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The lifetime of the soliton in the improved Davydov model at the biological temperature 300 K for protein molecules

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Abstract. We study the effects of quantum fluctuations and thermal perturbations on the lifetime of the soliton in the improved Davydov model proposed by us with two-quanta and with an added interaction. By using quantum perturbation theory, we compute the soliton lifetime for a wide ranges of parameter values relevant for protein molecules. The lifetime of the new soliton at the biological temperature 300 K is of the order of 10^{-10} second or $\tau/\tau_0 \geq 500$ for parameters appropriate to α-helical protein molecules. This shows clearly that the new soliton in the improved model is a viable mechanism for the bio-energy transport in the α-helix region of proteins.

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1 Physical and biological background

A lot of biological processes are associated with energy transport through protein molecules, where the bio-energy is released by hydrolysis of adenosine triphosphate (ATP). The transport is a fundamental problem in biology, but the mechanism is an open problem which continues to be of great interest. As an alternative to electronic mechanisms [1], one can assume that the energy is stored as vibrational energy in the C=O stretching mode (amide-I) of a polypeptidic chain. Following Davydov [2], one can take into account the coupling between the amide-I vibrational quantum exciton and the acoustic phonon (molecular displacements) in the lattice. This non linear interaction leads to a self-trapped state of the vibrational quanta. The latter together with the deformational lattice can move over a macroscopic distance along the molecular chain retaining wave shape, energy, momentum and other quasiparticle properties. In this way the bio-energy can be transported as a localized "wave packet" in solitary waves. This is the Davydov model for the bio-energy transport, which was first proposed in the 1970s [2]. The Hamiltonian describing such system has the form

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

where $\varepsilon_0 = 0.205$ eV is the amide-I quantum energy, $-J$ is the dipole-dipole interaction energy between neighbouring sites, $B_n^+(B_n)$ is the creation (annihilation) operator for an amide-I quantum excitation (exciton) in the site n, u_n is the displacement operator of 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 an nonlinear coupling parameter related to the interaction of the exciton-phonon. The wave function proposed by Davydov is

$$|D_2(t)\rangle = |\varphi_{\mathrm{D}}(t)\rangle 1\beta(t)\rangle = \sum_n \varphi_n(t)B_n^+ \exp\left(-\frac{\mathrm{i}}{\hbar}\sum_n [\beta_n(t)P_n - \pi_n(t)u_n]\right)|0\rangle \tag{2}$$

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or

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

where $|0\rangle = |0\rangle_{\rm ex}|0\rangle_{\rm ph}, |0\rangle_{\rm ex}$ and $|0\rangle_{\rm ph}$ are the ground states of the exciton and phonon, respectively, $a_q(a_q^+)$ is annihilation (creation) operator of the phonon with ware vector q, $\varphi_n(t)$ 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, $|\varphi_{\rm D}(t)\rangle = \sum_n \varphi_n(t) B_n^+ |0\rangle_{\rm ex}$ in equation (2) is an eigenstate of the number operator, $\hat{N} = \sum_n B_n^+ B_n$, corresponding to a single excitation, *i.e.*, $\hat{N}|\varphi_{\rm D}(t)\rangle = |\varphi_{\rm D}(t)\rangle$.

The Davydov soliton obtained from equations (1) and (2) in the semiclassical limit and using the continuum approximation has the from

$$\varphi_{\rm D}(x,t) = \left(\frac{\mu_{\rm D}}{2}\right)^{1/2} {\rm sech}\left[\frac{\mu_{\rm D}}{r_0}(x - x_0 - vt)\right] \times \exp\left\{ {\rm i} \left[\frac{\hbar v}{2 J r_0^2}(x - x_0) - E_v t/\hbar \right] \right\} \quad (3)$$

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

$$E_{\rm BD} = \frac{-\chi_1^4}{3Jw^2} \cdot \quad (4)$$

The above idea about the soliton mechanism of bioenergy transport in protein molecules has been subject of a large body of work [3–23]. A lot of issues related to the Davydov model, including the foundation and accuracy of the theory, the quantum and classical properties and the thermal stability and lifetimes of the Davydov soliton have extensively been studied by many scientists [3–23]. 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 the quantum fluctuations and thermal perturbations are expected to cause the Davydov soliton to decay into a delocalized state. Some numerical simulations indicated that the Davydov soliton is not stable at the biological temperature 300 K [12–14,23]. Other simulations showed that the Davydov soliton is stable at 300 K [7–10], but they were based on classical equations of motion which are likely to yield unreliable estimates for the stability of the soliton [3]. The simulations based on the $|D_2\rangle$ state generally show that the stability of the soliton decreases with increasing temperatures and that the soliton is not sufficiently stable in the region of biological temperature. Since the dynamical equations used in the simulations are not equivalent to the Schrödinger equation, the stability of the soliton obtained by these numerical simulations is not reliable. The simulation [9] based on the $|D_1\rangle$ state with the thermal treatment of Davydov [8] yields the wondering result that the stability of the soliton increases with increasing temperature, predicting that $|D_1\rangle$-type soliton is stable in the region of biological temperature. Evidently, the conclusion is doubtful because the Davydov procedure does not use a density matrix which is the correct method. Therefore, there exists no exact quantum mechanical treatment for the numerical simulation of the Davydov soliton. However, for the thermal equilibrium of the Davydov soliton one can use quantum Monte Carlo simulation [13]. In the simulation, correlations characteristic of solitonlike quasiparticles occur only at low temperature about $T < 10$ K for the widely accepted parameter values. This is consistent at a qualitative level with the Cottingham *et al.*'s result [14], arising from a quantum-mechanical perturbation calculation. The lifetime of the Davydov soliton computed by using this method is too small (about 10^{-12}–10^{-13}s) to be useful in biological processes. This shows clearly that the Davydov solution is not a true wave function of the system. However, a thorough study in terms of parameter values, different types of disorder, different thermalization schemes, different wave functions and different associated dynamics leads to a very complicated picture for the Davydov model [10–12]. The results do not completely rule out the Davydov theory. Indeed it is possible that using another wave function and a more sophisticated Hamiltonian we can find a soliton with good thermal stability and a suitably long lifetime. As a matter of fact, Takeno's [22] and Pang's [23] studies show that considering different couplings between the relevant modes in the vibronic Hamiltonian can enhance the binding energy and stability of the soliton. On the other hand, some scientists thought that the soliton with multiquanta state ($n \geq 2$), *e.g.*, Brown *et al.*'s coherent state [4], Kerr *et al.*'s [12] and Schweitzer *et al.*' s [14] multiquanta state, Cruzeiro-Hansson's [10] and Förner's [21] two-quanta state, would be thermally stable in the region of biological temperature, and could provide a realistic mechanism for the bioenergy transport in protein molecules. However, the standard coherent state is unsuitable for the biological protein molecules because the number of particles in this state is innumerable, violating the conservation of the number of particles of the systems. The assumption of a multiquanta state ($n > 2$) is also at odds with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) can only excite two quanta of amide-I vibration. The numerical study of a two-quanta model by Förner [21] reveals remarkable differences from one-quantum dynamics, *i.e.*, the soliton with two-quanta is more stable than that with one-quantum. Cruzeiro-Hansson reconstructed a two-quanta state of the semiclassical Davydov system, and also showed that the resulting soliton is thermally more stable than the one-quantum state [10]. However,

we proved [24] that the Hansson's ansatz contains exactly four quanta, instead of two quanta, which is impossible because the energy released in ATP hydrolysis can only excite two quanta. Therefore, Hansson's improvement is still not successful and the exact wave function of the model remains unknown.

On the basis of the work of Cruzeio-Hansson, Förner, Schweitzer and Takeno and Pang, we have improved both the Hamiltonian and the wave function of the model [24]. A new coupling interaction between the acoustic and amide-I vibrational modes was added to the original Davydov's Hamiltonian which takes into account relative displacement of the neighbouring peptide groups resulting from dipole-dipole interaction of the neighbouring amide-1 vibrational quanta. We also replaced the Davydov's wave function with a quasi-coherent two-quanta state for exhibiting the coherent behaviors of collective excitations [25,26] which are a feature of the energy released in ATP hydrolysis in the systems. The equation of motion and the properties of the new soliton in the new model are different from that in the Davydov model and as a result the soliton lifetime and stability are greatly enhanced. We suggest that this model can resolve the controversy on the thermal stability and lifetime of the soliton excited in the protein molecules. In the previous paper we studied only the quantum properties of the new soliton [24], but here we are more interested in the problem of its lifetime and thermal stability at biological temperature 300 K. In the present paper we shall calculate in detail the lifetime of the new soliton at 300 K by using the generally accepted values of the parameters appropriate to the α-helical protein molecules in terms of the quantum perturbation theory developed by Cottingham *et al.* [14], which can take simultaneously into account the quantum and thermal effects. We will see that the lifetime of the new soliton at 300 K is long enough to provide a viable explanation of the bio-energy transport in the proteins. The plan of this paper is as follows. In Section 2 and Section 3 we shall describe the new model, the properties of the new soliton and the partially diagonalized form of the model-Hamiltonian. In Section 4 we shall compute the transition probability from soliton state to the delocalized state and the lifetime of the new soliton by using quantum-mechanical perturbation methods. The detailed discussion of the properties and changes of the lifetimes of the soliton for a large range of parameter values is presented in Section 5. The conclusions of this investigation are also given in this section.

2 New model and the properties of the new soliton

The question of the lifetime of the soliton in the protein molecules is twofold. In the Langevin dynamics unpredictable effects arise from the semiclassical approximation. In the quantum treatment there is the problem that an exact wave function is lacking. In the Davydov model in equations (1–4), both the wave function and the Hamiltonian of the systems, is too simple. A first problem of the model concerns the Davydov wave functions, both $|D_1\rangle$ and $|D_2\rangle$. These are asymmetric since the phononic part is a coherent state, while, the excitonic part is an excitation state of a single-particle. It is not reasonable that the nonlinear interaction generated by the coupling between the excitons and phonons produces different states for the phonon and the exciton. Thus, the Davydov's wavefunction should be modified [23], *i.e.*, the excitonic part in it should also be coherent or quasi-coherent [25,26]. However, the standard coherent state [4] and large – n excitation state are not appropriate to the protein molecules due to the reasons mentioned above. Similarly, Förner's and Cruzeiro-Hansson's two-quanta states do not fulfill the above criteria.

