to describe the states of the fully quantum-mechanical systems [19–23, 24–26]. Although some of these wave functions lead to exact quantum states and exact quantum dynamics in the $J = 0$ state, they also share a problem with the original Davydov's 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 thought that the soliton with a multiquantum ($n \geqslant 2$), such as the coherent state of Brown *et al*. [9–23], the multiquantum state of Kerr *et al*. [46, 47] and Schweitzer *et al*. [50, 51], the two-quantum state of Cruzeiro-Hansson [35–39] and Forner [58], etc. would be thermally stable in the region of biological temperature and could provide a realistic mechanism for bio-energy transport in protein molecules. However, the assumption of the standard coherent state is unsuitable or impossible for biological protein molecules because there are innumerable particles in this state and the conservation of the number of particles of the system could not be maintained. The assumption of a multi-quantum state ($n > 2$) along with a coherent state is also inconsistent with the fact that the bio-energy released in ATP hydrolysis can excite only two quanta of amide-I vibration. On the other hand, the numerical result indicates that the soliton of the two-quantum state is more stable than that with a one-quantum state.

Cruzeiro-Hansson [35–39] thought that Forner's two-quantum state in the semiclassical case was not exact. Therefore, he constructed again a so-called exact two-quantum state for the semiclassical Davydov system as follows [35–39]:

$$|\varphi(t)\rangle = \sum_{n,m=1}^{N} \varphi_{nm}\left(\{u_1\},\{P_1\},t\right) B_n^t B_m^t |0\rangle_{\mathrm{ex}} \tag{5}$$

where $B_n(B_n^t)$ is the annihilation (creation) operator for an amide-I vibration quantum (exciton), u_1 is the displacement of the lattice molecules, P_1 is its conjugate momentum, and $|0\rangle_{\mathrm{ex}}$ is the ground state of the exciton. He calculated the average probability distribution of the exciton per site, and average displacement difference per site, and the thermodynamics average of the variable, $P = B_1^t B_1 - B_2^t B_2$, as a measure of the localization of the exciton, versus quantity $\nu = JW/\chi_1^2$ and $\ln\beta$ [$\beta = 1/(K_{\mathrm{B}}T)$] in the so-called two-quantum state, Eq. (5), where χ_1 is a nonlinear coupling parameter related to the interaction of the exciton-phonon coupling in Davydov's model. Their energy and stability are compared with those of the one-quantum state. From the results of the

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

However, by checking carefully Eq. (5) [35–39], it can be found that the Cruzeiro-Hansson wave function does not represent exactly the two-quantum state. To find out how many quanta the state Eq. (1) indeed contains, the expectation value of the exciton number operator has to be computed. $N=\sum_n B_n^t B_n$, in this state Eq. (5), and sum over the sites, i.e., the exciton numbers N are

$$\begin{aligned} N &= \langle\varphi \mid \sum_n B_n^t B_n \mid \varphi\rangle \\ &= \sum_{ijlmn} \varphi_{im}^* \varphi_{jl} {}_{\mathrm{ex}}\langle 0 \left| B_i B_m B_n^t B_n B_j^t B_l^t \right| 0\rangle_{\mathrm{ex}} \\ &= \sum_{nj} \left(\varphi_{nj}^* \varphi_{jn} + \varphi_{jn}^* \varphi_{jn}\right) + \sum_{nl} \left(\varphi_{nl}^* \varphi_{nl} + \varphi_{ln}^* \varphi_{nl}\right) = 4 \end{aligned} \tag{6}$$

where the following relationships are used:

$$[B_n, B_j^t] = \sigma_{nj} \sum_{nt} \left|\varphi_{nl}\right|^2 = 1 \tag{7}$$

$$\begin{aligned} {}_{\mathrm{ex}}\langle 0 \left| B_n^t \right| 0\rangle_{\mathrm{ex}} &= {}_{\mathrm{ex}}\langle 0 \left| B_n^t B_n \right| 0\rangle_{\mathrm{ex}} \\ &= {}_{\mathrm{ex}}\langle 0 \left| B_n^t B_m B_1 \right| 0\rangle_{\mathrm{ex}} = \cdots = 0 \end{aligned} \tag{8}$$

Therefore, the state Eq. (5), as it is put forward in Ref. [35–39], deals with four excitons (quanta) instead of two in contradiction to the author's statements. Obviously, it is impossible to create four excitons by the energy released in the ATP hydrolysis (about 0.43 eV). Thus the author's wave function is still not suitable for protein molecules, and his discussion and conclusion are all unreliable and implausible in that paper [35–39].

It is believed that the physical significance of the wave function, Eq. (5), is also unclear, or at least very difficult to understand. As far as the physical significance of Eq. (5) is concerned, it represents only a combinational state of single-particle excitation with two quanta created at sites n and m; $\varphi_{nm}\left(\{u_1\},\{P_1\},t\right)$ is the probability amplitude of particles occurring at sites n and m simultaneously. In general, $n=m$ and $\varphi_{nm} \neq \varphi_n \varphi_m$ are in accordance with the author's idea. In such a case, it is very difficult to imagine the form of the soliton by the mechanism of the 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 not explained the physical and biological reasons and the meaning for the proposed trial state. Therefore, it is believed that the Cruzeiro-Hansson representation is still not an exact wave function suitable for protein molecules. Thus, the wave function of the systems is still an open problem today.

On the basis of the works of Cruzeio-Hansson, Förner, Schweitzer and Takeno and Pang, both the Hamiltonian and the wave function of the mode [81–97] have been improved. A new coupling interaction between the acoustic and amide-I vibrational modes has been added to the original Davydov's Hamiltonian which takes into account the relative displacement of the neighboring peptide groups resulting from the dipole-dipole interaction of the neighboring amide-1 vibrational quanta. Davydov's wave function has been replaced with a quasi-coherent two-quanta state to exhibit the coherent behavior of collective excitations [98–102] which are a feature of the energy released in the ATP hydrolysis in the systems. The equation of motion and the properties of the new soliton in the new model are different from those in Davydov's model and as a result the lifetime and stability of the soliton are greatly enhanced. It is suggested that this model can resolve the controversy on the thermal stability and lifetime of the soliton excited in protein molecules. The quantum properties of the new soliton are studied here [81–97], but here attention is paid to the problem of its lifetime and thermal stability at biological temperature of 300 K and the lifetime of the new soliton at 300 K is calculated in detail by using the generally accepted values of the parameters appropriate to α-helical protein molecules in terms of the quantum perturbation theory developed by Cottingham *et al*. [50, 51], which can take simultaneously into account the quantum and thermal effects. It can be seen that the lifetime of the new soliton at 300 K is long enough to provide a viable explanation of bio-energy transport in proteins. The plan of this paper is as follows. In Section 2, the new model, including the extended Hamiltonian and the wave function, is presented. The equations of motion and the new soliton solution in this model are given in Section 3. In Section 4, the properties and thermal stability of the new soliton are discussed, and the possibility of the soliton being a suitable candidate for the mechanism of bio-energy transport in protein molecules is predicted on the basis of the results obtained in this paper. In Section 5, the properties of the new soliton are described and its lifetime is calculated by using quantum-mechanical perturbation methods. The detailed discussion of the properties and changes of the lifetime of the soliton and the conclusions of this investigation are presented in Section 6.

2 Construction of new model for the systems

Results obtained by many scientists over the years indicate that Davydov's model, whether it is the wave function or the Hamiltonian, is indeed too simple, i.e., it does not denote the elementary properties of collective excitations occurring in protein molecules, and many improvements of it have been unsuccessful, as mentioned above. What is the source of this problem? It is well known that the Davydov theory on bio-energy transport was introduced into protein molecules

from an exciton-soliton model in generally one-dimensional molecular chains [81–97]. 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, and ACN is the structure of two peptide channels [103–107]. If comparing the structure of the alpha-helix protein with ACN, it can be found that the hydrogen-bond 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 those of the latter. The protein molecules are both a kind of soft condensed matter and bio-self-organization with active functions, for instance, self-assembling and self-renovating. The physical concepts of coherence, order, collective effect, and mutual correlation are very important in bio-self-organization, including the protein molecules, when compared with generally molecular systems [98–102]. Therefore, it is worth studying how these properties can be physically described. It is noted that Davydov's operation is not strictly correct. Therefore, it is believed that a basic reason for the failure of Davydov's model is just that it completely ignores the above important properties of the protein molecules.

Let us consider Davydov's model with the present viewpoint. First, as far as the Davydov wave function, both $|D_1\rangle$ and $|D_2\rangle$, are concerned, they are not true solutions of the protein molecules. On the one hand, there is obviously asymmetry in the Davydov wave function since the phononic part is in a coherent state, while the excitonic part is only in an excitation state of a single particle. It is not reasonable that the same nonlinear interaction generated by the coupling between excitons and phonons produces different states for phonons and excitons. Thus, Davydov's wave function should be modified [62–80], 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 [19–23] and large-n excitation states [46, 47] are not appropriate for protein molecules due to the reasons mentioned above. Similarly, Forner's and Cruzeiro-Hansson's two-quantum states do not fulfill the above request. In view of the above discussion, the following wave function of protein molecular systems is proposed [81–97]:

$$\begin{aligned}|\Phi(t)\rangle &= |\varphi(t)\rangle|\beta(t)\rangle \\ &= \frac{1}{\lambda}\left[I + \sum_n \varphi_n(t) B_n^t + \frac{1}{2!}\left(\sum_n \varphi_n(t) B_n^t\right)^2\right]|0\rangle_{\text{ex}} \\ &\quad \cdot \exp\left\{-\frac{\mathrm{i}}{h}\sum_n\left[\beta_n(t) P_n - \pi_n(t) u_n\right]\right\}|0\rangle_{\text{ph}} \end{aligned} \tag{9}$$

here B_n^t and B_n are the creation and annihilation operators for the exciton, $|0\rangle_{\text{ex}}$ and $|0\rangle_{\text{ph}}$ are the ground states of excitons and phonons, respectively, and u_n and P_n are the displacement and momentum operators of the lattice oscillator at site n respectively. λ is a normalization constant. It is assumed hereafter that $\lambda = 1$ for the convenience of calculation, except that when explicitly mentioned, the $\varphi_n(t)\cdot\beta_n(t) = \langle\Phi(t)|u_n|\Phi(t)\rangle$ and $\pi_n(t) = \langle\Phi(t)|P_n|\Phi(T)\rangle$ are three sets of unknown functions.

A second problem arises for the Davydov Hamiltonian [62–80]. The Davydov Hamiltonian takes into account the resonant or dipole-dipole interaction of neighboring amide-I vibrational quanta in neighboring peptide groups with an electrical moment of about 3.5 D, but why not consider the changes of the relative displacement of the neighboring peptide groups arising from this interaction? It is reasonable to add the new interaction term $\chi_2(u_{n+1} - u_n)(B_{n+1}^t B_n + B_m^t B_{n+1})$ into the Davydov Hamiltonian to represent the correlations of collective excitations and collective motions in protein molecules, as is mentioned above [62–80]. Although the dipole-dipole interaction is small as compared with the energy of the amide-I vibrational quantum, the change of the relative displacement of neighboring peptide groups resulting from this interaction cannot be ignored due to the sensitive dependence of the dipole-dipole interaction on the distance between amino acids in protein molecules, which is a kind of soft condensed matter and bio-self-organization. Thus, the Davydov Hamiltonian is replaced by [81–97]

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

where $\varepsilon_0 = 0.205$ eV is the energy of the exciton (the $C = 0$ strechiong mode). The present nonlinear coupling constants are χ_1 and χ_2. They represent the modulations of the on-site energy and resonant (or dipole-dipole) interaction energy of excitons caused by molecular displacements, respectively. M is the mass of an amino acid molecule and w is the elasticity constant of protein molecular chains. J is the energy of the dipole-dipole interaction between neighboring sites. The physical meanings of the other quantities in Eq. (6) are the same as those in the above explanations.

The Hamiltonian and wave function shown in Eqs. (9), (10) are different from Davydov's. A new interaction term, $\sum_n \chi_2(u_{n+1} - u_n)(B_{n+1}^t B_n + B_n^t B_{n+1})$, is added into the original Davydov Hamiltonian [4–12]. Thus the Hamiltonian now has better symmetry and can also represent the features of the mutual correlations of collective excitations and motions in protein molecules. It should be pointed out here that the dif-

ferent coupling between the relevant modes was also considered by Takeno *et al*. [59–61, 108, 109] and Pang [62–80] in the Hamiltonian of the vibron-soliton model for one-dimensional oscillator-lattice and protein systems, respectively, but the wave functions of the systems they used are different from Eqs. (9), (10).