In view of the above discussion, we propose the following wave function for the system [24]

$$|\Phi(t)\rangle = |\varphi(t)\rangle|\beta(t)\rangle = U_1|0\rangle_{\rm ex}U_2|0\rangle_{\rm ph}, \tag{5}$$

where

$$U_1 = \frac{1}{\lambda}\left[1 + \sum_n \varphi_n(t)B_n^+ + \frac{1}{2!}\left(\sum_n \varphi_n(t)B_n^+\right)^2\right], \tag{5a}$$

$$U_2 = \exp\left\{-\frac{\mathrm{i}}{\hbar}\sum_n [\beta_n(t)P_n - \pi_n(t)u_n]\right\} \tag{5b}$$

$$= \exp\left\{\frac{1}{\sqrt{N}}\sum_q \alpha_q(t)a_q^+ - \alpha_q^*(t)a_q\right\} \tag{5c}$$

where $a_q(a_q^+)$ is annihilation (creation) operator of the phonon with wavevector q in the lattice, the meaning of $B_n(B_n^+)$ is the same as that in equation (1). The $\varphi_n(t)$, $\alpha_q(t) = \langle\Phi|a_q|\Phi\rangle$ and $\beta_n(t) = \langle\Phi|u_n|\Phi\rangle$ and $\pi_n(t) = \langle\Phi|P_n|\Phi\rangle$ are four sets of unknown functions, λ is a normalization constant, we assume in follows that $\lambda = 1$ for convenience of calculation, except when explicitly mentioned. N is total number of the amino acids in the protein molecular chain.

The present wave function of the exciton in equation (5a) is not an excitation state of single-particle, but a coherent state, accurately speaking, a quasi-coherent state. To see this point we can represent it by

$$\begin{aligned}|\varphi(t)\rangle &= \frac{1}{\lambda}\left[1 + \sum_n \varphi_n(t)B_n^+ + \frac{1}{2!}\left(\sum_n \varphi_n(t)B_n^+\right)^2\right]|0\rangle_{\rm ex} \\ &\sim \frac{1}{\lambda}\exp\left\{\sum_n \varphi_n(t)B_n^+\right\}|0\rangle_{\rm ex} \\ &= \frac{1}{\lambda}\exp\left\{\sum_n [\varphi_n(t)B_n^+ - \varphi_n^*B_n]\right\}|0\rangle_{\rm ex}. \end{aligned} \tag{6}$$

The last representation in equation (6) is a standard coherent state. However, the new wave function retains only three terms of a standard coherent state, which mathematically is justified for the case of small $\varphi_n(t)$ (*i.e.*, $|\varphi_n(t)| \ll 1$). Therefore we call $|\varphi(t)\rangle$ a quasi-coherent

state. Obviously, it is not an eigenstate of the number operator $\hat{N} = \sum_n B_n^+ B_n$, since

$$\hat{N}|\varphi(t)\rangle = \sum_n B_n^+ B_n |\varphi(t)\rangle = 2|\varphi(t)\rangle - \left(2 + \sum_n \varphi_n(t) B_n^+\right)|0\rangle_{\rm ex}\cdot \quad (7)$$

Therefore, the $|\varphi(t)\rangle$ represents a superposition of multiquanta states. More precisely, it is a coherent superposition of the excitonic state with two quanta and the ground state of exciton. The average number of excitons for this state is

$$N = \langle\varphi(t)|\hat{N}|\varphi(t)\rangle = \left[\sum_n |\varphi_n|^2 + \left(\sum_n |\varphi_n|^2\right)\left(\sum_m |\varphi_m|^2\right)\right] = \left(\sum_n |\varphi_n|^2\right)\left(1 + \sum_m |\varphi_m|^2\right) = 2 \quad (8)$$

where we utilize the relations [24]

$$\begin{aligned} {}_{\rm ex}\langle 0|B_n^+|0\rangle_{\rm ex} &= {}_{\rm ex}\langle 0|B_n^+ B_n|0\rangle_{\rm ex} = {}_{\rm ex}\langle 0|B_n^+ B_m|0\rangle_{\rm ex} \\ &= {}_{\rm ex}\langle 0|B_n^+ B_m B_l|0\rangle_{\rm ex} = {}_{\rm ex}\langle 0|B_n^+ B_m B_l^+ B_n|0\rangle_{\rm ex} \\ &= {}_{\rm ex}\langle 0|B_n^+ B_m B_i^+ B_l B_j|0\rangle_{\rm ex} \\ &= {}_{\rm ex}\langle 0|B_n^+ B_m B_l^+ B_i B_j B_n|0\rangle_{\rm ex} .... = 0 \end{aligned} \quad (9)$$

$$\sum_n |\varphi_n|^2 = 1, \quad \sum_m |\varphi_m|^2 = 1. \quad (10)$$

Next, another problem arises for the Davydov's Hamiltonian [24]. The Davydov Hamiltonian takes into account the resonant dipole-dipole interaction of the neighbouring amide-I vibrational quanta in neighbouring peptide groups, but fails to consider the changes of relative displacement of the neighbouring peptide groups arising from this interaction. Hence it is very reasonable to add the new interaction term, $\chi_2 \sum_n (u_{n+1} - u_n)(B_{n+1}^+ B_n + B_m^+ B_{n+1})$, to the Davydov's Hamiltonian for representing correlations of the collective excitations and collective motions in the protein molecules as mentioned above [22,23]. Although the dipole-dipole interaction is small as compared with the energy of the amide-I vibrational quantum, the resulting change of relative displacement of neighbouring peptide groups resulting from this interaction cannot be ignored. This is due to the sensitive dependence of the dipole-dipole interaction with the distance (separation) in protein molecules. The electromagnetic interaction between the neighbouring peptide groups that can allow the peptide groups to change positions with relative ease. This is a feature of soft condensed matter and bio-self- organization. Thus, we replace the Davydov's Hamiltonian, equation (1), by [24]

$$\begin{aligned} H &= H_{\rm ex} + H_{\rm ph} + H_{\rm int} \\ &= \sum_n \left[\varepsilon_0 B_n^+ B_n - J\ (B_n^+ B_{n+1} + B_n B_{n+1}^+)\right] \\ &\quad + \sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2} w (u_n - u_{n-1})^2\right] \\ &\quad + \sum_n \left[\chi_1 (u_{n+1} - u_{n-1}) B_n^+ B_n + \chi_2 (u_{n+1} - u_n) \right. \\ &\quad \left. \times (B_{n+1}^+ B_n + B_n^+ B_{n+1})\right]. \end{aligned} \quad (11)$$

The linear coupling constants are χ_1 and χ_2, and the new coupling constant χ_2 arises from the modulation of resonant dipole-dipole interaction energy of the excitons by the molecular displacements, *i.e.*, χ_2 represents the change of the resonant dipole-dipole interaction resulting from unit extension of the molecular chain. The meanings of other physical quantities in equation (11) was explained in equations (1, 2).

Quite evidently, both the Hamiltonian and wave function of the system shown in equations (5) and (11) are different from the Davydov's model in equations (1, 2). For the Hamiltonian we add the new interaction term, $\sum_n \chi_2 (u_{n+1} - u_n) \times (B_{n+1}^+ B_n + B_n^+ B_{n+1})$, into the originally Davydov's Hamiltonian, equation (1). Thus the Hamiltonian, now, has better symmetry for the interactions, and can also represent the features of mutual correlations of the collective excitations and collective motions in the protein molecules. The new wave function is a quasi-coherent state. The new state contains only two excitons, which come from the second and third terms in equation (5a). Each term contributes only one quantum, but it is not an excitation state of two particles. Hence, as far as the form and meanings of the new wave function are concerned, it is not either Förner's [11] and Cruzeiro-Hansson's [10] two-quanta states and Kerr *et al.*'s [12] multiquanta state, or Brown *et al.*'s [4] standard coherent state and Schweitzer, *et al.*'s multiquanta state defined by relation $\sum_i |\varphi_i|^2 = n$. The wave function, equation (5), does not only exhibit coherent properties, but also 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 multiquanta ($n > 2$). Therefore, the Hamiltonian and wave function of the systems, equations (5, 6), are reasonable and appropriate to the protein molecules.

Using the standard transformation:

$$\begin{aligned} u &= \sum_q \left[\frac{\hbar}{2NM\omega_q}\right]^{1/2} {\rm e}^{{\rm i}qnr_0}(a_{-q}^+ + a_q), \\ P_n &= {\rm i}\sum_q \left[\frac{M\hbar\omega_q}{2N}\right]^{1/2} {\rm e}^{{\rm i}qnr_0}(a_{-q}^+ - a_q) \end{aligned} \quad (12)$$

where $\omega_q = 2(w/M)^{1/2}\sin(r_0 q/2)$, equation (1) becomes

$$H = \sum_n \left[\varepsilon_0 B_n^+ B_n - J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)\right] + \sum_q \hbar\omega_q \left(a_q^+ a_q + \frac{1}{2}\right) + \frac{1}{\sqrt{N}}\sum_{qn}[g_1(q)B_n^+ B_n + g_2(q)(B_n^+ B_{n+1} + B_n^+ B_{n+1})](a_q + a_{-q}^+)\mathrm{e}^{\mathrm{i}nr_0 q} \quad (13)$$

where

$$g_1(q) = 2\chi_1 \mathrm{i}\left[\frac{\hbar}{2M\omega_q}\right]^{1/2}\sin r_0 q;$$
$$g_2(q) = \chi_2\left[\frac{\hbar}{2M\omega_q}\right]^{1/2}(\mathrm{e}^{\mathrm{i}r_0 q} - 1). \quad (14)$$

In a semiclassical and continuum approximations, from equation (13) we can obtain the envelope soliton solution in the new model, the calculation of which is described in Appendix A. The soliton is of the form [2,27,28]

$$\varphi(x,t) = \left(\frac{\mu_\mathrm{p}}{2}\right)^{1/2}\mathrm{sech}\left[\frac{\mu_\mathrm{p}}{r_0}(x - vt)\right] \times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{\hbar^2 vx}{2Jr_0^2} - E_\mathrm{sol}t\right)\right] \quad (15)$$

where

$$\mu_\mathrm{p} = \frac{2(\chi_1 + \chi_2)^2}{w(1-s^2)J}. \quad (16)$$

The energy of the new soliton is

$$E_\mathrm{S01} = 2\left[(\varepsilon_0 - 2J) + \frac{\hbar^2 v^2}{4Jr_0^2} - \frac{2\mu_\mathrm{p}^2}{3}J\right]. \quad (17)$$