Obviously, the wave function of excitons in Eq. (9) is not an excitation state of a single particle, but a coherent state [110], more accurately, a quasicoherent state. Seen from this, $|\varphi(t)\rangle$ can be represented by [81–97]

$$\begin{aligned}|\varphi(t)\rangle &= \frac{1}{\lambda}\left[1+\sum_n \varphi_n(t)B_n^t+\frac{1}{2\mathrm{i}}\left(\sum_n \varphi_n(t)B_n^t\right)^2\right]|0\rangle_{\mathrm{ex}} \\ &\sim \frac{1}{\lambda}\exp\left[-\frac{1}{2}|\varphi_n(t)|^2\right]\exp\left\{\sum_n \varphi(t)B_n^t\right\}|0\rangle_{\mathrm{ex}} \\ &= \frac{1}{\lambda}\exp\left\{\sum_n\left[\varphi_n(t)B_n^t-\varphi_n^*(t)B_n\right]\right\}|0\rangle_{\mathrm{ex}} \end{aligned} \tag{11}$$

The last representation in Eq. (11) is a standard coherent state. More precisely, the new wave function has relationships to only three terms of the expansion of a standard coherent state [110], which is mathematically justified in the case of small $\varphi_n(t)$ [i.e.,$[\varphi_n(t)]\ll 1$], which can be viewed as an effective truncation of a standard coherent state. Therefore, $|\varphi(t)\rangle$ is called a quasicoherent state. However, it is not an eigenstate of the number operator

$$\begin{aligned}\hat{N}|\varphi(t)\rangle &= \sum_n B_n^t B_n\,|\varphi(t)\rangle \\ &= \left\{\sum_n \varphi_n(t)B_n^t+\left(\sum_n \varphi_n\varphi_n(t)B_n^t\right)^2\right\}|0\rangle_{\mathrm{ex}} \\ &= 2|\varphi(t)-\left(2+\sum_n \varphi_n(t)B_n^t\right)|0\rangle_{\mathrm{ex}} \end{aligned} \tag{12}$$

Therefore, $|\varphi(t)\rangle$ indeed represents a superposition of multiquantum states. In other words, it is a coherent superposition of the excitonic state with two quanta and the ground state of excitons. However, in this state the number of quanta is determinate instead of innumerable. To find out how many excitons this state contains, the expectation value of the number operator N has to be computed in this state and the states summed over. The average number of excitons in this state is

$$\begin{aligned}N &= \langle\varphi(t)|\hat{N}|\varphi(t)\rangle = \sum_n \langle\varphi(t)|B_n^t B_n|\varphi(t)\rangle \\ &= \left\{\sum_n|\varphi_n(t)|^2+\left(\sum_n|\varphi_n(t)|^2\right)\left(\sum_m|\varphi_m(t)|^2\right)\right\} \\ &= \left(\sum_n|\varphi_n(t)|^2\right)\left(1+\sum_m|\varphi_m(t)|^2\right)=2 \end{aligned} \tag{13}$$

where Eq. (8) is utilized and the following relationships can be obtained [81–97]:

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

$$\begin{aligned}{}_{\mathrm{ex}}\langle 0|B_n^+|0\rangle_{\mathrm{ex}} &= {}_{\mathrm{ex}}\langle 0|B_n^+B_n|0\rangle_{\mathrm{ex}} \\ &= {}_{\mathrm{ex}}\langle 0|B_n^+B_m|0\rangle_{\mathrm{ex}} = {}_{\mathrm{ex}}\langle 0|B_n^+B_mB_l|0\rangle_{\mathrm{ex}} \\ &= {}_{\mathrm{ex}}\langle 0|B_n^+B_mB_l^+B_n|0\rangle_{\mathrm{ex}} = {}_{\mathrm{ex}}\langle 0|B_n^+B_mB_i^+B_lB_j|0\rangle_{\mathrm{ex}} \\ &= {}_{\mathrm{ex}}\langle 0|B_n^+B_mB_l^+B_iB_jB_n|0\rangle_{\mathrm{ex}}\cdots=0 \end{aligned}$$

Therefore, the new wave function is completely different from Davydov's. The latter is an excitation state of a single particle with one quantum and an eigenstate of the number operator, but the former is not. The new state is a quasicoherent state. It contains only two excitons, which come from the second and third terms in Eq. (9), in which each term contributes only one exciton, but it is not an excitation state of two single particles. Hence, as far as the form of the new wave function in Eq. (9) is concerned, it is either the two-quantum state proposed by Forner [58] and Cruzeiro- Hansson [35–39] or a standard coherent state proposed by the multiquanta states of Brown *et al*. [19–23] and Kerr *et al*. [46, 47] and Schweitzer *et al*. [50, 51]. Therefore, the wave function in Eq. (9) is new for protein molecular systems. It not only exhibits the coherent features of the collective excitation of excitons and phonons caused by the nonlinear interaction generated by the exciton-phonon interaction, which, thus, also makes the wave function of the states of the system symmetrical, but it also agrees with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) may only create two amide-I vibrational quanta which, thus, can also maintain the number of excitons in the Hamiltonian of Eq. (10). Meanwhile, the new wave function has another advantage, i.e., the equation of motion of the soliton can also be obtained from the Heisenberg equations of the creation and annihilation operators in quantum mechanics by using Eqs. (9) and (10), but the wave function of the states of the system in other models could not, including the one-quantum state [4–12] and the two-quantum state [35–47]. Therefore, the above Hamitonian and wave function, Eqs. (9) and (10), are reasonable and appropriate for protein molecules.

3 Equations of moton and the soliton solution

Now the equations of motion are derived from the improved Davydov's model. First of all, the interpretation of $\beta_n(t)$ and $\pi_n(t)$ is given in Eq. (9). It is known that the phonon part of the new wave function in Eq. (9) depending on displacement and momentum operators is a coherent state of the normal model of creation and annihilation operators. A coherent state for the mode with wave vector q is [4–12, 46,

47, 62–80, 111–113]

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

Utilizing the standard transformations

$$u_n = \sum_q \left(\frac{\hbar}{2NM\omega_q}\right)^{1/2} {\rm e}^{{\rm i}qnr_0}(a_{-q}^+ + a_q)$$

$$P_n = {\rm i}\sum_q \left(\frac{M\hbar\omega_q}{2N}\right)^{1/2} {\rm e}^{{\rm i}qnr_0}(a_{-q}^+ - a_q) \tag{16}$$

$|\alpha(t)\rangle = |\beta(t)\rangle$ can be obtained [46, 47, 62–80], where $|\beta(t)\rangle$ is in Eq. (9), and $\omega_q = 2(w/M)^{1/2}\sin(r_0 q/2)$, r_0 is the distance between neighboring amino acid molecules, and $a_{\rm q}(a_{\rm q}^+)$ is the annihilation (creation) operator of the phonon with wave vector q, where

$$\langle\alpha(t)|a_{\rm q}|\alpha(t)\rangle = a_{\rm q}(t)$$
$$= \left(\frac{M\omega_{\rm q}}{2\hbar}\right)^{1/2}\beta_{\rm q}(t) + {\rm i}\left(\frac{1}{2M\hbar\omega_{\rm q}}\right)^{1/2}\pi_{\rm q}(t)$$
$$\langle\Phi(t)|u_n|\Phi(t)\rangle = \beta_n(t)$$
$$\beta_q(t) = \frac{1}{\sqrt{N}}\sum_n {\rm e}^{-{\rm i}qnr_0}\beta_n(t)$$
$$\pi_{\rm q}(t) = \frac{1}{\sqrt{N}}\sum_n {\rm e}^{-{\rm i}qnr_0}\pi_n(t)$$
$$\langle\Phi(t)|P_n|\Phi(t)\rangle = \pi_n(t) \tag{17}$$

Utilizing the above results again and the formulas of the expectation values of the Heisenberg equations of operators [111–113], u_n and P_n in the state $|\Phi(t)\rangle$

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

the equation of motion for the $\beta_n(t)$ can be obtained as

$$M\ddot{\beta}_n(t) = w[\beta_{n+1}(t) - 2\beta_n(t) + \beta_{n-1}(t)]$$
$$+2\chi_1\left[|\varphi_{n+1}(t)|^2 - |\varphi_{n-1}(t)|^2\right]$$
$$+2\chi_2\left\{\varphi_n^*(t)[\varphi_{n+1}(t) - \varphi_{n-1}(t)]\right.$$
$$\left.+\varphi_n(t)\left[\varphi_{n+1}^*(t) - \varphi_{n-1}^*(t)\right]\right\} \tag{19}$$

From Eq. (15), it can be seen that the presence of two quanta for the oscillators increases the driving force in the phonon field by that factor when compared with the Davydov theory.

Now the equation of motion for $\varphi(t)$ is derived. A basic assumption in the derivation is that $|\Phi(t)\rangle$ in Eq. (9) is a solution of the time-dependent Shrödinger equation [81–97, 111–113]:

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

The left-hand side of Eq. (16) has [46, 47, 62–80]

$${\rm i}\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle$$
$$= \left\{{\rm i}\hbar\left(\sum_n \dot{\varphi}_n(t)B_n^+ + \sum_n \dot{\varphi}_n(t)\varphi_n(t)B_n^+B_n^+|0\rangle_{\rm ex}\right)\right\}|\beta(t)\rangle$$
$$+|\varphi(t)\rangle\left\{\sum_n\left\{\beta_n(t)P_n - \pi_n(t)u_n\right.\right.$$
$$\left.\left.+\frac{1}{2}\left[\beta_n(t)\dot{\pi}_n(t) - \dot{\beta}_n(t)\pi_n(t)\right]\right\}|\beta(t)\rangle\right\} \tag{21}$$

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

$${\rm i}\hbar\langle\Phi(t)|u_n|\Phi(t)\rangle$$
$$= {\rm i}\hbar\sum_n \varphi_n^*(t)\varphi_n(t)\left(\sum_m \varphi_m^*(t)\varphi_m(t) + 1\right)$$
$$= \frac{5}{4}\sum_n\left[\dot{\beta}_n(t)\pi_n(t) - \dot{\pi}_n(t)\beta_n(t)\right]\sum_n|\varphi_n(t)|^2 \tag{22}$$

Similarly, for the right-hand side of Eq. (21) the following can be obtained [46, 47, 62–80]:

$$\langle\Phi({\rm t})|\left(H_{\rm ex} + H_{\rm ph} + H_{\rm int}\right)|\Phi(t)\rangle$$
$$= \left\{\sum_n\left\{\varepsilon_0|\varphi_n(t)^2| - J\varphi_n^*(t)[\varphi_{n+1}(t) - \varphi_{n-1}(t)]\right\}\right.$$
$$\times\left(1 + \sum_m|\varphi_m(t)|^2\right) + \left\{\sum_n\left\{\chi_1[\beta_{n+1}(t) - \beta_{n-1}(t)]|\varphi_n(t)|^2\right.\right.$$
$$\left.\left.+\chi_2[\beta_{n+1}(t) - \beta_{n-1}(t)]\times\varphi^*(t)[\varphi_{n+1}(t) - \varphi_{n-1}(t)]\right\}\right\}$$
$$\cdot\left(1 + \sum_m|\varphi_m(t)|^2\right) + \frac{5}{2}W(t)\sum_n|\varphi n(t)|^2 \tag{23}$$

where

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

and utilizing Eqs. (11)–(14), the relationships can be obtained:

$$\sum_n[\beta_{m+1}(t) - 2\beta_m(t) + \beta_{m-1}(t)]\beta_m(t)$$

$$
\begin{aligned}
&= -\sum_n \left[\beta_{m+1}(t) - \beta_{m-1}(t)\right]^2 \\
&\cdot \langle \Phi(t) \mid \sum_n \left(B_n^+ B_{n-1} + B_n B_{n-1}^+ \right) \mid \Phi(t) \rangle \\
&= \sum_n \left[\varphi_n^*(t)\varphi_{n+1}(t) + \varphi_{n-1}^*(t)\varphi(t) \right] \left(1 + \sum_m \left|\varphi_m(t)\right|^2 \right) \\
&\cdot \langle \Phi(t) \mid \sum_n \left(u_{n+1} - u_{n-1} \right) \left(B_n^+ B_n \right) \mid \Phi(t) \rangle \\
&= \sum_n \left\{ \left[\beta_{m+1}(t) - \beta_{m-1}(t)\right] \left|\varphi_n(t)\right|^2 \right\} \left(1 + \sum_m \left|\varphi_m(t)\right|^2 \right) \\
&\cdot \langle \Phi(t) \mid \sum_n \left(u_{n-1} - u_n \right) \left(B_n^+ B_{n-1} + B_n B_{n-1}^+ \right) \mid \Phi(t) \rangle \\
&= \sum_n \left\{ \left[\beta_{m+1}(t) - \beta_{m-1}(t)\right] \left[\varphi_n^*(t)\varphi_{n+1}(t) + \varphi_{n-1}^*(t)\varphi(t) \right] \right\} \\
&\cdot \left(1 + \sum_m \left|\varphi_m(t)\right|^2 \right) \qquad (25)
\end{aligned}
$$

From Eqs. (20)–(23), the following equation can be obtained:

$$
\begin{aligned}
&\mathrm{i}\hbar \frac{\partial}{\partial t} \varphi_n(t) \\
&= \varepsilon_0 \varphi_n(t) - J\left[\varphi_{n+1}(t) + \varphi_{n-1}(t)\right] \\
&+ \chi_1 \left[\beta_{n+1}(t) + \beta_{n-1}(t)\right] \varphi_n(t) \\
&- \chi_2 \left[\beta_{n+1}(t) + \beta_n(t)\right] \times \left[\varphi_{n+1}(t) + \varphi_{n-1}(t)\right] \\
&+ \frac{5}{2} \left\{ W(t) - \frac{1}{2} \sum_m \left[\dot{\beta}_m(t)\pi_m(t) - \dot{\pi}_m(t)\beta(t) \right] \right\} \varphi_n(t) \qquad (26)
\end{aligned}
$$

In the continuum approximation, the following equations can be obtained from Eqs. (19) and (26)

$$
\begin{aligned}
\mathrm{i}\hbar \frac{\partial}{\partial t} \varphi(x,t) &= R(t)\varphi(x,t) - Jr_0^2 \frac{\partial^2}{\partial x^2} \varphi(x,t) \\
&\quad - G_p \left|\varphi(x,t)\right|^2 \varphi(x,t) \qquad (27)
\end{aligned}
$$

and

$$
\frac{\partial \beta(x,t)}{\partial \xi} = \frac{\partial \beta(x,t)}{\partial x} = -\frac{4(\chi_1 + \chi_1)}{w(1-s^2)r_0} \left|\varphi(x,t)\right|^2 \qquad (28)
$$

here $\xi = x - v_t$, $R(t) = \varepsilon_0 - 2J + \frac{5}{2}\left\{ W(t) - \frac{1}{2}\sum_m [\dot{\beta}_m(t)\pi_m(t) - \dot{\pi}_m(t)\beta(t)] \right\}$, and $s = V/V_0$. The soliton solution of Eq. (27) is in the form of [81–97, 111–113]

$$
\varphi(x,t) = \left(\frac{\mu_p}{2} \right)^{1/2} \operatorname{sech}\left[\left(\mu_p / r_0 \right) \left(x - x_0 - V_t \right) \right]
$$

$$
\cdot \exp\left\{ \mathrm{i} \left[\frac{\hbar V}{2Jr_0^2} \left(x - x_0 \right) - E_v \frac{t}{\hbar} \right] \right\} \qquad (29)
$$

with

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

Although the forms of the above equations of motion and the corresponding solution, Eqs. (27)–(30), are quite similar to that of the Davydov soliton ,the properties of our soliton have very large differences from the latter because the parameter values in the equation of motion and the solution Eqs. (27) and (29), including $R(t), G_p$, and μ_p, have obvious distinctions from that of Davydov's model. A straightforward result of our model is to increase the nonlinear interaction energy $G_p (G_p = 2G_{\mathrm{D}}[1 + 2(\chi_2/\chi_1) + (\chi_2/\chi_1)^2])$ and the amplitude of the new soliton and decrease its width due to an increase of $\mu_p (\mu_p = 2\mu_{\mathrm{D}}[1 + 2(x_2/x_1) + (x_2/x_1)^2])$ when compared with the soliton in Davydov's model, where $\mu_D = x_1^2/[w(1-s^2)J]$, and $G_{\mathrm{D}} = 4x_1^2/[w(1-s^2)]$ are the corresponding values. Thus the localized feature of the new soliton is enhanced. Therefore, its stability against quantum fluctuations and thermal perturbations increases considerably as compared with the Davydov soliton.

4 Properties of the new model and soliton

The energy of solitons in the improved model becomes [111–113]

$$
\begin{aligned}
E &= \langle \Phi(t) \mid H \mid \Phi(t) \rangle \\
&= \frac{1}{r_0} \int_{-\infty}^{\infty} 2\left[Jr_0^2 \left(\frac{\partial \varphi}{\partial x} \right)^2 + R\left|\varphi(x,t)\right|^2 - G_p \left|\varphi(x,t)\right|^4 \right] \mathrm{d}x \\
&\quad + \frac{1}{r_0} \int_{-\infty}^{\infty} \frac{1}{2} \left[M \left(\frac{\partial \beta(x,t)}{\partial t} \right)^2 + w r_0 \left(\frac{\partial \beta(x,t)}{\partial x} \right)^2 \right] \mathrm{d}x \\
&= E_0 + \frac{1}{2} M_{\mathrm{sol}} v^2 \qquad (31)
\end{aligned}
$$

The rest energy of the new soliton is

$$
E_0 = 2(\varepsilon_0 - 2J) - \frac{8(x_1 + x_2)^4}{3w^2 J} = E_s^0 - W \qquad (32)
$$

where $W = [8(x_1 + x_2)^4]/(3w^2 J)$ is the energy of the deformation of the lattice. The effective mass of the new soliton is

$$
M_{\mathrm{sol}} = 2m_{\mathrm{ex}} + \frac{8(x_1 + x_2)^4 (9s^2 + 2 - 3s^4)}{3w^2 J (1-s^2)^3 V_0^2} \qquad (33)
$$

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

$$E_{\mathrm{B}p} = \frac{-8\left(x_1 + x_2\right)^4}{3Jw^2} \tag{34}$$

$E_{\mathrm{B}p}$ is larger than that of the Davydov soliton. The latter is $E_{\mathrm{BD}} = -x_1^4/(3Jw^2)$. They have the following relationship

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

It can be estimated that the binding energy of the new soliton is about several decades larger than that of the Davydov soliton. This is a very interesting result. It is helpful to enhance the thermal stability of the new soliton. Obviously, the increase of the binding energy of the new soliton comes from its two-quantum nature and the added interaction. $\sum_n \chi_2\left(u_{n+1} - u_n\right)\left(B_{n+1}^{+}B_n + B_n^{+}B_{n+1}\right)$, in the Hamiltonian of the systems, Eq. (10). However, it can be seen from Eq. (35) that the former plays the main role in the increase in the binding energy and the enhancement of the thermal stability for the new soliton relative to the latter due to $\chi_2 < \chi_1$. The increase of the binding energy results in significant changes of the properties of the new soliton, which are discussed as follows.

In comparing various correlations to this model, it is helpful to consider them as a function of a composite coupling parameter like that of Young *et al*. [114] and Scott [13–18] that can be written as

$$4\pi\alpha_p = \left(\chi_1 + \chi_2\right)^2/(2w\hbar\omega_{\mathrm{D}}) \tag{36}$$

where $\omega_{\mathrm{D}} = \left(w/M\right)^{1/2}$ is the band edge for acoustic phonons (Debye frequency). If $4\pi\alpha_p$=1, it is said to be weak. Using widely accepted values for the physical parameters for the alpha-helix protein molecule [4–97],

$$\begin{aligned} &J = 1.55\times10^{-22}\,\mathrm{J}, \quad w = (13-19.5)\,N/m \\ &M = (1.17-1.91)\times10^{-25}\,\mathrm{kg}, \quad \chi_1 = 62\times10^{-12}\,\mathrm{N} \\ &\chi_2 = (10-18)\times10^{-12}\,\mathrm{N}, \quad r_0 = 4.5\times10^{-10}\,\mathrm{m} \end{aligned} \tag{37}$$

it can be estimated that the coupled constant lies in the region of $4\pi\alpha_p = 0.11-0.273$, which is still a weakly coupled theory, but the coupling strength is enhanced as compared with that of the Davydov model, the latter is $4\pi\alpha_p = 0.036-0.045$. Using the notation of Venzel and Fischer [115], Nagy [116], and Wagner and Kongeter [117] again, it is convenient to define another com- posite parameter [13–18]:

$$\gamma = \frac{J}{2\hbar w_{\mathrm{D}}} \tag{38}$$

In terms of the two composite parameters $4\pi\alpha_p$ and γ, the binding energy of the soliton in the new model can be written as

$$\begin{aligned} &E_{\mathrm{B}p}/J = 8\left(4\pi\alpha_p/\gamma\right)^2/3 \\ &M_{\mathrm{sol}} = 2m_{\mathrm{ex}}\left[1 + 32\left(4\pi\alpha_p\right)^2/3\right] \end{aligned} \tag{39}$$

From the above parameter values, $\gamma = 0.08$ can be obtained. Thus the $E_{\mathrm{B}p}/J$ versus $4\pi\alpha$ relationships in Eq. (39) are plotted in Fig. 1. However, $E_{\mathrm{B}p}/J = \left(4\pi\alpha_p/\gamma\right)^2/3$ for Davydov's model [here $M'_{\mathrm{sol}} = m_{\mathrm{ex}}[1 + 2(4\pi\alpha_p/\gamma)^2/3], 4\pi\alpha_{\mathrm{D}} = \chi_1^2/(2w\hbar\omega_{\mathrm{D}})$], then the E_{BD}/J versus $4\pi\alpha_{\mathrm{D}}$ relationship is also plotted in Fig. 2. From this figure, it can be seen that the difference of soliton binding energies between the two models becomes larger with increasing $4\pi\alpha$.

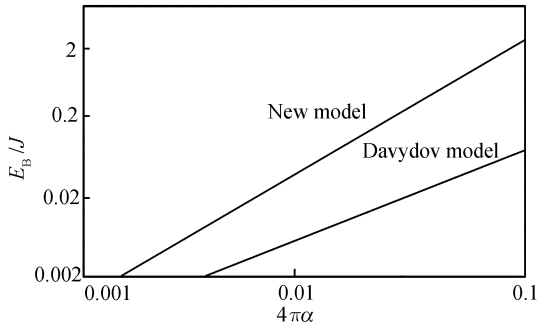

Fig. 2 Binding energy (E_{B}) of the solitons in our model and the Davydov model in units of the dipole-dipole interaction energy (J) vs. the coupled constant, $4\pi\alpha$ relationship.

Also, it can be seen clearly from Eqs. (28)–(32) and (35) that the localized feature of our soliton is enhanced due to the increases of the nonlinear interaction and the binding energy of the new soliton resulting from the increases of the exciton-phonon interaction in the improved model. Thus, the stability of the soliton against quantum and thermal fluctuations is also enhanced considerably.

As a matter of fact, the nonlinear interaction energy forming this siliton in the new model is $G_p = 8(\chi_1 + \chi_2)^2/(1-S^2)w = 3.8\times10^{-32}\,\mathrm{J}$, and it is larger than the linear dispersion energy, $J = 1.55\times10^{-32}\,\mathrm{J}$, i.e., the nonlinear interaction in this model is so large that it can actually cancel or suppress the linear dispersion effect in the equation of motion, thus the soliton is stable in such a case according the soliton theory [4–12, 115]. On the other hand, the nonlinear interaction energy in Davydov's model is only $G_{\mathrm{D}} = 4\chi_1^2/(1-S^2)w = 1.8\times10^{-21}\,\mathrm{J}$, and it is about 3–4 times smaller than G_p. Therefore, the stability of the Davydov soliton is weaker than the new one. Moreover, the binding energy of the new soliton in the improved model is $E_{\mathrm{B}p}$= (4.16–4.3)$\times10^{-21}$ J in Eq. (31), which is somewhat larger than the thermal perturbation energy, $k_{\mathrm{B}}T = 4.13\times10^{-21}\,\mathrm{J}$, at 300 K

and about four times larger than the Debye energy, $k\Theta = \hbar\omega_{\mathrm{D}} = 1.2\times10^{-21}$ J (ω_{D} is the Debye frequency). This shows that the transition of the new soliton to a delocalized state can be suppressed by the large energy difference between the initial (solitonic) state and the final (delocalized) state, which is very difficult to compensate for with the energy of the absorbed phonon. Thus, the new soliton is robust against quantum fluctuations and thermal perturbations; therefore, it has long lifetime and good thermal stability in the region of biological temperature. In practice, according to the studies of Schweitzer *et al*. (i.e., the lifetime of the soliton increases as μ_p and $T_0 = \hbar V_0 \mu_p / (k_{\mathrm{B}}\pi)$ increase at a given temperature) [50, 51] and the above obtained results, an inference could be roughly be drawn that the lifetime of the new soliton will increase considerably as compared with that of the Davydov soliton due to the increase of μ_P and T_0, because the latter is about three times larger than that in the Davydov model. On the other hand, the binding energy of the Davydov soliton $E_{\mathrm{BD}} = \chi_1^4 / (3w^2 J) = 0.188\times10^{-21}$ J, and it is about 23 times smaller than that of the new soliton, about 22 times smaller than $k_{\mathrm{B}}T$, and about six times smaller than $k_{\mathrm{B}}\Theta$, respectively. Therefore, the Davydov soliton [4–12] is easily destroyed by the thermal perturbation energy and quantum transition effects. Thus it indicates that the Davdov soliton has a very short lifetime, and it is unstable at the biological temperature of 300 K. This conclusion is consistent at a qualitative level with the results of Wang *et al*. [48, 49] and Cottingham *et al*. [50, 51].

One can sum up the differences between our model and Davydov's model, Eqs. (1)–(4), as follows. First, the parameter μ_p is increased ($\mu_p = 2\,\mu_{\mathrm{D}}\left[1+2\left(\frac{\chi_2}{\chi_1}\right)+\left(\frac{\chi_2}{\chi_1}\right)^2\right]$). Second, the non-linear coupling energy becomes $G_p = \frac{8(\chi_1+\chi_2)^2}{w(1-s^2)}$ ($G_p = 2G_{\mathrm{D}}\left[1+2\left(\frac{\chi_2}{\chi_1}\right)+\left(\frac{\chi_2}{\chi_1}\right)^2\right]$, where $G_{\mathrm{D}} = \frac{4\chi_1^2}{w(1-s^2)}$ is the non-linear interaction in Davydov's model resulting from the two-quantum nature and the enhancement of the coupling coefficient $(\chi_1+\chi_2)$. In fact, the non-linear interaction G_p is increased by about a factor of over 3–4 times larger than that of the Davydov soliton and larger than the dispersion energy J in the equation of motion. A straightforward consequence of these effects is that the binding energy of the new soltion or, in other words, the energy gap between the solitonic and excitonic states are greatly increased or $E_{\mathrm{B}p} = -4\mu_p^2 J/3 = -G_p^2/(12J) = 16E_{\mathrm{BD}}\left[1+4\left(\frac{\chi_2}{\chi_1}\right)^4+6\left(\frac{\chi_2}{\chi_1}\right)^2+4\left(\frac{\chi_2}{\chi_1}\right)^3+\left(\frac{\chi_2}{\chi_1}\right)\right]$, where E_{BD} is given in Eq. (4). For α-helical protein molecules and using the parameter values listed in Eq. (37) the values of the main parameters in this model can be calculated by the above values. These values and the corresponding values in Davydov's model are simultaneously listed in Table 1.