Thus we can also find out that

$$\alpha_q(t) = \frac{\mathrm{i}\pi(\chi_1 + \chi_2)}{w\mu_\mathrm{p}(1 - v^2/v_0^2)}\left[\frac{M}{2\hbar\omega_q}\right]^{1/2} \times (\omega_q + qv)\mathrm{csch}(\pi q r_0/2\mu_\mathrm{p})\mathrm{e}^{\mathrm{i}qvt} = \alpha_q \mathrm{e}^{\mathrm{i}qvt}. \quad (18)$$

This treatment yields a localized coherent structure with size of order $2\pi r_0/\mu_\mathrm{p}$ that propagates with velocity v and can transfer energy $E_\mathrm{S01} < 2\epsilon_0$. Unlike bare excitons that are scattered by the interactions with the phonons, this soliton state describes a quasi-particle consisting of the two excitons plus a lattice deformation and hence a priori includes interaction with the acoustic phonons. So the soliton is not scattered and spread by this interaction, and can maintain its form, energy, momentum and other quasi-particle properties moving over a macroscopic distance. The bell-shaped form of the soliton (15) does not depend on the excitation method. It is self-consistent. Since the soliton always move with velocity less than that of longitudinal sound in the chain they do not emit phonons, *i.e.*, their kinetic energy is not transformed into thermal energy. This is one important reason for the high stability of the new soliton. In addition the energy of the soliton state is below the bottom of the bare exciton bands, the energy gap being $4\mu_\mathrm{p}^2 J/3$ for small velocity of propagation. Hence there is an energy penalty associated with the destruction with transformation from the soliton state to a bare exciton state, *i.e.*, the destruction of the soliton state requires simultaneous removal of the lattice distortion. We know in general that the transition probability to a lattice state without distortion is very small, in general, being negligible for a long chain. Considering this it is reasonable to assume that such a soliton is stable enough to propagate through the length of a typical protein structure. However, the thermal stability of the soliton state must be calculated quantitatively. The following calculation addresses this point explicitly.

One can sum up the differences between our model and the Davydov model, equations (1–4), as follows. Firstly the parameter μ_p is increased $\left(\mu_\mathrm{p} = 2\mu_\mathrm{D}\left[1 + 2(\frac{\chi_2}{\chi_1}) + (\frac{\chi_2}{\chi_1})^2\right]\right)$. Secondly the non-linear coupling energy becomes $G_\mathrm{p} = \frac{8(\chi_1+\chi_2)^2}{w(1-s^2)}$ ($G_\mathrm{p} = 2G_\mathrm{D} \times \left[1 + 2(\frac{\chi_2}{\chi_1}) + (\frac{\chi_2}{\chi_1})^2\right]$), where $G_\mathrm{D} = \frac{4\chi_1^2}{w(1-s^2)}$ is the non-linear interaction in the Davydov model) resulting from the two-quanta nature and the enhancement of the coupling the coefficient $(\chi_1 + \chi_2)$. In fact, the non-linear interaction, G_p, is increased by about a factor of 3 over that of the Davydov soliton and is larger than the dispersion energy J in the equation of motion, equation (A4). A straightforward consequence of these effect is that the binding energy of the new soliton or, in other words, the energy gap between the solitonic and excitonic states are greatly increased or

$$E_\mathrm{BP} = -4\mu_\mathrm{p}^2 J/3 = -G_\mathrm{p}^2/12J = 16E_\mathrm{BD} \times \left[1 + 4\left(\frac{\chi_2}{\chi_1}\right) + 6\left(\frac{\chi_2}{\chi_1}\right)^2 + 4\left(\frac{\chi_2}{\chi_1}\right)^3 + \left(\frac{\chi_2}{\chi_1}\right)^4\right] \quad (19)$$

where E_BD is given in equation (4).

We will now evaluate the main parameters of the new model using generally accepted values of physical parameters appropriate to α-helical protein molecules. The parameter values used in the calculation are listed below

$$J = 1.55\times10^{-22}\ \mathrm{J},\quad w = (13{-}19.5)\ \mathrm{N/m},$$
$$M = (1.17{-}1.91)\times10^{-25}\ \mathrm{kg},\quad \chi_1 = 62\times10^{-12}\ \mathrm{N}$$
$$\chi_2 = (10{-}18)\times10^{-12}\ \mathrm{N}\quad r_0 = 4.5\times10^{-10}\ \mathrm{m}. \quad (20)$$

Note χ_2 was roughly estimated by referring Takeno *et al.*'s papers [22,23]. We can calculate the values of the main parameters in this model by above values. These values and the corresponding values in the Davydov model are simultaneously listed in Table 1.

From Table 1 we can see clearly that the new model produces considerable changes in the properties of the new soliton, for example, 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

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

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

soliton. This shows that the soliton in the new model is more localized and more robust against quantum and thermal fluctuations and has enhanced stability [2,27,28] which implies an increase in lifetime for the new soliton. From equation (19) we also find that the effect of the two-quanta nature is larger than that of the added interaction. We can therefore refer to the new soliton as quasi-coherent.

In the above studies, in order to investigate the influences of quantum and thermal effects on soliton state, which are expected to cause the soliton to decay into delocalized states, we postulate that the model Hamiltonian and the wavefunction in the new model together give a complete and realistic picture of the interaction properties and allowed states of the protein molecules. The additional interaction term in the Hamiltonian gives better symmetry of interactions. The new wavefunction is a reasonable choice for the protein molecules because it not only can exhibit the coherent features of collective excitations arising from the nonlinear interaction between the excitons and phonons, but also retain the conservation of number of particles and fulfil the fact that the energy released by the ATP hydrolysis can only excite two quanta. In such a case, using a standard calculating method [2,26] and widely accepted parameters we can calculate the region encompassed of the excitation or the linear extent of the new soliton, $\Delta X = 2\pi r_0/\mu_{\rm p}$, to be greater than the lattice constant r_0 *i.e.*, $\Delta X > r_0$ as shown in Table 1. Conversely we can explicitly calculate the amplitude squared of the new soliton using equation (15) in its rest frame as $|\varphi(X)|^2 = \mu_{\rm p}/2{\rm sech}^2(\mu_{\rm p}X/r_0)$. Thus the probability to find the new soliton outside a range of width r_0 is about 0.10. This number can be compatible with the continuous approximation since the quasi-coherent soliton can spread over more than one lattice spacing in the system in such a case. This proves that assuming the continuous approximation used in the calculation is still qualitatively valid for soliton widths of the order of the lattice spacing, soliton stability is still improved. There may however be considerable corrections to the quantitative values.

3 Partially diagonalized form of the model Hamiltonian

We now diagonalize partially the model Hamiltonian in order to calculate the lifetime of the soliton, equation (15), using the quantum perturbation method [14]. Since one is interested in investigating the case where there is initially a soliton moving with a velocity v on the chains, it is convenient to do the analysis in a frame of reference where the soliton is at rest. We should then consider the Hamiltonian in this rest frame of the soliton, $H - vP$, where P is the total momentum, and $P = \sum_q \hbar q(a_q^+ a_q - B_q^+ B_q)$, where $B_q^+ = \frac{1}{\sqrt{N}} \sum_n {\rm e}^{{\rm i}qnr_0} B_n^+$. Also, in order to have simple analytical expressions we make the usual continuum approximation. This gives

$$\widetilde{H} = \int_0^L {\rm d}x 2 \left[(\varepsilon_0 - 2J)\varphi^+(x)\varphi(x) + Jr_0^2 \frac{\partial \varphi^+}{\partial x}\frac{\partial \varphi}{\partial x} - \frac{{\rm i}\hbar v}{2} \times \left(\frac{\partial \phi^+}{\partial x}\varphi(x) - \varphi^+(x)\frac{\partial \varphi}{\partial x} \right) \right] + \sum_q \hbar(\omega_q - qv) a_q^+ a_q + \frac{1}{\sqrt{N}} \sum_q 2[g_1(q) + 2g_2(q)](a_{-q}^+ + a_q) \times \int_0^L {\rm d}x {\rm e}^{{\rm i}kx} \varphi^+(x)\varphi(x) \quad (21)$$

where $\varphi(x)$ represents now the field operator corresponding to $B_{\rm n}$ in the continuum limit (whereas before it only indicated a numerical value). Here $L = Nr_0$, $-\pi < kr_0 < \pi$, and $\omega_q \approx (w/M)^{1/2} r_0 |q|$, $x = nr_0$. Since the soliton excitation is connected with the deformation of intermolecular spacing, it is necessary to pass in equation (21) to new phonons taking this deformation into account. Such a transformation can be realized by means of the following transformation of phonon operators [29]

$$b_q = a_{\rm p} - \frac{1}{\sqrt{N}}\alpha_q, \quad b_q^+ = a_q^+ - \frac{1}{\sqrt{N}}\alpha_q^*, \quad (22)$$

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

$$|\widetilde{0}\rangle_{\rm ph} = \exp\left[\frac{1}{\sqrt{N}} \sum_q (\alpha_q(t) a_q^+ - \alpha_q^*(t)) a_q \right] |0\rangle_{\rm ph} \quad (23)$$

which is a coherent phonon state [30], *i.e.*, $b_q|\widetilde{0}\rangle_{\rm ph} = 0$. The Hamiltonian $\widetilde{H}$ can now be rewritten as

$$\widetilde{H} = \int_0^L 2{\rm d}x \varphi(x) \left[\varepsilon_0 - 2J + V(x) - Jr_0^2 \frac{\partial}{\partial x^2} + {\rm i}\hbar \frac{\partial}{\partial x} \right] \times \varphi(x) + \sum_q \hbar(\omega_q - qv)[b_q^+ b_q + \frac{1}{\sqrt{N}}(\alpha_q b_q^+ + \alpha_q^* b_q^+)] + w + \frac{1}{\sqrt{N}} \sum_q 2[g_1(q) + 2g_2(q)](b_{-q}^+ + b_q) \times \int_0^L {\rm d}x {\rm e}^{{\rm i}qx} \varphi^+(x)\varphi(x) \quad (24)$$

where

$$W = \frac{1}{N}\sum_q \hbar(\omega_q - qv)|\alpha_q|^2,\ V(x)$$
$$= \frac{1}{N}\sum_q [g_1(q) + 2g_2(q)](\alpha^*_{-q} + \alpha_{-q})\mathrm{e}^{\mathrm{i}qx}. \quad (25)$$

To describe the deformation corresponding to a soliton in the subspace where there is $\int_0^L \mathrm{d}x\varphi^+(x)\varphi(x) = 1$ from equation (11) in such a case. From the above formulae we can obtain

$$V(x) = -2J\mu_\mathrm{p}^2\ \mathrm{sech}^2(\mu_\mathrm{p}x/r_0). \quad (26)$$

In order to partially diagonalize the Hamiltonian equation (24) we introduce the following canonical transformation [14,23]

$$\varphi(x) = \sum_j A_j C_j(x), \quad \varphi^+(x) = \sum_j C_j^*(x)A_j^+ \quad (27)$$

where

$$\int C_1^*(x)C_j(x)\mathrm{d}x = \delta_{lj}, \sum_j C_j^*(x')C_j(x)$$
$$= \delta(x - x'), \int \mathrm{d}x|C_j(x)|^2 = 1. \quad (28)$$

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

$$\widetilde{H} = W + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - qv)b_q^+ b_q$$
$$+ \frac{1}{\sqrt{N}}\sum_q \hbar(\omega_q - qv)(b_q^+\alpha_q + \alpha_q^* b_q)(1 - A_s^+ A_s)$$
$$+ \frac{1}{\sqrt{N}}\sum_{kk'q} F(k,k',q)(b_{-q}^+ + b_q)A_{k'}^+ A_k$$
$$- \frac{1}{\sqrt{N}}\sum_{kq} \widetilde{F}(k,q)(b_{-q}^+ + b_q)(A_s^+ A_{-k} - A_k^+ A_s) \quad (29)$$

and

$$C_s(x) = \left(\frac{\mu_\mathrm{p}}{2r_0}\right)^{1/2} \mathrm{sech}(\mu_\mathrm{p}x/r_0)\exp[\mathrm{i}\hbar xv/2Jr_0^2],$$

with

$$E_s = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - \mu_\mathrm{p}J\right] \quad (30a)$$

$$C_k(x) = \frac{\mu_\mathrm{p}\tanh(\mu_\mathrm{p}x/r_0) - \mathrm{i}kr_0}{\sqrt{Nr_0}[\mu_\mathrm{p} - \mathrm{i}kr_0]}\exp\left[\mathrm{i}kx + \frac{\mathrm{i}\hbar vx}{2Jr_0^2}\right],$$

with $$E_k = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2 V^2}{2Jr_0^2} - J(kr_0)^2\right] \quad (30b)$$

where

$$F(k,k',q) = 2[g_1(q) + 2g_2(q)]\int_0^L \mathrm{d}x\mathrm{e}^{\mathrm{i}qx}C_{k'}^*(x)C_k(x)$$
$$\approx 2[g_1(q) + 2g_2(q)]\left\{1 - \frac{\mathrm{i}\mu_\mathrm{p}qr_0}{[\mu_\mathrm{p} + \mathrm{i}(k+q)r_0][\mu_\mathrm{p} - \mathrm{i}kr_0]}\right\}$$
$$\approx F[k,(k+q),q]\delta_{k'k+q} \quad (31)$$

$$\widetilde{F}(k,q) = 2[g_1(q) + 2g_2(q)]\int_0^L \mathrm{d}x\mathrm{e}^{\mathrm{i}qx}C_{k'}^*(x)C_s(x)$$
$$= \frac{2\pi}{\sqrt{2\mu_\mathrm{p}}}[g_1(q) + 2g_2(q)]\left\{\frac{\mathrm{i}qr_0}{[\mu_\mathrm{p} + \mathrm{i}kr_0]}\right\}$$
$$\times \mathrm{sech}[\pi(k-q)r_0/2\mu_\mathrm{p}] \quad (32)$$

where α_q is determined by $V(x)$ and the condition, $(\omega_q - vq)\alpha_q = (\omega_q + qv)\alpha_q^*$, which is required to get the factor, $(1 - A_s^+A_s)$, in the $\widetilde{H}$ in equation (29). Thus we find

$$\alpha_q = \frac{\mathrm{i}\pi(\chi_1 + \chi_2)}{w\mu_\mathrm{p}(1 - s^2)}\left[\frac{M}{2\hbar\omega_q}\right]^{1/2}(\omega_q + qv)\mathrm{csch}(\pi qr_0/2\mu_\mathrm{p}) \quad (33)$$

and $W = \frac{2}{3}\mu_\mathrm{p}^2 J$.

For this α_q the $|\widetilde{0}\rangle_\mathrm{ph}$ in equation (23) is just the coherent phonon state introduced by Davydov. However, the bound state $C_s(x)$ in equation (30a), unlike the unbounded state $C_k(x)$ in equation (30b), is self-consistent with the deformation. Such a self-consistent state of the intramolecular excitation and deformation forms a soliton which in the intrinsic reference frame is stationary. For the new soliton described by the state vector $|\psi\rangle = \frac{1}{\sqrt{2!}}(A_s^+)^2|0\rangle_\mathrm{ex}|\widetilde{0}\rangle_\mathrm{ph}$ the average energy of $\widetilde{H}$ in equation (29) is

$$\langle\psi|\widetilde{H}|\psi\rangle = 2(\varepsilon_0 - 2J - \frac{\hbar^2 v^2}{4Jr_0^2}) - \frac{4}{3}J\mu_\mathrm{p}^2. \quad (34)$$

Evidently, the average energy of $\widetilde{H}$ in the soliton state $|\psi\rangle$, equation (34), is just equal to the above soliton energy E_sol, or the sum of the energy of the bound state in equation (30a), E_s, and the deformation energy of the lattice, W, *i.e.*, $\langle\psi|\widetilde{H}|\psi\rangle = E_\mathrm{sol} = E_s + W$. This is an interesting result, which shows clearly that the quasi-coherent soliton formed by this mechanism is just a self-trapping state of the two excitons plus the corresponding deformation of the lattice. However, it should be noted that $|\psi\rangle$ is not an exact eigenstate of $\widetilde{H}$ owing to the presence of the terms in $\widetilde{H}$ with $A_k^+A_s$ and $A_s^+A_{-k}$.

4 Transition probability and decay rate of the new soliton

We now calculate the transition probability and decay rate of the quasi-coherent soliton arising from the perturbed potential by using the first-order quantum perturbation theory developed by Cottingham *et al.* [14], in which the influences of the thermal and quantum effects on the properties of the soliton can be taken into account simultaneously.

For the discussion of the decay rate and lifetime of the new soliton state it is very convenient to divide $\widetilde{H}$ in equation (29) into $H_0 + V_1 + V_2$, where

$$H_0 = W + E_s A_s^+ A_s + \sum_k E_k A_k^+ A_k + \sum_q \hbar(\omega_q - vq) b_q^+ b_q + \frac{1}{\sqrt{N}} \sum_q \hbar(\omega_q - vq)(\alpha_q b_q^+ + \alpha_q^* b_q)(1 - A_s^+ A_s) \tag{35}$$

$$V_1 = \frac{1}{\sqrt{N}} \sum_{kk'q} F(k, k+q, q)(b_{-q}^+ + b_q) A_{k'}^+ A_k \tag{36}$$

$$V_2 = \frac{1}{N} \sum_{kq} \widetilde{F}(k, q)(b_{-q}^+ + b_q)(A_s^+ A_k - A_s^+ A_{-k}),$$

$$V = V_1 + V_2. \tag{37}$$

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

We now calculate the decay rate of the new soliton along the following lines by using equation (35) and V_2 in equation (37) and quantum perturbation theory. Firstly, we compute a more general formula for the decay rate of the soliton containing n quanta in the system in which the three terms contained in equation (5a) is replaced by $(n+1)$ terms of the expression of a coherent state $\frac{1}{\lambda}\exp\left[\sum_n \varphi_n(t) B_n^+\right]|0\rangle_{\rm ex}$. Finally we find out the decay rate of the new soliton with two-quanta. In such a case H_0 is chosen such the ground state, $|n\rangle$ has energy $W + nE_s'$ in the subspace of excitation number equal to n, *i.e.*, $\langle n|\sum_i B_i^+ B_i|n\rangle = \langle n|(A_s^+ A_s + \sum_k A_k^+ A_k)|n\rangle = n$. In this subspace the eigenstates have the simple form

$$|n-m, k_1 K_2 \ldots k_m,\ \{n_q\}\rangle = \frac{1}{\sqrt{(n-m)!}}(A_s^+)^{n-m} \times A_{k_1}^+ A_{k_2}^+ \ldots A_{k_m}^+ |0\rangle_{\rm ex} \prod_q \frac{(d_q^+)^{n_q}}{\sqrt{n_q!}} |\widetilde{0}\rangle_{\rm ph}^{n-m} \tag{38}$$

where

$$d_q = b_q + \frac{m}{n}\frac{1}{\sqrt{N}}\alpha_q = a_q - \frac{n-m}{n}\frac{1}{\sqrt{N}}\alpha_q \quad (m \le n,\ n \text{ and } m \text{ are all integers}) \tag{39}$$

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

$$E_{n-m;k_1\ldots k_{m_1};\{n_q\}}^{(0)} = (1 - (m/n)^2)W + (n-m)E_s' + \sum_{j=1}^{m} E_{k_1}' + \sum_q \hbar(\omega_q - vq) n_q \tag{40}$$

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

$$|n\rangle = \frac{1}{\sqrt{n!}} \prod_q \frac{(b_q^+)^{n_q}}{(n_q!)^{1/2}} (A_s^+)^n |0\rangle_{\rm ex} |\widetilde{0}\rangle_{\rm ph} \tag{41}$$

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:

$$|\alpha k\rangle = \prod_q \frac{(a_q^+)^{n_q}}{\sqrt{n_q!}} |0\rangle_{\rm ph}\ (A_k^+)^n |0\rangle_{\rm ex} \tag{42}$$