From Table 1, it can be seen clearly that the new model produces considerable changes in the properties of the new soliton, such as large increase of the non-linear interaction, binding energy and amplitude of the soliton, and decrease of its width as compared to that of the Davydov soliton. This indicates that the soliton in the new model is more localized and more robust against quantum and thermal fluctuations and the stability has been enhanced [4–12, 103–109], which implies an increase in the lifetime of the new soliton. From Eq. (19), it can also be found that the effect of the two-quantum nature is larger than that of the added interaction. Therefore, the new soliton can be considered as quasi- coherent.

Table 1 Comparison of parameters used in Davydov's model and our new model.

Parameters / Models	μ	$G/(10^{-21}\mathrm{J})$	Amplitude of soliton A'	Width of soliton $\Delta X/(10^{-10}\mathrm{m})$	Binding energy of soliton $E_{\mathrm{B}}/(10^{-21}\mathrm{J})$
Our model	5.94	3.8	1.72	4.95	–7.8
Davydov's model	1.90	1.18	0.974	14.88	–0.188

In the above studies, in order to investigate the influences of quantum and thermal effects on the soliton state, which are expected to cause the soliton to decay into a delocalized state, it is postulated that the model Hamiltonian and the wave function in the new model together give a complete and realistic picture of the interaction properties and allowed states of protein molecules. The additional interaction term in the Hamiltonian gives more symmetrical interactions. The new wave function is a reasonable choice for protein molecules because it not only exhibits the coherent features of collective excitations arising from the nonlinear interaction between excitons and phonons, but also maintains the conservation of the number of particles and fulfills the fact that the energy released by the ATP hydrolysis can only excite two quanta. In such a case, using a standard calculating method [4–12, 101, 102] and widely accepted parameters, the region encompassed of the excitation or the linear extent of the new soliton, $\Delta X = 2\pi r_0 / \mu_p$ can be calculated to be greater than the lattice constant r_0, i.e., $\Delta X > r_0$ as shown in Table 1. Conversely, the amplitude squared of the new soliton can be explicitly calculated using Eq. (29) in its rest frame as $|\varphi(x)|^2 = \frac{\mu_p}{2}\mathrm{sech}^2\left(\frac{\mu_p x}{r_0}\right)$. Thus the probability of finding the new soliton outside a range of width r_0 is about 0.10. This number can be compatible with the continuous approximation since the quasi-coherent soliton can spread over more than one lattice spacing in the system in such a case.

This proves that assuming the continuous approximation used in the calculation is still qualitatively valid for the soliton width of the order of the lattice spacing, and soliton stability is still improved. However, there may be considerable corrections to the quantitative values.

5 Lifetime of the soliton at biological temperature

5.1 Partially diagonalized form of the model Hamiltonian

The lifetime of the soliton in protein molecules is an central problem in the process of bio-energy transport because the soliton possess certain biological meanings and can play an important role in biological process, only if it has sufficiently long lifetime. However, this question about the 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 Davydov's model in Eqs. (1)–(4), both the wave function and the Hamiltonian of the systems are too simple. The first problem of the model concerns the Davydov wave functions, both $|D_1\rangle$ and $|D_2\rangle$ [4–12]. These are asymmetric since the phononic part is in a coherent state, while the excitonic part is in an excitation state of a single-particle. It is unreasonable that the nonlinear interaction generated by the coupling between excitons and phonons produces different states for phonons and the excitons. Thus, Davydov's wave function should be modified [62–80], i.e., the excitonic part in it should also be coherent or quasi-coherent [81–97]. However, the standard coherent state [19–23] and the large-`n excitation state are not appropriate to protein molecules due to the above-mentioned reasons. Similarly, Förner's and Cruzeiro-Hansson's two-quantum states [35–45] do not fulfill the above criteria.

For the convenience of calculation, the wave function of the system in Eq. (9) is represented by [81–97]

$$|\Phi(t)\rangle = |\varphi(t)\rangle\,|\beta(t)\rangle = U_1\,|0\rangle_{\rm ex}\,U_2\,|0\rangle_{\rm ph} \tag{40}$$

where

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

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

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

where $\sum_i |\varphi_i|^2 = n$ is assumed, where n is an integer, denoting the number of particles. The wave function of Eq. (40) does not only exhibit coherent properties, but agrees with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) excites only two amide-I vibrational quanta, instead of multi-quanta ($n > 2$). Therefore, the Hamitonian and wave function of the systems, Eqs. (9), (10), or (40) are reasonable and appropriate to protein molecules. Using the standard transformation in Eq. (16), where $\omega_q = 2(w/M)^{1/2}\sin\frac{r_0 q}{2}$, Eq. (10) becomes

$$\begin{aligned} H = &\sum_n\left[\varepsilon_0 B_n^+ B_n - J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)\right] \\ &+\sum_q \hbar\omega_q\left(a_q^+ a_q + \frac{1}{2}\right) + \frac{1}{\sqrt{N}}\sum_{q,n}[g_1(q)B_n^+ B_n \\ &+g_2(q)(B_n^+ B_{n+1} + B_n^+ B_{n+1})](a_q + a_{-q}^+)\mathrm{e}^{\mathrm{i}nr_0 q} \end{aligned} \tag{41}$$

where

$$\begin{aligned} g_1(q) &= 2\chi_1 \mathrm{i}\left(\frac{\hbar}{2M\omega_q}\right)^{1/2}\sin(r_0 q) \\ \mathrm{g}_2(q) &= \chi_2\left(\frac{\hbar}{2M\omega_q}\right)^{1/2}(\mathrm{e}^{\mathrm{i}r_0 q} - 1) \end{aligned} \tag{42}$$

In a semiclassical and continuum approximation from Eq. (41), the envelope soliton solution of Eq. (29) can be obtained in the new model, and Eq. (29) can be represented by the following form [81–97]:

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

where

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

The energy of the new soliton is

$$E_{S01} = 2\left[(\varepsilon_0 - 2J) + \frac{\hbar^2 v^2}{4Jr_0^2} - \frac{2\mu_p^2}{3}J\right] \tag{45}$$

Thus it can also be found out that

$$\begin{aligned} \alpha_q(t) = &\frac{\mathrm{i}\pi(\chi_1+\chi_2)}{w\mu_p(1-v^2/v_0^2)}\left(\frac{M}{2\hbar\omega_q}\right)^{1/2} \\ &\cdot(\omega_q + qv)\mathrm{csch}(\pi q r_0/2\mu_p)\mathrm{e}^{\mathrm{i}qvt} = \alpha_q \mathrm{e}^{\mathrm{i}qvt} \end{aligned} \tag{46}$$

This treatment yields a localized coherent structure with the size of order $2\pi r_0/\mu_{\rm p}$ that propagates with velocity v and can transfer energy $E_{S01} < 2\varepsilon_0$. Unlike bare excitons scattered by the interactions with phonons, this soliton state describes a quasi-particle consisting of two excitons plus a lattice deformation and hence a priori includes the interac-

tion with acoustic phonons. So the soliton is not scattered and spread by this interaction of lattice vibration, so it can maintain its form, energy, momentum and other quasi-particle properties when 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 moves with a velocity less than that of longitudinal sound in the chain, they do not emit phonons, i.e., their kinetic energy is not transformed into thermal energy. This is one important reason for the high stability of the new soliton. In addition, the energy of the soliton state is below the bottom of bare exciton bands with the energy gap $4\mu_p^2 J/3$ at a low velocity of propagation. Hence there is an energy penalty associated with the destruction of the 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. It is known in general that the probability of the transition to a lattice state without distortion is very small, which, in general, is negligible in a long chain. 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 problem explicitly.

Now the model Hamiltonian is partially diagonalized in order to calculate the lifetime of the soliton [Eq. (43)], using the quantum perturbation method [50, 51]. Since attention is paid to the investigation of the case where there is initially a soliton moving with velocity v in the chains, it is convenient to do the analysis in a frame of reference where the soliton is at rest. The Hamiltonian should then be considered in this rest frame of the soliton, $\tilde{H} - vP$, where P is the total momentum, and $P = \sum_q \hbar q(a_q^+ a_q - B_q^+ B_q)$, where $B_q^+ = \frac{1}{\sqrt{N}}\sum_n e^{iqnr_0} B_n^+$. Also, in order to have simple analytical expressions, the usual continuum approximation is made. This yields

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

where $\varphi(x)$ represents the field operator corresponding to B_n in the continuum limit (whereas it only indicated a numerical value before). Here $L = Nr_0$, $-\pi < kr_0 < \pi$, and $\omega_q \approx (w/M)^{1/2} r_0 \cdot |q|$, $x = nr_0$. Since the soliton excitation is connected with the deformation of intermolecular spacing, it is necessary to pass in Eq. (47) to new phonons when this deformation is taken into account. Such a transformation can be realized by means of the following transformation of phonon operators [118]:

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

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

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

which is a coherent phonon state [111, 112], i.e., $b_q|\tilde{0}\rangle_{ph} = 0$. The Hamiltonian $\tilde{H}$ can now be rewritten as

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

where

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

$$V(x) = \frac{1}{N}\sum_q [g_1(q) + 2g_2(q)](\alpha_{-q}^* + \alpha_{-q})e^{iqx} \quad (51)$$

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

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

from Eq. (45) in such a case. From the above formulae, it can be obtained

$$V(x) = -2J\mu_p{}^2 \mathrm{sech}^2(\mu_p x/r_0) \quad (52)$$

In order to partially diagonalize the Hamiltonian Eq. (50), the following canonical transformation is introduced [50, 51, 81–97]:

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

where

$$\int C_1^*(x)C_j(x)dx = \delta_{lj}, \quad \sum_j C_j^*(x')C_j(x) = \delta(x - x')$$

$$\int dx|C_j(x)|^2 = 1 \quad (54)$$

The operators A_s^+ and A_k^+ are the creation operators for the bound state $C_s(x)$ and delocalized state $C_k(x)$, respectively. The detailed calculation of the partial diagonalization and corresponding $C_s(x)$ and $C_k(x)$ are described in Appenix A. The obtained partially diagonalized Hamiltonian is as follows

$$\tilde{H} = W' + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - qv) b_q^+ b_q + \frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - qv)(b_q^+ \alpha_q + \alpha_q^* b_q)(1 - A_s^+ A_s) + \frac{1}{\sqrt{N}} \sum_{kk'q} F(k,k',q)(b_{-q}^+ + b_q) A_{k'}^+ A_k - \frac{1}{\sqrt{N}} \sum_{kq} \tilde{F}(k,q)(b_{-q}^+ + b_q)(A_s^+ A_{-k} - A_k^+ A_s) \quad (55)$$

and

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

with $E_s = 2\left(\varepsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - \mu_p^2 J\right)$ (56a)

$$C_k(x) = \frac{\mu_p \tanh(\mu_p x / r_0) - \mathrm{i}kr_0}{\sqrt{Nr_0}[\mu_p - \mathrm{i}kr_0]} \exp\left(\mathrm{i}kx + \frac{\mathrm{i}\hbar v x}{2Jr_0^2}\right) \quad (56b)$$

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

where

$$F(k,k',q) = 2[g_1(q) + 2g_2(q)] \int_0^L \mathrm{d}x \mathrm{e}^{\mathrm{i}qx} C_{k'}^*(x) C_k(x) \approx 2[g_1(q) + 2g_2(q)] \left\{1 - \frac{\mathrm{i}\mu_p q r_0}{[\mu_p + \mathrm{i}(k+q)r_0][\mu_p - \mathrm{i}kr_0]}\right\} \approx F[k,(k+q),q]\delta_{k'k+q} \quad (57)$$

$$\tilde{F}(k,q) = 2[g_1(q) + 2g_2(q)] \int_0^L \mathrm{d}x \mathrm{e}^{\mathrm{i}qx} C_{k'}^*(x) C_s(x) = \frac{2\pi}{\sqrt{2\mu_p}}[g_1(q) + 2g_2(q)] \cdot \frac{\mathrm{i}qr_0}{\mu_p + \mathrm{i}kr_0} \operatorname{sech}[\pi(k-q)r_0/(2\mu_p)] \quad (58)$$

where α_q is determined by $V(x)$ and the condition $(\omega_q - vq)\alpha_q = (\omega_q + qv)\alpha_q^*$, which is required to obtain the factor $(1 - A_s^+ A_s)$ in the $\tilde{H}$ in Eq. (55). Thus the following is obtained

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

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

For this α_q the $|\tilde{0}\rangle_{\mathrm{ph}}$ 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 frame of reference is stationary. For the new soliton described by the state vector $|\psi\rangle = \frac{1}{\sqrt{2!}}(A_s^+)^2 |0\rangle_{\mathrm{ex}} |\tilde{0}\rangle_{\mathrm{ph}}$ the average energy of $\tilde{H}$ in Eq. (55) is

$$\langle\psi|\tilde{H}|\psi\rangle = 2\left(\varepsilon_0 - 2J - \frac{\hbar^2 v^2}{4Jr_0^2}\right) - \frac{4}{3}J\mu_p^2 \quad (60)$$

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

5.2 Transition probability and decay rate of the new soliton

Now the transition probability and decay rate of the quasi-coherent soliton arising from the perturbed potential are calculated by using the first-order quantum perturbation theory developed by Cottingham *et al*. [50, 51], in which the influences of thermal and quantum effects on the properties of the soliton can be taken into account simultaneously.