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

$$\bar{W} = \frac{1}{\hbar^2}\int_0^t {\rm d}t' \int_0^t {\rm d}t'' \left\{ \sum_{\alpha k'} \sum_1 P_1^{({\rm ph})} \langle n| \exp\left(\frac{{\rm i}H_0 t''}{\hbar}\right) V_2 \times \exp\left(\frac{-{\rm i}H_0 t''}{\hbar}\right) |\alpha k'\rangle\langle \alpha k'| \exp\left(\frac{{\rm i}H_0 t'}{\hbar}\right) V_2 \times \exp\left(\frac{-{\rm i}H_0 t'}{h}\right) |n\rangle \right\}. \tag{43}$$

We should calculate the transition probability of the soliton resulting from the perturbed potential, $(V_1 + V_2)$, at first-order in perturbation theory. Following Cottingham and Schweitzer [14], we estimate only the transition from the soliton state to delocalized exciton

$$\Gamma_n = \lim_{t\to\infty}\frac{\mathrm{d}\overline{W}}{\mathrm{d}t} = \frac{4}{\hbar}\left[\frac{\pi^2}{2n\mu_1 N^2}\right]\sum_{kk'k''}[g_1^*(k)+2g_2^*(k)][g_1(k'')+2g_2(k'')]\frac{(kr_0)(k''r_0)}{(n\mu_1)^2+(k'r_0)^2}\quad \mathrm{sech}\left[\frac{\pi r_0}{2n\mu_1}(k-k')\right]$$

$$\times\,\mathrm{sech}\left[\frac{\pi r_0}{2n\mu_1}(k''-k')\right]\mathrm{Re}\left\{\int_0^\infty \mathrm{d}t\exp\left[-\frac{\mathrm{i}}{\hbar}\left(n\left(n^2-\frac{2}{3}n\right)\mu_1^2 J+\ nJ(k'r_0)^2\right)t\right]\langle\langle\exp\left[\mathrm{i}\sum_q(\omega_q-qv)b_q^+b_qt\right](b_k^++b_{-k})\right.$$

$$\left.\times\exp\left[-\mathrm{i}\sum_q(\omega_q-qv)a_q^+a_qt\right](b_{-k''}^+ +\ b_{k''})\rangle\rangle\right\} = \frac{4}{\hbar^2}\frac{\pi^2}{2n\mu_1N^2}\sum_{kk'k''}\left\{[g_1^*(k)+2g_2^*(k)][g_1(k'')+2g_2(k'')]\frac{(kr_0)(k''r_0)}{(n\mu_1)^2+(k'r_0)^2}\right.$$

$$\left.\times\,\mathrm{sech}\left[\frac{\pi r_0(k-k')}{2n\mu_1}\right]\mathrm{sech}\left[\frac{\pi r_0}{2n\mu_1}(k''-k')\right]\mathrm{Re}\int_0^\infty \mathrm{d}tU(k,k''t)\exp\left[-\frac{\mathrm{i}}{\hbar}\left(n\left(n^2-\frac{2}{3}n\right)\mu_1^2J+\ nJ(k'r_0)^2\right)t\right]\right\} \tag{46}$$

states caused by the potential V_2, which can satisfactorily be treated by means of perturbation theory since the coefficient $\widetilde{F}(k,q)$ defined by equation (32) is proportional to an integral over the product of the localized state, and a delocalized state, and therefore is of order $1/\sqrt{N}$. The V_1 term in the Hamiltonian is an interaction between the delocalized excitons and the phonons. The main effect of V_1 is to modify the spectrum of the delocalized excitons in the weak coupling limit ($J\mu_\mathrm{p}/K_\mathrm{B}T_0 \ll 1$), the definition of T_0 is given below). As a result the delocalized excitons and phonons will have their energies shifted and also have finite lifetimes. These effects are ignored in our calculation since they are only of second order in V_1.

The sum over l in equation (43) 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 taken to be the thermal equilibrium distribution for a given temperature T. Since

$$\mathrm{e}^{-\mathrm{i}H_0t}|n,\{n_q\}\rangle = \exp\Big\{-\mathrm{i}(W+nE_q')t/\hbar-\mathrm{i}\times\sum_q(\omega_q-qv)b_q^+b_qt\Big\}|n,\{n_q\}\rangle$$

and

$$\mathrm{e}^{\mathrm{i}H_0t}|n-1,\{n_q'\}\rangle = \exp\left\{-\mathrm{i}\left[\left(1-\frac{1}{n^2}\right)W+(n-1)E_s'+E_k'\right]t/\hbar-\mathrm{i}\sum_q(\omega_q-qv)d_q^+d_qt\right\}|n-1,\{n_q'\}\rangle$$

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 values of k', one can rewrite $\overline{W}$ as

$$\overline{W} = \frac{1}{\hbar^2}\frac{\pi^2}{2n\mu_1N^2}\sum_k\sum_{k'}\sum_{k''}[g_1^*(k)+2g_2^*(k)][g_1(k'')+2g_2(k'')]\frac{(kr_0)(k''r_0)}{(n\mu_1)^2+(k'r_0)^2}\mathrm{sech}\left[\frac{\pi r_0}{2n\mu_1}(k-k')\right]$$
$$\times\,\mathrm{sech}\left[\frac{\pi r_0}{2n\mu_1}(k''-k')\right]\int_0^t\mathrm{d}t'\int_0^t\mathrm{d}t''\times\left\{\exp\left[\frac{-\mathrm{i}}{\hbar}\left(n\left(n^2-\frac{2}{3}n\right)\mu_1^2J+nJ(k'r_0)^2\right)\right.\right.$$
$$\times(t'-t'')]\,\langle\langle\exp\left[\mathrm{i}\sum_q(\omega_q-qv)b_q^+b_q(t'-t'')\right]$$
$$\left.\left.\times\,(b_k^++b_{-k})\exp\left[\mathrm{i}\sum_q(\omega_q-qv)a_q^+a_q(t'-t'')\right]\right.\right.$$
$$\left.\left.\times\,(b_{-k''}^++b_{-k''})\rangle\rangle\right\}. \tag{44}$$

where

$$g_1(k)+2g_2(k) = \ 2\chi_1\left(\frac{\hbar}{2M\omega_k}\right)^{1/2}[A(\cos(r_0k)-1)+\mathrm{i}(A+1)\sin(r_0k)] \approx 2\mathrm{i}(A+1)(r_0k)\chi_1\left(\frac{\hbar}{2M\omega_k}\right)^{1/2},$$
$$\mu_1 = \frac{\chi_1^2(1+A^2)}{\omega(1-s^2)J},\quad A=\chi_2/\chi_1. \tag{45}$$

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

To estimate the lifetime of the soliton we are interested in the long-time behaviour of $\frac{\mathrm{d}\overline{W}}{\mathrm{d}t}$. By straightforward calculation, the average transition probability or decay rate of the soliton is given by

see equation (46) above

where the thermal average is

$$U(k,k'',t) = \langle\langle \exp\left[\mathrm{i}\sum_q(\omega_q - qv)b_q^+ b_q t\right](b_k^+ + b_{-k}) \times \exp\left[-\mathrm{i}\sum_q(\omega_q - qv)a_q^+ a_q t\right](b_{-k''}^+ + b_{k''})\rangle\rangle$$

with

$$\langle\langle A\rangle\rangle = \mathrm{Tr}\left\{A\exp\left[-\beta\sum_q \hbar(\omega_q - qv)b_q^+ b_q\right]\right\} \times \mathrm{Tr}\left\{\exp\left[-\beta\sum_q \hbar(\omega_q - qv)b_q^+ b_q\right]\right\} = \mathrm{Tr}\left\{A\exp\left[-\beta\sum_q \hbar(\omega_q - qv)b_q^+ b_q\right]\right\}/Z_{\mathrm{ph}} \quad (47)$$

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

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 we use the coherent state to calculate the $U(k,k'',t)$ as it is described in Appendix C. The decay rate obtained finally is

$$\Gamma_n = \lim_{1\to\infty}\frac{\mathrm{d}\overline{W}}{\mathrm{d}t} = \frac{2}{n\mu_1\hbar^2}\frac{\pi^2}{N^2}\sum_{kk'}\Bigg[|g_1(k) + 2g_2(k)|^2 \times \frac{(r_0k)^2\mathrm{sech}^2[\pi(k-k')r_0/2n\mu_1]}{(n\mu_1)^2 + (k'r_0)^2}\mathrm{Re}\int_0^\infty \mathrm{d}t \times \Bigg\{\exp[-\mathrm{i}(nJ(k'r_0)^2 + n\left(n^2 - \frac{2}{3}n\right) \times\mu_1^2 Jt/\hbar + R_n(t) + \xi_n(t)]\frac{\exp[\mathrm{i}(\omega_k - kv)t]}{\exp[\beta\hbar(\omega_k - kv)] - 1}\Bigg\}\Bigg] \quad (48)$$

where

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

$$\xi_n(t) = -\frac{4}{n^2N}\sum_k \frac{|\alpha_k|^2\sin^2\left[\frac{1}{2}(\omega_k - kv)t\right]}{\exp[\beta\hbar(\omega_k - kv)] - 1}. \quad (49)$$

This is just a generally analytical expression for the decay rate of the soliton containing n quanta at any temperature within lowest order perturbation theory. Note that in the case where a phonon with wavevector k in equation (49) is absorbed, the delocalized excitation produced does not need to have wavevector equal to k. The wavevector 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, we do not find the usual energy conservation. The terms $R_n(t)$ and $\xi_n(t)$ occur because the phonons in the initial and final states are defined relative to different deformations.

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

From equations (48) and (49) we see that the Γ_n and $R_n(t)$ and $\xi_n(t)$ and $\mu = n\mu_1$ mentioned above are all changed by increasing the number of quanta, n. Therefore, the approximation methods used to calculate Γ_n and related quantities (especially the integral contained in Γ_n) should be different for different n. We now calculate the explicit formula of the decay rate of the new soliton with two-quanta ($n = 2$) by using equations (48, 49). In such a case we can compute explicitly the expressions of this integral and $R_2(t)$ and $\xi_2(t)$ contained in equations (48, 49) by means of approximation. As a matter of fact, in equation (49) 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 it is shown in Appendix D. For $t \to \infty$ (because we are interested in the long-time steady behaviour) the asymptotic forms of $R_2(t)$ and $\xi_2(t)$ are

$$R_2(t) = -R_0\left[\ln\left(\frac{1}{2}\omega_\alpha t\right) + 1.578 + \frac{1}{2}\mathrm{i}\pi\right] \quad (50)$$

$$\xi_2(t) \approx -\pi R_0 k_{\mathrm{B}}Tt/\hbar \ \ (\text{where } \coth\frac{1}{2}\omega_\alpha t \sim 1) \quad (51)$$

i.e.,

$$\lim_{t\to\infty}\xi_2(t) = -\eta t, \eta = \pi R_0/\beta\hbar = \pi R_0 k_{\mathrm{B}}T/\hbar \quad (52)$$

where

$$R_0 = \frac{4(\chi_1 + \chi_2)^2}{\pi\hbar w}(M/w)^{1/2} = \frac{2J\mu_{\mathrm{p}}r_0}{\pi\hbar v_0},$$
$$\omega_\alpha = \frac{2\mu_{\mathrm{p}}}{\pi}\left(\frac{w}{M}\right)^{1/2}, \quad T_0 = \hbar\omega_\alpha/K_{\mathrm{B}}. \quad (53)$$

At $R_0 < 1$ and $T_0 < T$ and $R_0\ T/T_0 < 1$ for the protein molecules, one can evaluate the integral including in equation (48) by using the approximation which is shown

$$\Gamma_2 = \lim_{t\to\infty}\frac{\mathrm{d}\overline{W}}{\mathrm{d}t} = \frac{2}{\mu_\mathrm{p}}\left(\frac{\pi}{N}\right)^2\sum_{kk'}\left[\frac{(kr_0)^2|g_1(k)+2g_2(k)|^2\mathrm{sech}^2[(\pi r_0/2\mu_\mathrm{p})(k-k')]}{[\mu_\mathrm{p}^2+(k'r_0)^2][\exp(\beta\hbar\omega_k)-1]}(2.43\omega_\alpha)^{-R_0}\right.$$
$$\times\left\{\frac{\left(\eta^2+\frac{1}{\hbar^2}\left[\frac{4}{3}\mu_\mathrm{p}^2J+2(k'r_0)^2J-\hbar\omega_k\right]^2\right)^{(1+R_0)/2}}{\hbar^2\eta^2+\left[\frac{4}{3}\mu_\mathrm{p}^2J+2(k'r_0)^2J-\hbar\omega_k\right]^2}\right\}\left\{1-\frac{1}{2}\left[\frac{R_0\pi}{2}+(1-R_0)\left[\frac{\frac{4}{3}\mu_\mathrm{p}^2J+2(k'r_0)^2J-\hbar\omega_k}{\hbar\eta}\right]\right]^2\right\}\Bigg]. \quad (56)$$

in Appendix D. The result is

$$\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t\exp\Bigg\{-\mathrm{i}\left[2J(k'r_0)^2+\frac{4}{3}J\mu_\mathrm{p}^2-\hbar\omega_k\right]t/\hbar + R_2(t)+\xi_2(t)\Bigg\}$$
$$\approx\frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\left[\eta^2+(\delta(k,k')/\hbar)^2\right]^{-(1-R_0)/2}\times\left[1-\frac{1}{2}\left[\frac{\pi R_0}{2}+(1-R_0)\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]^2\right], \quad (54)$$

where

$$\delta(k,k')=2J(k'r_0)^2+\frac{4}{3}\mu_\mathrm{p}^2J-\hbar\omega_k, \Phi_1=\frac{R_0\pi}{2},$$
$$\Phi_2=\left[(1-R_0)\tan^{-1}\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right] \quad (55)$$

The decay rate of the soliton, in such an approximation, can be represented, from equations (48) and (54), by

see equation (56) above.

This is the final analytical expression for the decay rate of the quasi-coherent soliton with two-quanta. Evidently, it is different from that in the Davydov model [14]. To emphasis the difference of the decay rate between the two models we rewrite down the corresponding quantity for the Davydov soliton [14]

$$\Gamma_\mathrm{D}=\frac{1}{\hbar^2}\frac{\chi_1^2}{\mu_\mathrm{D}}\left(\frac{2\pi}{N}\right)^2\sum_{kk'}\left(\frac{\hbar}{2M\omega_k}\right)\times\frac{(kr_0)^2\sin^2(kr_0)\mathrm{sech}^2[(\pi r_0/2\mu_\mathrm{D})(k-k')]}{[\mu_\mathrm{D}^2+(k'r_0)^2][\exp(\beta\hbar\omega_k)-1]}\times\left(\frac{\omega_\alpha^\mathrm{D}}{\eta_\mathrm{D}}\right)^{-R_0^D}\frac{\hbar^2\eta_\mathrm{D}}{\hbar^2\eta_\mathrm{D}^2+[J\mu_\mathrm{D}^2/3+J(k'r_0)^2-\hbar\omega_k]} \quad (57)$$

where

$$\eta_\mathrm{D}=\pi R_0^\mathrm{D}K_\mathrm{B}T/\hbar,\ R_0^\mathrm{D}=\frac{2\chi_1^2}{\pi\hbar w}\left(\frac{M}{w}\right)^{1/2},$$
$$\omega_\alpha^\mathrm{D}=\frac{2\mu_\mathrm{D}}{\pi}\left(\frac{M}{w}\right)^{1/2}. \quad (58)$$

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

	R_0	T_0(K)	$\eta(\times10^{13}/\mathrm{s})$
New model	0.529	294	6.527
Davydov model	0.16	95	2.096

Equation (57) can also be found out from equation (48) at $n=1$ by using the Cottingham *et al.*'s approximation.

The two formulae above equations (56) and (57) are completely different, not only for the parameter's values, but also the factors contained in them. In equation (56) the factor, $\left\{1-\frac{1}{2}\left[\frac{R_0\pi}{2}+(1-R_0)\left[\left(\frac{4}{3}\mu_\mathrm{p}^2J+2(k'r_0)^2J-\hbar\omega_k\right)/\hbar\eta\right]\right]^2\right\}$ is added, while in equation (57) the factor, $(\omega_\alpha/\eta_\mathrm{D})^{-R_0^\mathrm{D}}\eta_\mathrm{D}$ replaces the term $(2.43\omega_d)^{-R_0}\times(\eta^2+1/\hbar^2[4/3\mu_\mathrm{p}^2J+2(k'r_0)^2J-\hbar\omega_k]^2)^{(\frac{1+R_0}{2})}$ in equation (56) due to the two-quanta nature of the new wavefunction and the additional interaction term in the new Hamiltonian. In equation (56) the η, R_0 and T_0 are not small, unlike in the Davydov model. Using equation (20) and Table 1 we find out the values of η, R_0 and T_0 at $T=300$ K in both models, which are listed in Table 2. From this table we see that the η, R_0 and T_0 for the new model are about 3 times larger than the corresponding values in the Davydov model due to the increases of μ_p and of the non-linear interaction coefficient G_p. Thus the approximations used in the Davydov model by Cottingham, *et al.* [14] can not be applied in our calculation of lifetime of the new soliton, although we utilized the same quantum-perturbation scheme. Hence we can audaciously suppose that the lifetimes of the quasi-coherent soliton will greatly change.

5 Discussion for the lifetime of the new soliton and results

The above expression, equation (56), allows us to compute numerically the decay rate, Γ_2, and the lifetimes of the new soliton, $\tau=1/\Gamma_2$, for values of the physical parameters appropriate to α-helical protein molecules. Using the parameter values given in equation (20), Tables 1 and 2, $v=0.2v_0$ and assuming the wavevectors are

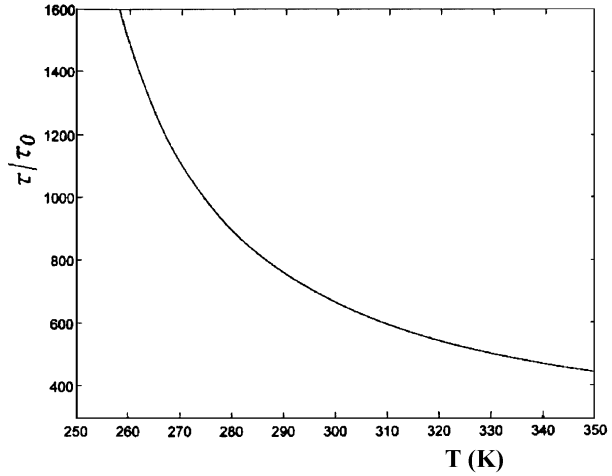

Fig. 1. Soliton lifetime τ relatively to τ_0 as a function of the temperature T for parameters appropriate to the α-helical molecules in the new model in equation (5).

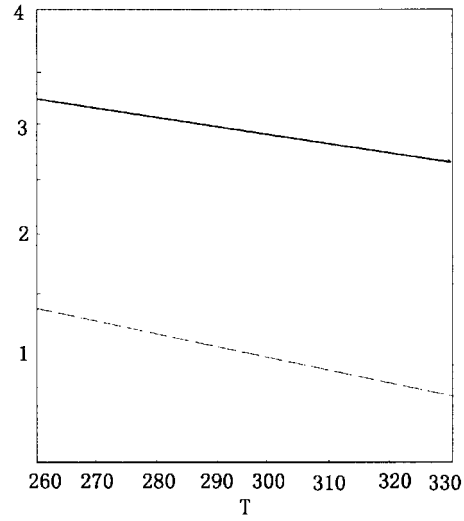

Fig. 2. $\log(\tau/\tau_0)$ *versus* the temperature for the soliton. The solid line is the result of the new model, the dashed line is the result of the Davydov model.

in the Brillouin zone we obtain values of Γ_2 between $1.54 \times 10^{10}\text{s}^{-1} - 1.89 \times 10^{10}\text{s}^{-1}$. This corresponds to the soliton lifetimes τ, of between $0.53\times10^{-10}\text{s}-0.65\times10^{-10}\text{s}$ at $T = 300$ K, or $\tau/\tau_0 = 510 - 630$, where $\tau_0 = r_0/v_0$ is the time for travelling one lattice spacing at the speed of sound, equal to $(M/w)^{1/2} = 0.96 \times 10^{-13}$s. In this amount of time the new soliton, travelling at two tenths of the speed of sound in the chain, would travel several hundreds of lattice spacings, that is several hundred times more than the Davydov soliton for which $\tau/\tau_0 < 10$ at 300 K [14] (*i.e.*, the Davydov soliton traveling at a half of the sound speed can cover less than 10 lattice spacing in its lifetime). The lifetime is sufficiently long for the new soliton excitation to be a carrier of bio-energy. Therefore the quasi-coherent soliton is a viable mechanism for the bio-energy transport at biological temperature in the above range of parameters.