For the discussion of the decay rate and lifetime of the new soliton state, it is very convenient to divide $\tilde{H}$ in Eq. (55) into $H_0 + V_1 + V_2$, where

$$H_0 = W' + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - vq) b_q^+ b_q + \frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - vq)(\alpha_q b_q^+ + \alpha_q^* b_q)(1 - A_s^+ A_s) \quad (61)$$

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

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

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

Now the decay rate of the new soliton along the following lines is calculated by using Eq. (61) and V_2 in Eq. (63) and the quantum perturbation theory. First, a more general formula is computed for the decay rate of the soliton containing n quanta in the system in which the three terms contained in Eq. (40a) are replaced by (n+1) terms of the expression of a coherent state $\frac{1}{\lambda}\exp\left[\sum_n \varphi_n(t)B_n^{+}\right]|0\rangle_{\text{ex}}$. Finally, the decay rate of the new soliton with two quanta is found out. In such a case H_0 is chosen as the ground state, $|n\rangle$ has energy $W+nE_s'$ in the subspace of excitation equal to n, i.e., $\langle n|\sum_i B_i^{+}B_i|n\rangle = \langle n|A_s^{+}A_s + \sum_k A_k^{+}A_k)|n\rangle = n$. In this subspace, the eigenstates have the simple form

$$|n-m, k_1k_2,\cdots,k_m,\{n_q\}\rangle$$
$$= \frac{1}{\sqrt{(n-m)!}}(A_s^{+})^{n-m}A_{k_1}^{+}A_{k_2}^{+}\cdots A_{k_m}^{+}|0\rangle_{\text{ex}}\prod_q\frac{(d_q^{+})^{n_q}}{\sqrt{n_q!}}|\tilde{0}\rangle_{\text{ph}}^{n-m} \tag{64}$$

where

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

($m \leqslant n$, n and m are all intgers)

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

$$E_{n-m;k_1,\cdots,k_{m_1};\{n_q\}}^{(0)} = [1-(m/n)^2]W' + (n-m)E_s' + \sum_{j=1}^{m}E_{k_1}' + \sum_q \hbar(\omega_q - vq)n_q \tag{66}$$

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 an 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

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

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

$$|\alpha k\rangle = \Pi_q\frac{(a_q^{+})^{n_q}}{\sqrt{n_q!}}|0\rangle_{\text{ph}}(A_k^{+})^n|0\rangle_{\text{ex}} \tag{68}$$

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

$$\bar{W} = \frac{1}{\hbar^2}\int_0^t dt'\int_0^t dt''\left\{\sum_{\alpha k'}\sum_l P_l^{(\text{ph})}\langle n|\exp\left(\frac{iH_0t''}{\hbar}\right)V_2 \cdot\exp\left(\frac{-iH_0t''}{\hbar}\right)|\alpha k'\rangle\cdot\langle\alpha k'|\exp\left(\frac{iH_0t'}{\hbar}\right)V_2 \cdot\exp\left(\frac{-iH_0t'}{h}\right)|n\rangle\right\} \tag{69}$$

The transition probability of the soliton resulting from the perturbed potential (V_1+V_2) should be calculated at the first order by the perturbation theory. Following Cottingham and Schweitzer [50, 51], only the transition from the soliton state to the delocalized exciton state caused by the potential V_2 is estimated, which can satisfactorily be treated by means of the perturbation theory since the coefficient $\tilde{F}(k, q)$ defined by Eq. (58) is proportional to an integral over the product of the localized state and a delocalized state, and therefore is of order $1/\sqrt{N}$. The V_1 term in the Hamiltonian is an interaction between delocalized excitons and the phonons. The main effect of V_1 is to modify the spectrum of delocalized excitatons in the weak coupling limit [$J\mu_p/(K_B T_0) \ll 1$, the definition of T_0 is given below]. As a result, delocalized excitons and phonons will have their energies shifted and also have finite lifetime. These effects are ignored in our calculation since they are only of second order in V_1.

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

$$e^{-iH_0t}|n,\{n_q\}\rangle = \exp\left\{-i(W'+nE_q')t/\hbar - i\sum_q(\omega_q - qv)b_q^{+}b_qt\right\}|n,\{n_q\}\rangle$$

and

$$e^{iH_0 t}\,|\,n-1,\{n_q'\}\rangle = \exp\left\{-i\left[\left(1-\frac{1}{n^2}\right)W' + (n-1)E_s' + E_k'\right]t/\hbar - i\sum_q(\omega_q - qv)d_q^+ d_q t\right\}|\,n-1,\{n_q'\}\rangle$$

where

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

using the explicit form for V_2 and the fact that the sum over states $|\,k'\alpha,\ \{n_q'\}\rangle$ contains a complete set of phonons for each value of k', $\bar{W}$ can be rewritten as

$$\begin{aligned}\bar{W} = {} & \frac{1}{\hbar^2}\frac{\pi^2}{2n\mu_1 N^2}\sum_k\sum_{k'}\sum_{k''}[g_1^*(k)+2g_2^*(k)] \\ & \cdot[g_1(k'')+2g_2(k'')]\frac{(kr_0)(k''r_0)}{(n\mu_1)^2+(k'r_0)^2} \\ & \cdot\operatorname{sech}\left[\frac{\pi r_0}{2n\mu_1}(k-k')\right] \\ & \cdot\operatorname{sech}\left[\frac{\pi r_0}{2n\mu_1}(k''-k')\right]\int_0^t dt'\int_0^t dt'' \\ & \cdot\left\{\exp\left[\frac{-i}{\hbar}\left(n\left(n^2-\frac{2}{3}n\right)\mu_1^2 J + nJ(k'r_0)^2\right)(t'-t'')\right]\right. \\ & \cdot\langle\langle\exp[i\sum_q(\omega_q - qv)b_q^+ b_q(t'-t'')](b_k^+ + b_{-k}) \\ & \left.\cdot\exp[i\sum_q(\omega_q - qv)a_q^+ a_q(t'-t'')](b_{-k''}^+ + b_{k''})\rangle\rangle\right\} \end{aligned} \quad (70)$$

where

$$\begin{aligned} & g_1(k)+2g_2(k) \\ & = 2\chi_1\left(\frac{\hbar}{2M\omega_k}\right)^{1/2}\{A[\cos(r_0 k)-1]+i(A+1)\sin(r_0 k)\} \\ & \approx 2i(A+1)(r_0 k)\chi_1\left(\frac{\hbar}{2M\omega_k}\right)^{1/2} \\ & \mu_1 = \frac{\chi_1^2(1+A^2)}{\omega(1-s^2)J},\quad A=\chi_2/\chi_1 \end{aligned} \quad (71)$$

here A is a new parameter introduced to describe the rate between the new nonlinear interaction term and that in Davydov's model.

To estimate the lifetime of the soliton, attention should be paid to the long-time behavior of $\frac{d\bar{w}}{dt}$. By straightforward calculation, the average transition probability or decay rate of the soliton is given by

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

where the thermal average is

$$\begin{aligned} U(k,k'',t) = {} & \langle\langle\exp[i\sum_q(\omega_q - qv)b_q^+ b_q t](b_k^+ + b_{-k}) \\ & \cdot\exp[-i\sum_q(\omega_q - qv)a_q^+ a_q t](b_{-k''}^+ + b_{k''})\rangle\rangle \end{aligned}$$

with

$$\begin{aligned}\langle\langle A\rangle\rangle = {} & \operatorname{Tr}\left\{A\exp[-\beta\sum_q\hbar(\omega_q - qv)b_q^+ b_q]\right\} \\ & /\operatorname{Tr}\left\{\exp[-\beta\sum_q\hbar(\omega_q - qv)b_q^+ b_q]\right\} \\ = {} & \operatorname{Tr}\left\{A\exp\left[-\beta\sum_q\hbar(\omega_q - qv)b_q^+ b_q\right]\right\}/Z_{ph} \end{aligned} \quad (73)$$

and $Z_{ph}=\prod_q\left\{1-\exp[-\beta\hbar(\omega_q - qv)]\right\}^{-1}$, $\beta = \frac{1}{k_B T}$.

This rather unusual expression of Γ_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 Γ_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 the improved model. Here the coherent state is used to calculate the $U(k,k'',t)$ as it is described in Appendix B. The decay rate is finally obtained:

$$\begin{aligned}\Gamma_n = \lim_{t\to\infty}\frac{\mathrm{d}\bar{W}}{\mathrm{d}t} = \frac{2}{n\mu_1\hbar^2}\frac{\pi^2}{N^2}\sum_{kk'}\Big[|\, g_1(k)+2g_2(k)\,|^2 \\ \cdot\frac{(r_0k)^2\sec h^2[\pi(k-k')r_0/(2n\mu_1)]}{(n\mu_1)^2+(k'r_0)^2}\mathrm{Re}\int_0^\infty \mathrm{d}t \\ \cdot\Big\{\exp\Big[-\mathrm{i}nJ(k'r_0{}^2+n\Big(n^2-\frac{2}{3}n\Big)\mu_1^2\,\mathrm{J}\,t/\hbar \\ +R_n(t)+\xi_n(t)\Big]\frac{\exp[\mathrm{i}(\omega_k-kv)t]}{\exp[\beta\hbar(\omega_k-kv)]-1}\Big\}\Big]\end{aligned} \tag{74}$$

where

$$\begin{aligned}R_n(t) = -\frac{1}{n^2N}\sum_k |\,\alpha_k\,|^2\,\{\mathrm{i}-\exp[-\mathrm{i}(\omega_k-kv)t]\} \\ \xi_n(t) = -\frac{4}{n^2N}\sum_k\frac{|\,\alpha_k\,|^2\,\sin^2\Big[\frac{1}{2}(\omega_k-kv)t\Big]}{\exp[\beta\hbar(\omega_k-kv)]-1}\end{aligned} \tag{75}$$

This is just a generally analytical expression for the decay rate of the soliton containing n quanta at any temperature within the lowest order perturbation theory. It is noted that in the case where a phonon with wave vector k in Eq. (75) is absorbed, the delocalized excitation produced does not need to have any wave vector equal to k. The wave vector here is only approximately conserved by the $\mathrm{sech}^2[\pi(k–k')\,r_0/2n\mu_1]$ term. This is, of course, a consequence of the breaking of the translation symmetry by the deformation. Consequently, the usual energy conservation is not found. The terms $R_n(t)$ and $\xi_n(t)$ occur because the phonons in the initial and final states are defined relative to different deformations.

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

From Eqs. (74) and (75), it can be seen that the Γ_n and $R_n(t)$ and $\xi_n(t)$ and $\mu = n\mu_1$ mentioned above are all changed by increasing the number of quanta, n. Therefore, the approximation methods used to calculate Γ_n and related quantities (especially the integral contained in Γ_n) should be different for different n. The explicit formula of the decay rate of the new soliton with two-quanta (n = 2) is calculated by using Eqs. (74), (75). In such a case we can the expressions of this integral and $R_2(t)$ and $\xi_2(t)$ contained in Eqs. (74), (75) are explicitly computed 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 ω_q is approximated by $\sqrt{w/M}\,|q|r_0$, as is shown in Appendix *C*. For $t\to\infty$ (because attention is being paid to the long-time steady behavior) the asymptotic forms of $R_2(t)$ and $\xi_2(t)$ are

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

$$\xi_2(t)\approx -\pi R_0k_\mathrm{B}Tt/\hbar,\quad \text{where } \coth\left(\frac{1}{2}\omega_\alpha t\right)\sim 1 \tag{77}$$

i.e.,

$$\lim_{t\to\infty}\xi_2(t) = -\eta t\,,\quad \eta = \pi R_0/(\beta\hbar) = \pi R_0k_BT/\hbar \tag{78}$$

where

$$\begin{aligned}R_0 = \frac{4(\chi_1+\chi_2)^2}{\pi\hbar w}(M/w)^{1/2} = \frac{2J\mu_pr_0}{\pi\hbar v_0} \\ \omega_\alpha = \frac{2\mu_p}{\pi}\left(\frac{w}{M}\right)^{1/2},\quad T_0 = \hbar\omega_\alpha/k_\mathrm{B}\end{aligned} \tag{79}$$

At $R_0 < 1$ and $T_0 < T$ and $R_0\,T/T_0 < 1$ for protein molecules, the integral included in Eq. (74) can be evaluated by using the approximation which is shown in Appendix C. The result is

$$\begin{aligned}\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t \\ \cdot\exp\Big\{-\mathrm{i}[2J(k'r_0)^2+\frac{4}{3}J\mu_p^2-\hbar\omega_k]t/\hbar+R_2(t)+\xi_2(t)\Big\} \\ \approx\frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\Big\{\eta^2+[\delta(k,k')/\hbar]^2\Big\}^{-(1-R_0)/2} \\ \cdot\Big\{1-\frac{1}{2}\Big[\frac{\pi R_0}{2}+(1-R_0)\Big(\frac{\delta(k,k')}{\eta\hbar}\Big)\Big]^2\Big\}(54)\end{aligned} \tag{80}$$

here

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

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

$$\begin{aligned}\Gamma_2 = \lim_{t\to\infty}\frac{\mathrm{d}\overline{W}}{\mathrm{d}t} &= \frac{2}{\mu_p}\left(\frac{\pi}{N}\right)^2 \\ &\cdot\sum_{kk'}\left[\frac{(kr_0)^2\,|\,g_1(k)+2g_2(k)\,|^2\ \mathrm{sech}^2[(\pi r_0/2\mu_p)(k-k')]}{[\mu_p^2+(k'r_0)^2][\exp(\beta\hbar\omega_k)-1]}\right. \\ &\cdot(2.43\omega_\alpha)^{-R_0} \\ &\cdot\frac{\left\{\eta^2+\frac{1}{\hbar^2}\left[\frac{4}{3}\mu_p^2 J+2(k'r_0)^2 J-\hbar\omega_k\right]^2\right\}^{(1+R_0)/2}}{\hbar^2\eta^2+\left[\frac{4}{3}\mu_p^2 J+2(k'r_0)^2 J-\hbar\omega_k\right]^2} \\ &\cdot\left.\left\{1-\frac{1}{2}\left[\frac{R_0\pi}{2}+(1-R_0)\frac{\frac{4}{3}\mu_p^2 J+2(k'r_0)^2 J-\hbar\omega_k}{\hbar\eta}\right]^2\right\}\right.\end{aligned} \tag{82}$$

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 Davydov's model [50, 51]. To emphasize the difference of the decay rate between the two models, the corresponding quantity for the Davydov soliton is re-written as [50, 51]

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

where

$$\eta_{\mathrm{D}} = \pi R_0^{\mathrm{D}} K_{\mathrm{B}} T/\hbar,\quad R_0^{\mathrm{D}} = \frac{2\chi_1^2}{\pi\hbar w}\left(\frac{M}{w}\right)^{1/2}$$

$$\omega_\alpha^{\mathrm{D}} = \frac{2\mu_{\mathrm{D}}}{\pi}\left(\frac{M}{w}\right)^{1/2} \tag{84}$$

Eq. (83) can also be found out from Eq. (74) at $n = 1$ by using the Cottingham *et al.*'s approximation.