We are very interested in the relation between the lifetime of the quasi-coherent soliton and temperature. Figure 1 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 equation (20). Since one assumes that $v < v_0$, the soliton will not travel the length of the chain unless τ/τ_0 is large compared with L/r_0, where $L = Nr_0$ is the typical length of the protein molecular chains. Hence for $L/r_0 \approx 100$, $\tau/\tau_0 > 500$ is a reasonable criterion for the soliton to be a possible mechanism of the bio-energy transport in protein molecules. The lifetime of the quasi-coherent soliton shown in Figure 1 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 roles in biological processes.

For comparison we plotted simultaneously $\log(\tau/\tau_0)$ *versus* the temperature relations for the Davydov soliton and the new soliton with a quasi-coherent two-quanta state in Figure 2. The temperature-dependence of $\log(\tau/\tau_0)$ of the Davydov soliton is obtained from equation (57). We find that the differences of values of τ/τ_0 between the two models are very large. The value of τ/τ_0 of the Davydov soliton really is too small, and it can only travel fewer than ten lattice spacings in half the speed of sound in the protein chain [14]. Hence it is true that the Davydov soliton is ineffective for biological processes [14].

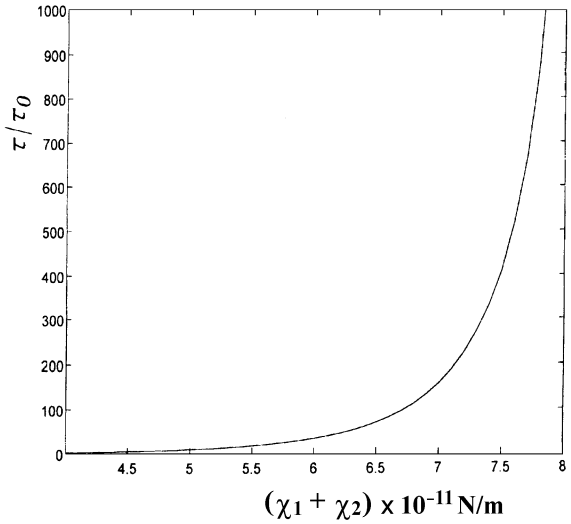

Fig. 3. τ/τ_0 *versus* $(\chi_1 + \chi_2)$ relation in equation (56).

We can also study the dependency of the soliton lifetime on the other parameters by using equation (56). We chose parameter values near the above accepted values shown in equation (20). In the new model we know from equation (56) that the lifetime of the soliton depends mainly on the following parameters: coupling constants $(\chi_1 + \chi_2)$, M, w, J, phonon energy $\hbar\omega_k$, as well as on the composite parameters $\mu(\mu = \mu_\text{p})$, 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 Figures 3 and 4, respectively. Since

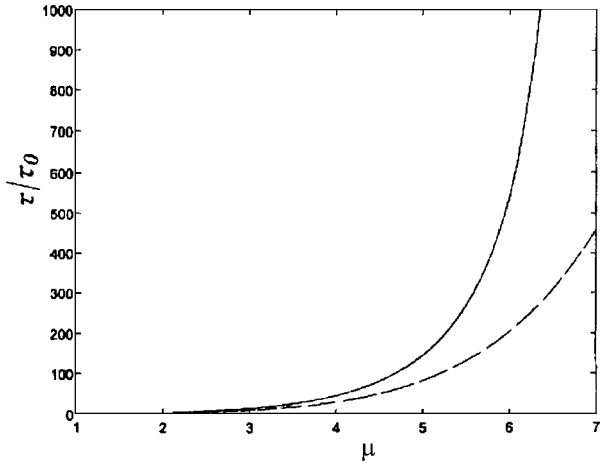

Fig. 4. τ/τ_0 *versus* μ relation. The solid and dashed lines are results of equations (56) and (57), respectively.

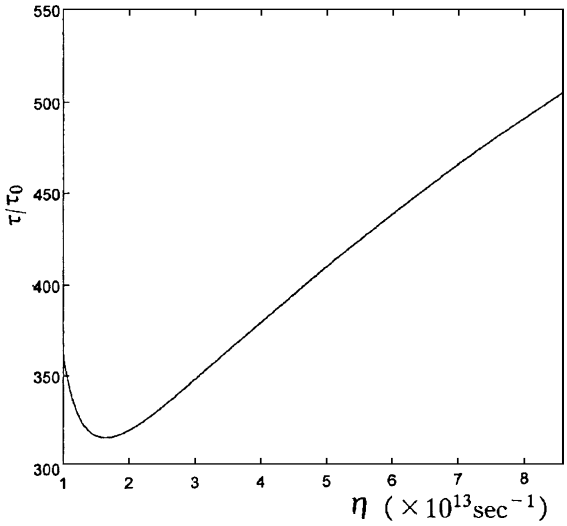

Fig. 5. τ/τ_0 *versus* η relation in equation (56).

μ is inversely proportional to the size of the soliton, and determining the binding energy in the new model, therefore it is an important quantity. We regard it as an independent variable. In such a case the other parameters in equation (56) adopt the values in equation (20). It is clear from Figures 3 and 4 that the lifetime of the soliton, τ/τ_0, increases rapidly with increasing μ and $(\chi_1+\chi_2)$. Furthermore, when $\mu \geqslant 5.8$ and $(\chi_1+\chi_2) \geq 7.5\times10^{-11}$ N, which are values appropriate to the new model, we find $\tau/\tau_0 > 500$. For comparison we show the corresponding result obtained using equation (57), for the original Davydov model as a dashed line in Figure 4. Here we see that the increase in lifetime of the Davydov soliton with increasing μ is quite slow and the difference between the two models increases rapidly with 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 Figure 3. These results show again that the quasi-coherent soliton in the new model is a likely candidate for the mechanism of bioenergy transport in the protein molecules. In addition it shows that a basic mechanism for increasing the lifetime of the soliton in the biomacromolecules is to enhance the strength of the exciton-phonon interaction.

In Figure 5 we plot τ/τ_0 *versus* η. Since $-\eta$ designates the influence of the thermal phonons on the soliton, it is also an important quantity. Thus, we regard it here as an independent variable. The other parameters in equation (56) take the values in equation (20). From this figure we see that τ/τ_0 increases with increasing η. Therefore, to enhance η can also increase the value of τ/τ_0.

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 equation (49) or equations (D1) and (D3) (*i.e.*, this is in the initial case) in which we can evaluate analytically the values of $R_2(t)$ and $\xi_2(t)$. In fact, for $\omega_a t < 1$ both $R_2(t)$ and $\xi_2(t)$ have power-series expansions. To lowest order as $\omega_a t \to 0$, one finds from equation (49)

$$R_2(t) \approx -R_0[\mathrm{i}\pi^2\,\omega_a t/6 + 3\zeta(3)(\omega_a t)^2] \tag{59}$$

$$\xi_2(t) \approx -\frac{R_0 K_\mathrm{B}^2 T T_0\,\pi^2}{3\hbar^2} t^2, \tag{60}$$

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

Thus

$$\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t \exp\left\{-\mathrm{i}\left[2J(k'r_0)^2 + \frac{4J\mu_\mathrm{p}^2}{3} - \hbar\omega_k\right]\frac{t}{\hbar} + R_2(t) + \xi_2(t)\right\} \approx [4\pi(3\zeta(3)R_0K_\mathrm{B}^2T_0^2 + R_0\pi^2K_\mathrm{B}^2TT_0/3]^{-1/2} \times \exp\left\{-\frac{[2J(k'r_0)^2 + \frac{4}{3}\mu_\mathrm{p}^2 J - \hbar\omega_k + \hbar(R_0\pi^2K_\mathrm{B}T)]^2]}{4[3\zeta(3)R_0K_\mathrm{B}^2T_0^2 + R_0\pi^2K_\mathrm{B}^2TT_0/3]}\right\} \tag{61}$$

when $T/T_0 > 1$ and $\pi^4 R_0 T/2\mu T_0 > 1$. The above integral is the generalization of the usual $\delta-$ function for energy conservation in zero-temperature perturbation theory. Thus we can obtain from equations (48) and (61)

at $n = 2$ the decay rate of the soliton as

$$\Gamma_2 = \frac{2\pi^3}{\mu_{\rm p}\hbar N^2 K_{\rm B}} \left(\frac{\pi}{R_0\, T_0[3\zeta(3)T_0 + \pi^2 T/3]}\right)^{-1/2} \times \sum_{kk'} \frac{(kr_0)^2 \mid g_1(k) + 2g_2(k)\mid^2}{\mu_{\rm p}^2 + (k'r_0)^2} \,\mathrm{sech}^2 \left[\left(\frac{\pi r_0}{2\mu_{\rm p}}\right)(k-k')\right] \times \left\{\exp\left[\frac{[2J(k'r_0)^2 + \frac{4}{3}\mu_{\rm p}^2 J - \hbar\omega_k + \frac{1}{6}R_0\pi^2 K_{\rm B}T_0]^2}{4[3\zeta(3)R_0K_{\rm B}^2T_0^2 + R_0K_{\rm B}^2TT_0\pi^2/3]}\right] \times [\exp(\beta\hbar\omega_k) - 1]\right\}^{-1}. \quad (62)$$

The expression of the decay rate of the quasi-coherent soliton in this limit is different from equation (56). Therefore, studying properties of the lifetime of the new soliton in such a case helps in understanding the behavior of the soliton. A summary of the results obtained from equation (62) are given in Figures 6–9. The dependency of lifetime on temperature T is shown in Figure 6, which has been obtained from the numerical evaluation of equation (62).