The two formulae above Eqs. (82) and (83) are completely different, not only in the parameter's values, but also in the factors contained in them. In Eq. (82), the factor $\left\{1-\frac{1}{2}\left[\frac{R_0\pi}{2}+(1-R_0)\left[\left(\frac{4}{3}\mu_p^2 J+2(k'r_0)^2 J-\hbar\omega_k\right)/(\hbar\eta)\right]\right]^2\right\}$ is added, while in Eq. (83), the factor $(\omega_\alpha/\eta_{\mathrm{D}})^{-R_0^{\mathrm{D}}}\eta_{\mathrm{D}}$ replaces the term $(2.43\omega_{\mathrm{d}})^{-R_0}\cdot\left\{\eta^2+\frac{1}{\hbar}\left[\frac{4}{3}\mu_p^2 J+2(k'r_0)^2 J-\hbar\omega_k\right]^2\right\}^{\left(\frac{1+R_0}{2}\right)}$ in Eq. (82) due to the two-quantum nature of the new wave function and the additional interaction term in the new Hamiltonian. In Eq. (82), η, R_0 and T_0 are not small, unlike those in Davydov's model. Using Eq. (72) and Table 1, the values of η, R_0 and T_0 are found out at $T = 300$ K in both models, which are listed in Table 2. From this table, it can be seen that η, R_0 and T_0 for the new model are about three times larger than the corresponding values in Davydov's model due to the increases of μ_p and the non-linear interaction coefficient G_p. Thus the approximations used in Davydov's model by Cottingham *et al.* [50, 51] can not be applied in our calculation of the lifetime of the new soliton, though the same quantum-perturbation scheme is utilized. Hence it can be audaciously supposed that the lifetime of the quasi-coherent soliton will be greatly changed.

Table 2 Comparison of characteristic parameters in Davydov's model and in our new model.

	R_0	T_0/K	$\eta/(10^{13}\mathrm{s}^{-1})$
New model	0.529	294	6.527
Davydov's model	0.16	95	2.096

5.3 Discussion for the lifetime of the new soliton and results

The above expression, Eq. (82), allows the decay rate Γ_2 to be numerically computed, and the lifetime of the new soliton $\tau = 1/\Gamma_2$ for the values of the physical parameters is appropriate to α-helical protein molecules. Using the parameter values given in Eq. (37), Tables 1 and 2, $v = 0.2\,v_0$ and assuming the wave vectors are in the Brillouin zone, the values of Γ_2 between 1.54×10^{10} and $1.89\times10^{10}\,\mathrm{s}^{-1}$ can be obtained. This corresponds to the soliton lifetime τ between 0.53×10^{-10} and 0.65×10^{-10} s at $T = 300$ K, or $\tau/\tau_0 =$ 510–630, where $\tau_0 = r_0/v_0$ is the time for traveling one lattice spacing at the speed of sound, equal to $(M/w)^{1/2} = 0.96\times10^{-13}$ s. In this amount of time, the new soliton, traveling at two tenths of the speed of sound in the chain, would travel several hundreds of lattice spacings, that is several hundred times more than the Davydov soliton for which $\tau/\tau_0 < 10$ at 300 K [50, 51] (i.e., the Davydov soliton traveling at half of the sound speed can cover less than ten lattice spacings in its lifetime). The lifetime is sufficiently long for the new soliton

excitation to be a carrier of bio-energy. Therefore, the quasi-coherent soliton is a viable mechanism for bio-energy transport at biological temperature in the above range of parameters.

Attention is being paid to the relationship between the lifetime of the quasi-coherent soliton and temperature. Figure 3 shows the relative lifetimes τ/τ_0 of the new soliton versus temperature T for a set of widely accepted parameter values as shown in Eq. (37). Since it is assumed that $v < v_0$, the soliton will not travel the length of the chain unless τ/τ_0 is large compared with L/r_0, where $L = Nr_0$ is the typical length of protein molecular chains. Hence for $L/r_0 \approx 100$, $\tau/\tau_0 > 500$ is a reasonable criterion for the soliton to be a possible mechanism of bio-energy transport in protein molecules. The lifetime of the quasi-coherent soliton shown in Fig. 4 decreases rapidly as temperature increases, but below $T = 310$ K it is still large enough to fulfill the criterion. Thus the new soliton can play an important role in biological processes.

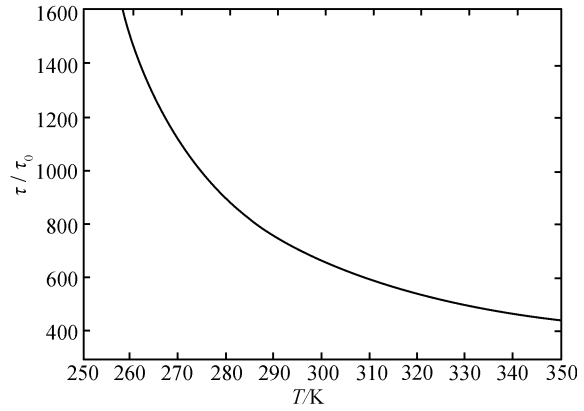

Fig.3 Soliton lifetime τ relatively to τ_0 as a function of the temperatureT for parameters appropriate to the α-helical molecules in the new model in Eq.(9).

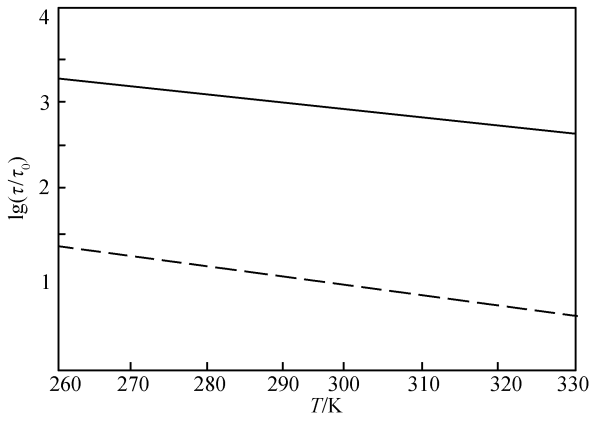

Fig. 4 $\lg(\tau/\tau_0)$ vs. the temperature for the soliton. Note: The solid line is the result of the new model, and the dashed line is the result of Davydov's model.

For comparison, $\lg(\tau/\tau_0)$ versus the temperature relationships was simultaneously plotted for the Davydov soliton and the new soliton with a quasi-coherent two-quantum state in Fig. 4. The temperature-dependence of $\lg(\tau/\tau_0)$ of the Davydov soliton is obtained from Eq. (83). It is found that the differences of the values of τ/τ_0 between the two models are very large. The value of τ/τ_0 of the Davydov soliton really is too small, and it travels less than ten lattice spacings at half the speed of sound in the protein chain [50, 51]. Hence it is true that the Davydov soliton is ineffective for biological processes [50, 51].

The dependency of the soliton lifetime on the other parameters can also be studied by using Eq. (82). Parameter values near the above accepted values shown in Eq. (37) are chosen. In the new model, it is known from Eq. (82) that the lifetime of the soliton mainly depends on the following parameters: coupling constants $(\chi_1 + \chi_2)$, M, w, J, phonon energy $\hbar\omega_k$, as well as composite parameters $\mu(\mu = \mu_p)$, R_0 and T/T_0. At a given temperature, τ/τ_0 increases as μ and T_0 increase. The dependences of the lifetime τ/τ_0 at 300 K on $(\chi_1+\chi_2)$ and μ are shown in Figs. 5 and 6, respectively. Since μ is inversely proportional to the size of the soliton, and determines the binding energy in the new model, it is an important quantity. It is regarded as an independent variable. In such a case, the other parameters in Eq. (82) adopt the values in Eq. (37). It is clear from Figs. 5 and 6 that the lifetime of the soliton τ/τ_0 increases rapidly with the increase of μ and $(\chi_1 + \chi_2)$. Furthermore, when $\mu \geqslant 5.8$ and $(\chi_1 + \chi_2) \geqslant 7.5 \times 10^{-11}$ N, which are values appropriate to the new model, $\tau/\tau_0 > 500$ can be found. For comparison, the corresponding result obtained by using Eq. (83) is shown for the original Davydov's model as the dashed line in Fig. 6. Here it can be seen that the increase in the lifetime of the Davydov soliton with the increase of μ is quite slow and the difference between the two models increases rapidly with the increase of μ. The same holds for the dependency on the parameter $(\chi_1 + \chi_2)$, but the result for the Davydov soliton is not drawn in Fig. 5. These results show again that the quasi-coherent soliton in the new model is a likely candidate for the mechanism of bio-energy transport in protein molecules. In addition, it indicates that a basic

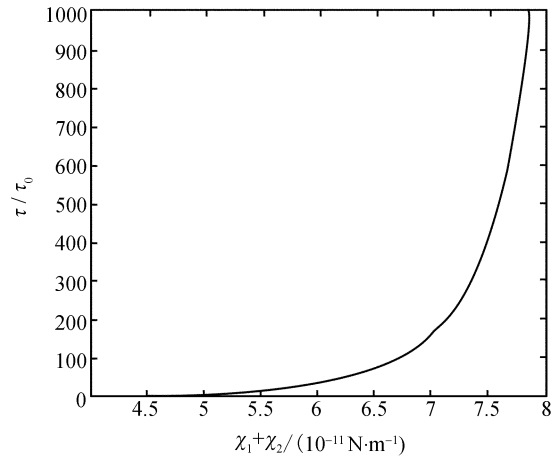

Fig. 5 τ/τ_0 versus $(\chi_1 + \chi_2)$ relationship in Eq. (82).

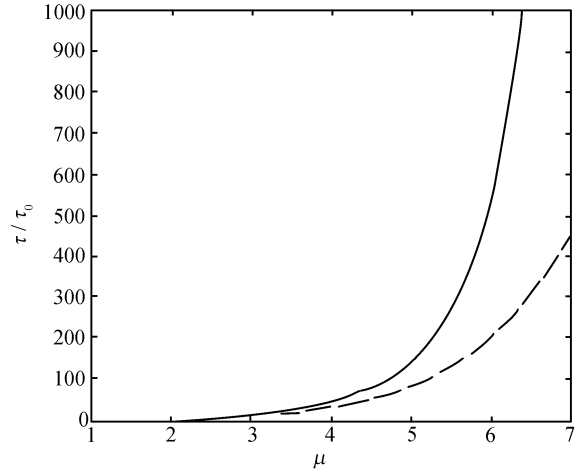

Fig. 6 τ/τ_0 vs. μ relationship. Note: The solid and dashed lines are results of Eqs. (82) and (83), respectively.

mechanism for increasing the lifetime of the soliton in biomacromolecules is to enhance the strength of the exciton-phonon interaction.

In Fig. 7, τ/τ_0 versus η is plotted. Since $-\eta$ designates the influence of thermal phonons on the soliton, it is also an important quantity. Thus, it is regarded here as an independent variable. The other parameters in Eq. (82) take the values in Eq. (37). From this figure, it can be seen that τ/τ_0 increases with the increase of η. Therefore, to enhance η can also increase the value of τ/τ_0.

In order to understand the behavior of the quasi-coherent soliton lifetime in very wide ranges, it is necessary to study τ/τ_0 in the limit $\omega_a t \to 0$ in Eq. (75) or Eqs. (C–1) and (C–3) (i.e., this is in the initial case) in which the values of $R_2(t)$ and $\xi_2(t)$ can be analytically evaluated. In fact, for $\omega_a t < 1$ both $R_2(t)$ and $\xi_2(t)$ have power-series expansions. To the lowest order as $\omega_a t \to 0$, it can be found from Eq. (75):

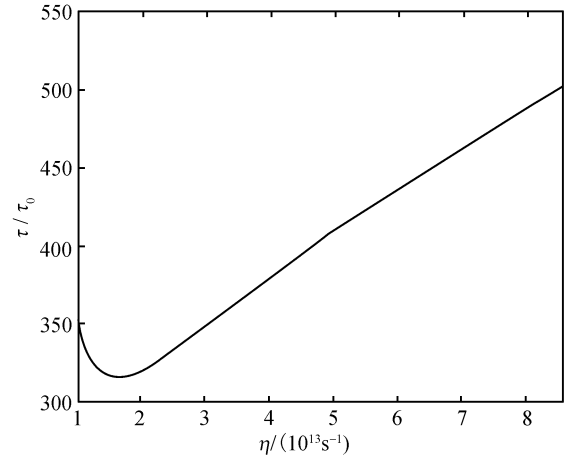

Fig. 7 τ/τ_0 vs. η relationship in Eq. (82).

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

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

using $\coth(\pi\omega_\alpha t) \approx (\pi\omega_\alpha t)^{-1} + \frac{\pi}{3}\omega_\alpha t$. Thus

$$\begin{aligned}
&\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t \\
&\cdot\exp\left\{-\mathrm{i}\left[2J(k'r_0)^2 + \frac{4J\mu_p^2}{3} - \hbar\omega_k\right]t/\hbar + R_2(t) + \xi_2(t)\right\} \\
&\approx \left[4\pi\cdot 3\zeta(3)R_0 k_B^2 T_0^2 + R_0\pi^2 k_B^2 T T_0/3)\right]^{-1/2} \\
&\cdot\exp\left\{-\frac{[2J(k'r_0)^2 + \frac{4}{3}\mu_p^2 J - \hbar\omega_k + \hbar(R_0\pi^2 k_B T)]^2}{4[3\zeta(3)R_0 k_B^2 T_0^2 + R_0\pi^2 k_B^2 T T_0/3]}\right\}
\end{aligned} \tag{87}$$

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 δ-function for energy conservation in the zero-temperature perturbation theory. Thus the decay rate of the soliton can be obtained from Eqs. (74) and (87) at $n = 2$ as

$$\begin{aligned}
\Gamma_2 = &\frac{2\pi^3}{\mu_p\hbar N^2 k_B}\left(\frac{\pi}{R_0 T_0[3\zeta(3)T_0 + \pi^2 T/3]}\right)^{-1/2} \\
&\cdot\sum_{kk'}\frac{(kr_0)^2 \mid g_1(k) + 2g_2(k)\mid^2}{\mu_p^2 + (k'r_0)^2}\sec h^2\left[\left(\frac{\pi r_0}{2\mu_p}\right)(k-k')\right] \\
&\cdot\exp\left\{\left[\frac{[2J(k'r_0)^2 + \frac{4}{3}\mu_p^2 J - \hbar\omega_k + \frac{1}{6}R_0\pi^2 k_B T_0]^2}{4[3\zeta(3)R_0 k_B^2 T_0^2 + R_0 k_B^2 T T_0\pi^2/3]}\right]\right. \\
&\left.\cdot\left[\exp(\beta\hbar\omega_k) - 1\right]\right\}^{-1}
\end{aligned} \tag{88}$$

The expression of the decay rate of the quasi-coherent soliton in this limit is different from Eq. (84). Therefore, studying the properties of the lifetime of the new soliton in such a case helps in understanding the behavior of the soliton. A summary of the results obtained from Eq. (88) is given in Figs. 8–11. The dependency of lifetime on temperature T is shown in Fig. 6, which has been obtained from the numerical evaluation of Eq. (88).

In Figs. 9 and 10, τ/τ_0 versus $(\chi_1+\chi_2)$ and versus μ are plotted respectively at $T = 300$ K. From Figs. 8–10, it can be seen that τ/τ_0 increases as T decreases and as μ and $(\chi_1+\chi_2)$ increase. Furthermore, it is clear from this the Gaussian expression in Eq. (88) that the lifetime of the new soliton will be large if μ and $(\chi_1+\chi_2)$ will be 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 de-

pendence of the lifetime of the new soliton is mainly due to the temperature dependence of the width of the Gaussian, which decreases with the decrease of temperature. The dashed line in Fig. 10 is the result for the Davydov soliton under the same conditions. It is clear that the lifetime of the Davydov soliton is shorter than that of the new soliton, especially at large μ, though at low μ the difference between them is small. Taking Fig. 4 also into account, it can be found that the lifetime of the Davydov soliton is indeed generally short. However this is not the case for the new soliton. In Fig. 11, τ/τ_0 is plotted as a function of T_0 at T = 300 K. T_0 is related to the Debye temperature of the systems; therefore, it is also an important quantity. It is regarded here as an independent variable which evaluates other parameters as in Eq. (21). From this figure, it can be seen that the lifetime of the new soliton is large if T_0 is either large or small, because the Gaussian expression in Eq. (88) is very small for k and k' between $-\pi/r_0$ and $+\pi/r_0$. As a point of reference, it is noted that these parameters have the values $T/T_0 \approx 1.03$ –1.06, $JT/(k_B T_0^2) = 4.10$ at 300 K and μ = 5.81–5.96 depending on whether the widely accepted or the "three-channel" parameter values for the protein are assumed. From these results, it is clear that using widely accepted, realistic parameter values, the new model can satisfy the relationship $\tau/\tau_0 \geqslant 500$ at 300 K and large μ and large T_0. Hence the proposed new soliton model provides a viable candidate for biological processes.

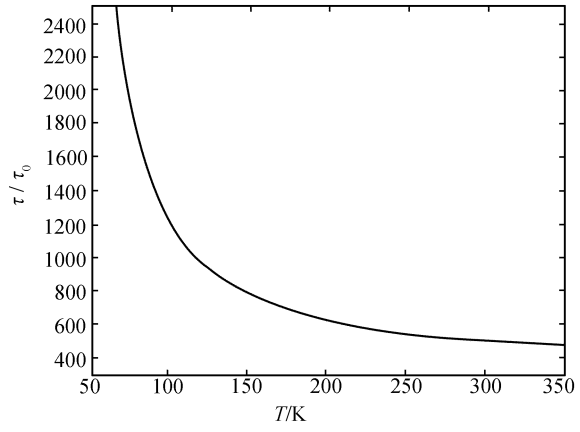

Fig. 8 τ/τ_0 vs. T relationship in the new model in Eq. (88).

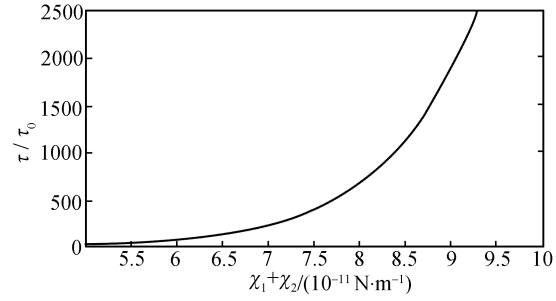

Fig. 9 τ/τ_0 vs. (χ_1+χ_2) relationships in the new model in Eq. (88).

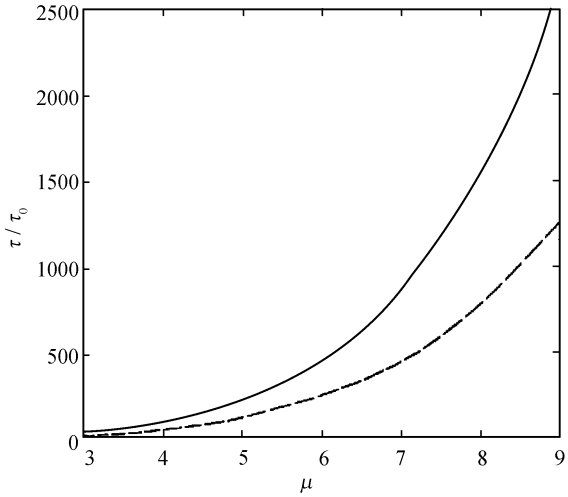

Fig. 10 τ/τ_0 vs. μ relationship in the new model in Eq. (88).

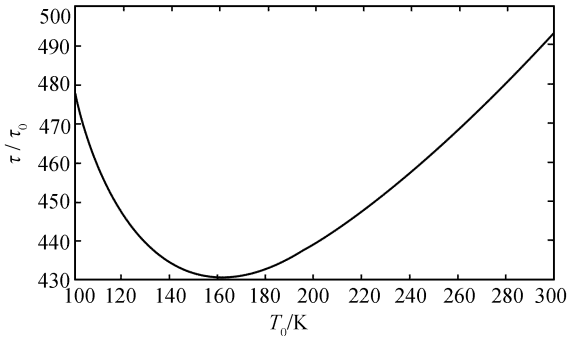

Fig. 11 τ/τ_0 vs. T_0 relationship. Note: Here the solid and dashed lines are the results in the new model in Eq. (62) and in Davydov's model, respectively.

6 Conclusion

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

Table 3 Comparison of features of the soliton between our model and Davydov's model

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

the properties of the soliton. In fact, the non linear interaction energy in the new model is $G_p = 8(\chi_1 + \chi_2)^2/(1 - S^2)w = 3.8 \times 10^{-21}$ J, and it is larger than the linear dispersion energy, $J = 1.55 \times 10^{-22}$ J, i.e., the non-linear interaction is so large that it can really cancel or suppress the linear dispersion effects in the equation of motion of this model. From this point, the soliton is stable according to the conditions of the formation and stability of the soliton in the soliton theory [27, 28]. By comparison, the non-linear interaction energy in Davydov's model is $G_D = 4\chi_1^2/(1–S^2)w \approx 1.18 \times 10^{-21}$ J and it is 3–4 times smaller than G_p. Thus the stability of the Davydov soliton is weak compared with that of the new soliton. Moreover, the binding energy of the quasi-coherent soliton in the new model is $E_{Bp} = 4\mu_p^2 J/3 = 7.8 \times 10^{-21}$ J in Eq. (19), which is about twice larger than the thermal energy, $K_B T = 4.14 \times 10^{-21}$ J, at 300 K, and about six times larger than the Debye energy, $k\Theta = \hbar\omega_D = 1.2\times10^{-21}$ J (here ω_D is Debye frequency), and it is approximately equal to $\varepsilon_0/4 = 8.2 \times 10^{-21}$ J, i.e., it has the same order of magnitude of the energy of the amide-I vibrational quantum, ε_0. This shows that the quasi-coherent soliton is robust due to the large energy gap between the solitonic ground state and the delocalized state. In contrast, the binding energy of the Davydov soliton is only $E_{BD} = \dfrac{\chi_1^4}{3w^2 J} = 0.188 \times 10^{-21}$ J which is about 23 times smaller than that of the new soliton, about 22 times smaller than $k_B T$ and about six times smaller than $k\Theta = \hbar\omega_D = 1.2\times10^{-21}$ J, respectively. Therefore, it is easily destroyed by thermal and quantum effects. Hence the Davydov soliton has very small lifetime (about 10^{-12}–10^{-13} s), and it is unstable at 300 K [50, 51]. In contrast, the quasi-coherent soliton can provide a realistic mechanism for bio-energy transport in protein molecules.

The two-quantum nature of the quasi-coherent soliton plays a more important role in the increase of lifetime than that of the added interaction because of the following facts. (1) The change of the nonlinear interaction energy $G_p = 2G_D\left[1 + 2\left(\dfrac{\chi_2}{\chi_1}\right) + \left(\dfrac{\chi_2}{\chi_1}\right)^2\right]$ by μ_p produced by the added interaction in the new model are $\Delta G = G_p(\chi_2 \neq 0) - G_p(\chi_2 = 0) = 1.08G_D < G_p(\chi_2 = 0) = 2G_D$ and $\Delta\mu = \mu_p(\chi_2 \neq 0) - \mu_p(\chi_2 = 0) = 1.08\,\mu_D < \mu_p(\chi_2 = 0) = 2\mu_D$, respectively, i.e., the roles of the added interaction on G_p and μ_p are smaller that of the two-quantum nature. The two parameters G_p and μ_p are responsible for the lifetime of the soliton. Thus the effect of the former on the lifetime is smaller than the latter. (2) The contribution of the added interaction to the binding energy of the soliton is about $E'_{BP} = E_{BD}\left[1 + \left(\dfrac{\chi_2}{\chi_1}\right)\right]^4 = 2.6E_{BD}$, which is smaller than that of the two-quantum nature which is $E''_{BD} = 16\,E_{BD}$. By putting them together in Eq. (35), it can be seen that $E_{BP} \approx 41E_{BD}$. (3) From the $(\chi_1 + \chi_2)$-dependence of τ/τ_0 in Fig. 5, $\tau/\tau_0 \approx 100$ has already been found directly at $\chi_2 = 0$ which is about 20 times larger than that of the Davydov soliton under the same conditions. This shows clearly that the major effect on the increase of lifetime is due to the modified wave function. Therefore, it is very reasonable to refer to the new soliton as the quasi-coherent soliton.

The above calculation helps to resolve the controversies on the lifetime of the Davydov soliton, which is too small in the region of biological temperature. However, by modifying the wave function and the Hamiltonian of the model, a stable soliton at biological temperature could be produced. This result was obtained considering a new coupled interaction between the acoustic and amide-I vibration modes and a wave function with a quasi-coherent two-quantum state. In such a way, the quasi-coherent soliton is a viable mechanism for bio-energy transport in living systems. Therefore, it can be seen that the improved model is completely different from Davydov's model. Thus, the equation of motion and the properties of the soliton occurring in the improved model are also different from that in Davydov's model. The distinction of the features of the soliton between the two models is shown in Table 3 [53]. From the Table 3, our new model repulse and refuse the shortcomings of Davydov's model [4–12], the new soliton in the improved model is thermally stable at biological temperature of 300 K, and has so sufficiently long lifetime; thus it plays important role in biological processes. It is supposed that this model could resolve the controversies on the thermal stability and lifetime of the soliton excited in protein molecules, and the new soliton is possibly an actual carrier of bio-energy transport in protein molecules in living systems.

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Appendix A

The partial diagonalization of the Hamiltonian implies the

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

$$2\left[-Jr_0^2\frac{\partial^2}{\partial x^2}+\mathrm{i}\hbar v\frac{\partial}{\partial x}+\varepsilon_0-2J+V(x)\right]C_j(x)=E_jC_j(x) \tag{A–1}$$

For the above expression of $V(x)$ in Eq. (52) there is only one bound state in Eq. (A–1),

$$C_\mathrm{s}(x)=\left(\frac{\mu_p}{2r_0}\right)^{1/2}\operatorname{sech}(\mu_p x/r_0)\exp[\mathrm{i}\hbar vx/(2Jr_0^2)] \tag{A–2}$$

with energy

$$E_\mathrm{s}=2\left(\varepsilon_0-2J-\frac{\hbar^2v^2}{4Jr_0^2}-J\mu_p^2\right) \tag{A–3}$$

and unbounded (delocalized) states

$$C_k(x)=\frac{\mu_p\tanh(\mu_p x/r_0)-\mathrm{i}kr_0}{\sqrt{Nr_0}(\mu_p-\mathrm{i}kr_0)}\exp[\mathrm{i}kx+\mathrm{i}\hbar vx/(2Jr_0^2)] \tag{A–4}$$

with energy

$$E_k=2\left(\varepsilon_0-2J-\frac{\hbar^2v^2}{2Jr_0^2}+J(kr_0)^2\right) \tag{A–5}$$

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

$$\int_{-\infty}^{\infty}\mathrm{d}xC_k^*(x)C_{k'}(x)=\delta(kr_0-k'r_0)$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\,|\,C_k(x)\,|^2=1,\quad\int_{-\infty}^{\infty}\mathrm{d}xC_s^*(x)C_k(x)=0$$

Therefore, A_s^+ is an excitation which is localized at the lattice distortion, while A_k^+ creates an unbounded excitation with wave vector k.

In getting Eq. (A–1) the variable x was assumed to be continuous and the chain length to tend to infinity $L=Nr_0\to\infty$. Thus this wave vector k has a continuous value between $-\infty$ and ∞. In the following, a discrete description is mainly used. The continuous description is transformed into a discrete one according to the rules

$$\int_{-\infty}^{\infty}\mathrm{d}x/r_0\to\sum_n,\quad\int_{-\infty}^{\infty}\mathrm{d}x\to\frac{2\pi}{Nr_0}\sum_k$$

$$\delta(kr_0-k'r_0)\to\frac{N}{2\pi}\delta_{kk'}$$

$$C_\mathrm{s}(x)\to C_s(n),\quad C_k(x)\to\left(\frac{N}{2\pi}\right)^{1/2}C_k(n)$$

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

Appendix B

Now $U(k, k'', t)$ in Eq. (72) is calculated utilizing the coherent state $|u\rangle$ [14, 30] defined by $b_q|u\rangle=u_q|u\rangle$ with

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

$$|u\rangle=\exp\left[\sum_q(u_qb_q^+-u_q^*b_q)\right]$$

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

$$\begin{aligned}U(k,k'',t)=\frac{1}{Z_{ph}}\int\mathrm{d}\Omega(u)\int\mathrm{d}\Omega(u'')(u_k''^*+u_{-k}'')(u_{-k''}^*+u_{-k''})\langle u|\\ \exp\left\{\sum_q(\omega_q-qv)(-\beta\hbar+\mathrm{i}t)b_q^+b_q\right\}|u''\rangle\\ \cdot\langle u''|\exp\left\{-\mathrm{i}\sum_q(\omega_q-qv)\left[(b_q^+b_q\right.\right.\\ \left.\left.+\frac{1}{n\sqrt{N}}(b_q^+\alpha_q+\alpha_q^*b_q)+\frac{1}{n^2}\frac{1}{N}|\alpha_q|^2\right]t\right\}|u\rangle\end{aligned} \tag{B–1}$$

where the integration measure is defined as

$$\mathrm{d}\Omega(u)=\prod_k\frac{1}{\pi}\mathrm{d}x_k\mathrm{d}y_k,\ \text{with}\ x_k+\mathrm{i}y_k=u_k$$

Since it can be shown that $\exp(\tau b_k^+b_k)|u_k\rangle=\exp\left\{\frac{1}{2}|u_k|^2(\mathrm{e}^{\tau+\tau^*}-1)\right\}|\mathrm{e}^\tau u_k\rangle$, it follows that the first matrix element in Eq. (B–1) equals

$$\langle u_k|\exp[\sum_q(\omega_q-qv)(-\beta\hbar+\mathrm{i}t)b_q^+b_q]|u_k''\rangle$$

$$=\exp\left\{-\sum_k\left(\frac{1}{2}|u_k|^2+\frac{1}{2}|u_k''|^2-u_k^*u_k''\exp[(\omega_q-qv)(-\beta\hbar+\mathrm{i}t)]\right)\right\}$$

The second matrix element in Eq. (B–1) can be represented as a path integral that can be evaluated exactly. Utilizing the general relationship between the matrix element and the path integral

$$\langle u_k''|\exp[-\mathrm{i}\omega(b_k^+b_k+\tau^*b_k+b_k^+\tau+\tau^*\tau]|u_k\rangle$$

$$=\exp\left[-\frac{1}{2}(|u_k''|^2+|u_k|^2)-\mathrm{i}\omega|\tau|^2t\right]$$

$$\cdot\int_{y^*(t)=u''^*}^{y(0)=u_q} D(y^*,y)\exp[\mathrm{i}T(y^*,y)] \tag{B–2}$$

where $T(y^*,y)=\int_0^t \mathrm{d}t'\left\{\mathrm{i}y^*(t')\frac{\mathrm{d}y}{\mathrm{d}t'}-\omega[y^*(t)y(t')+\tau^* y(t')+y^*(t')\tau]\right\}-\mathrm{i}u''_{k'}{}^* y(t).$

The path integral can be evaluated by standard techniques. The result for Eq. (B–2) is

$$\exp\left[-\frac{1}{2}(|u''_k|^2+|u_k|^2+u''_k{}^* u_k \mathrm{e}^{-\mathrm{i}\omega t} -(1-\mathrm{e}^{-\mathrm{i}\omega t})(u''_t{}^*\tau+\tau^* u_k+|\tau|^2)\right] \tag{B–3}$$

Substituting above the matrix elements obtained into Eq. (B–1) the following can be obtained:

$$\begin{aligned}U(k,k'',t)=&\frac{\mathrm{e}^{R_n(t)}}{Z_{ph}}\int \mathrm{d}\Omega(u)\int \mathrm{d}\Omega(u'')(u''_k{}^*+u''_{-k})(u_{-k''}{}^*+u_{k''})\\ &\cdot\exp\left\{-\sum_q(|u_q|^2+|u''_q|^2-u^*_q u''_q\right.\\ &\cdot\exp[(\omega_q-qv)(-\beta\hbar+\mathrm{i}t)]-u''_q{}^* u_q\\ &\cdot\exp[-\mathrm{i}(\omega_q-qv)t]+\frac{1}{n}\\ &\left.\cdot\frac{1}{\sqrt{N}}(u''_q\alpha_q+u^*_q\alpha^*_q)(1-\exp[\mathrm{i}(\omega_q-qv)t])\right\}\end{aligned} \tag{B–4}$$

where

$$R_n(t)=\frac{-1}{n^2N}\sum_k|\alpha_k|^2\{1-\exp[-\mathrm{i}(\omega_k-kv)t]\} \tag{B–5}$$

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

$$\begin{aligned}U_a(k,k'',t)=&\frac{\exp[\mathrm{i}(\omega_k-kv)t+R_n(t)+\xi_n(t)]}{\exp[\beta\hbar(\omega_k-vk)]-1}\\ &\cdot\left\{\delta_{kk''}-\left(\frac{1}{n^2}\frac{1}{N}\alpha^*_k\alpha_{k''}(\exp[\mathrm{i}(\omega_{k''}-k''v)t]-1\right)\right.\\ &\left.\cdot(\exp[-\mathrm{i}(\omega_k-kv)t]-1))/\exp[\beta\hbar(\omega_k-vk)]-1\right\}\end{aligned} \tag{B–6}$$

where

$$\xi_n(t)=\frac{-4}{n^2N}\sum_k\frac{|\alpha_k|^2\sin^2\left[\frac{1}{2}(\omega_k-vk)t\right]}{\exp[\beta\hbar(\omega_k-vk)]-1} \tag{B–7}$$

It is noted that the breaking of the translational symmetry by the deformation leads to off-diagonal terms corresponding to violation of wave vector conservation. However, it can be proved that these terms are proportional to $\frac{1}{N}\alpha^*_k\alpha_{k''}$ which can be neglected when either $|k|$ or $|k''|$ is large as compared with $4\mu_p/(\pi r_0)$ as can be seen in the definition of α_k in Eq. (59). Furthermore, when $-\pi \leqslant kr_0 \leqslant \pi$ and $\mu_p < \pi^2$ the off-diagonal terms are negligible except for a small region at the center of the Brillouin zone. Since the small wave vector terms do not significantly contribute to Γ_n due to the k-dependence of $\tilde{F}(q, k)$, and thus the off-diagonal terms can be neglected in $U_a(k,k'',t)$ in the calculation of Γ_n. The energy of the soliton state is less than that of unlocalized exciton in the uniform lattice. Therefore, the parts of $U_a(k,k'',t)$ corresponding to the absorption of a phonon make the major contributions to the sum in Eq. (72) at the temperature and the parameter values of interest, and their off-diagonal terms may also be neglected just as above. Using the result of the $U_a(k,k'',t)$ obtained from the above formulae of Eq. (72) the decay rate Eq. (74) can be obtained.

Appendix C

If the soliton velocity approaches zero, an analytical expression can be obtained for $R_2(t)$ and $\xi_2(t)$ at $n = 2$ defined in Eq. (75) or Eqs. (B–5) and (B–7) through inserting Eq. (59) into Eqs. (C–5) and (C–7) and applying the relationship of $\frac{1}{N}\sum_q \to \frac{r_0}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}q$, i.e.,

$$\begin{aligned}\lim_{v\to 0}R_2(t)=&-R_0\int_{-\infty}^{\infty}\frac{y}{\mathrm{sh}^2 y}\{[1-\cos(\omega_\alpha t y)]\\ &+\mathrm{i}\sin(\omega_\alpha t y)\}\mathrm{d}y\quad\left(\text{here}\quad y=\frac{\pi q r_0}{2\mu_p}\right)\\ =&-R_0[\mathrm{i}x'\psi'(1+\mathrm{i}x')+\psi(1+\mathrm{i}x')-\psi(1)]\end{aligned} \tag{C–1}$$

where

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

ψ is the digamma function, ψ' is its derivative and $x'=\omega_\alpha t = k_B T_0 t/\hbar$. $\xi_2(t)$ can be easily evaluated when $v\approx 0$ and $R_0 < 1$ at sufficiently high temperature $T > T_0 (T_0=\hbar\omega_\alpha/K_B)$:

$$\begin{aligned}\xi_2(t)=&\frac{-R_0}{\omega_\alpha}\frac{T}{T_0}\int_0^\infty \mathrm{d}\omega_k\frac{\sin^2\left(\frac{1}{2}\omega_k t\right)}{\mathrm{sh}^2(\omega_k/\omega_\alpha)}\\ =&\frac{R_0 T}{T_0}[1-\pi\omega_\alpha t\coth(\pi\omega_\alpha t)]\end{aligned} \tag{C–3}$$

where we use the relationship $\exp(\beta\hbar\omega_k) \approx 1 + \beta\hbar\omega_k$.

As $t \to \infty$ (because attention is paid to the long-time steady behavior) the leading terms in the above asymptotic formulae of $R_2(t)$ and $\xi_2(t)$ are

$$R_2(t) = -R_0\left[\ln\left(\frac{1}{2}\omega_\alpha t\right) + 1.578 + \frac{1}{2}\mathrm{i}\pi\right] \tag{C–4}$$

$$\xi_2(t) \approx -\pi R_0 k_\mathrm{B} T t/\hbar \tag{C–5}$$

where $\coth\ \frac{1}{2}\omega_\alpha t \sim 1$ is approximated, i.e.,

$$\lim_{t\to\infty} \xi_2(t) = -\eta t\ ,\quad \eta = \pi R_0/(\beta\hbar) = \pi R_0 k_\mathrm{B} T/\hbar \tag{C–6}$$

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

$$\begin{aligned}
&\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t \exp\left\{-\mathrm{i}[2J(k'r_0)^2 + \frac{4}{3}J\mu_p^2 - \hbar\omega_k]t/\hbar \right.\\
&\left. + R(t) + \xi(t)\right\}\\
&\approx \frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\{\eta^2 + [\delta(k,k')/\hbar]^2\}^{-(1-R_0)/2}\\
&\cdot\left\{\cos\left(\frac{\pi R_0}{2}\right)\cdot\cos\left[(1-R_0)\arctan\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]\right.\\
&\left. -\sin\frac{\pi R_0}{2}\sin\left[(1-R_0)\arctan\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]\right\}\\
&= \frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\left\{\eta^2 + [\delta(k,k')/\hbar]^2\right\}^{-(1-R_0)/2}\\
&\cdot\cos(\Phi_1 + \Phi_2)\\
&\approx \frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\left\{\eta^2 + [\delta(k,k')/\hbar]^2\right\}^{-(1-R_0)/2}\\
&\cdot\left\{1 - \frac{1}{2}\left[\frac{\pi R_0}{2} + (1-R_0)\frac{\delta(k,k')}{\eta\hbar}\right]^2\right\}
\end{aligned} \tag{C–7}$$

where

$$\delta(k,k') = 2J(k'r_0)^2 + \frac{4}{3}\mu_p^2 J - \hbar\omega_k,\quad \Phi_1 = \frac{R_0\pi}{2} \tag{C–8}$$

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