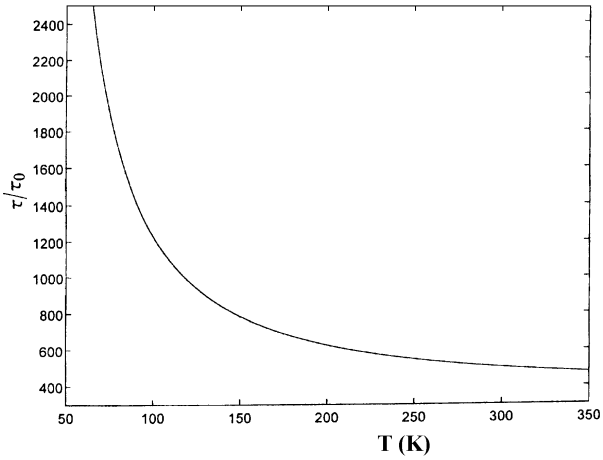

Fig. 6. τ/τ_0 *versus* T relation in the new model in equation (62).

In Figures 7 and 8 we plot τ/τ_0 *versus* $(\chi_1 + \chi_2)$ and *versus* μ, respectively, at $T = 300$ K. From Figures 6–8 we see that τ/τ_0 increases as T decreases and as μ and $(\chi_1 + \chi_2)$ increase. Furthermore, it is clear from this Gaussian expression in equation (62) that the lifetime of the new soliton will be large if μ and $(\chi_1 + \chi_2)$are larger, but the Gaussian expression is very small for k and k' between $-\pi/r_0$ and $+\pi/r_0$, *i.e.*, in the Brillouin zero. Obviously, the temperature dependence of the lifetime of the new soliton is mainly due to the temperature dependence of the width of the Gaussian, which decreases with decreasing temperature. The dashed line in Figure 8 is the result for the Davydov soliton under the same conditions. It is clear that the lifetime of the Davydov soliton is lower than that of the new soliton, especially at large, although at low μ the difference between them is small. Taking Figure 4 also into account we find that the lifetime of the Davydov soliton is indeed generally low. However this is not the case for the new soliton. In Figure 9 we plot τ/τ_0 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. We regard it here as an independent variable and evaluate other parameters as in equation (20). From this figure we see that the lifetime of the new soliton is large if T_0 is either large or small, because the Gaussian expression in equation (62) is very small for k and k' between $-\pi/r_0$ and $+\pi/r_0$. As a point of reference, note that these parameters have the values $T/T_0 \approx 1.03$–1.06, $JT/K_{\rm B}T_0^2 = 4.10$ at 300 K and $\mu = 5.81 - 5.96$ depending on whether the widely accepted or the "three-channel"parameter values for the protein are assumed. From these results it is clear that using widely accepted, realistic parameter values, the new model can satisfy the relation $\tau/\tau_0 \geqslant 500$ at 300 K and large μ and large T_0. Hence the proposed new soliton model provides a viable candidate for biological processes.

6 Conclusions

Why then does the quasi-coherent soliton have such high lifetime? From equations (A4) and (13) and Tables 1 and 2 we see that the binding energy and localization of the new soliton increase due to the increase of the nonlinear interactions of exciton-phonon interaction, *i.e.*, the new wave function with two-quanta state and the new Hamiltonian with the added interaction produce considerable changes to the properties of the soliton. In fact, the non linear interaction energy in the new model is $G_{\rm p} = 8(\chi_1+\chi_2)^2/(1-S^2)w = 3.8 \times 10^{-21}J$, 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 we can also say that the soliton is stable according to the conditions of formation and stability of the soliton in the soliton theory [27,28]. By comparison, the non-linear interaction energy in the Davydov model is $G_{\rm D} = 4\chi_1^2/(1-S^2)w \approx 1.18\times10^{-21}J$ and it is 3-4 times smaller than $G_{\rm p}$. Thus the stability of the Davydov soliton is weak compared to that of the new soliton. Moreover, the binding energy of the quasi-coherent soliton in the new model is $E_{\rm BP} = 4\mu_{\rm p}^2\, J/3 = 7.8 \times 10^{-21}J$ in equation (19), which is about 2 times larger than the thermal energy, $K_{\rm B}T = 4.14\times10^{-21}J$, at 300 K, and about 6 times larger than the Debye energy, $K_{\rm B}\Theta = \hbar\omega_{\rm D} = 1.2\times10^{-21}J$ (here $\omega_{\rm D}$ is Debye frequency), and it is approximately equal to $\varepsilon_0/4 = 8.2 \times 10^{-21}J$, *i.e.*, it has same order of magnitude of the energy of the amide-I vibrational quantum, ε_0. This shows that the 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

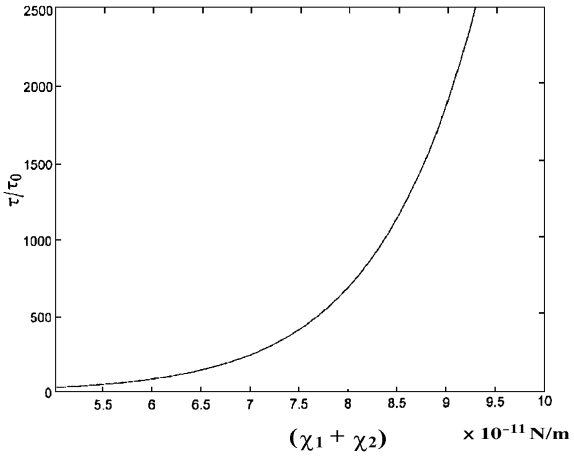

Fig. 7. τ/τ_0 *versus* $(\chi_1 + \chi_2)$ relation in the new model in equation (62).

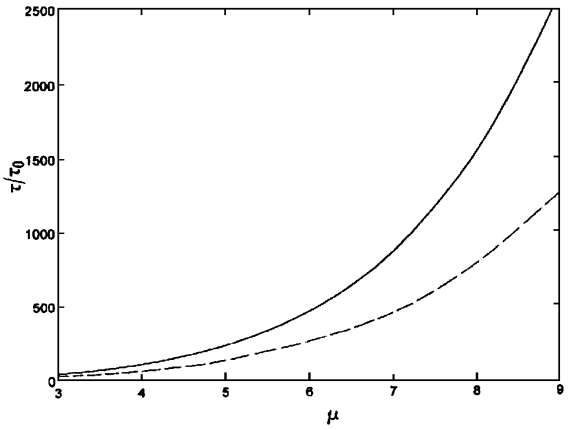

Fig. 8. τ/τ_0 *versus* μ relation in the new model in equation (62).

$E_{\rm BD} = (\chi_1^4/3w^2J) = 0.188 \times 10^{-21}J$ which is about 41 times smaller than that of the new soliton, about 23 times smaller than $K_{\rm B}T$ and about 6 times smaller than $K_{\rm B}\Theta$, respectively. Therefore, it is easily destroyed by thermal and quantum effects. Hence the Davydov soliton has very small lifetime (about $10^{-12} \sim 10^{-13}$s), and it is unstable at 300 K [14]. In contrast, the quasi-coherent soliton can provide a realistic mechanism for the bio-energy transport in protein molecules.

The two-quanta nature of the quasi-coherent soliton plays a more important role in the increase of lifetime than that of the added interaction because of the following facts. (1) The change of the nonlinear interaction energy $G_{\rm P} = 2G_{\rm D}\left[1 + 2\left(\frac{\chi_2}{\chi_1}\right) + \left(\frac{\chi_2}{\chi_1}\right)^2\right]$ and $\mu_{\rm p}$ produced by the added interaction in the new model are $\Delta G = G_{\rm P}(\chi_2 \neq 0) - G_{\rm P}(\chi_2 = 0) = 1.08G_{\rm D} < G_{\rm P}(\chi_2 = 0) = 2G_{\rm D}$, and $\Delta\mu = \mu_{\rm p}(\chi_2 \neq 0) - \mu_{\rm p}(\chi_2 = 0) = 1.08\mu_{\rm D} < \mu_{\rm p}(\chi_2 = 0) = 2\mu_{\rm D}$ respectively, *i.e.*, the roles of the added interaction on $G_{\rm P}$ and $\mu_{\rm p}$ are smaller than that of the two-quanta nature. The two parameters $G_{\rm P}$ and $\mu_{\rm p}$ are responsible for the lifetime of the soliton. Thus the effect of the former on the lifetimes is smaller than that of the latter. (2) The contribution of the added interaction to the binding energy of the soliton is about $E'_{\rm BP} = E_{\rm BD}\left[1 + \left(\frac{\chi_2}{\chi_1}\right)\right]^4 = 2.6E_{\rm BD}$, which is smaller than that of the two-quanta nature which is $E''_{\rm BD} = 16E_{\rm BD}$. Putting them together in equation (19) we see that $E_{\rm BP} \approx 41E_{\rm BD}$. (3) From the $(\chi_1 + \chi_2)$-dependence of τ/τ_0 in Figure 3 one finds directly already $\tau/\tau_0 \approx 100$ at $\chi_2 = 0$ which is about 20 times larger than that of the Davydov soliton under the same conditions. This shows clearly that the major effect in the increase of the lifetime is due to the modified wave function. Therefore, it is very reasonable to refer to the new soliton as the quasi-coherent soliton.

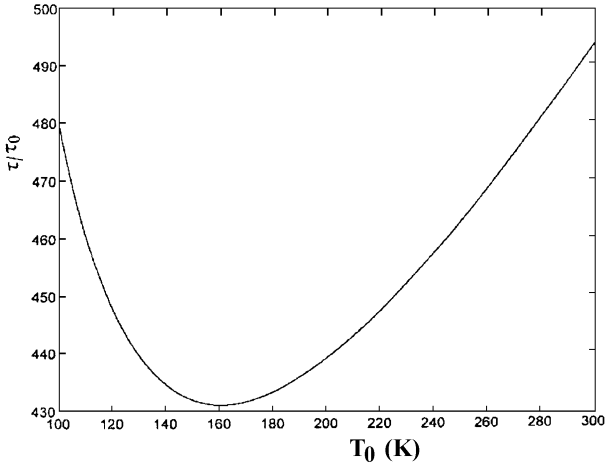

Fig. 9. τ/τ_0 *versus* T_0 relation. Here the solid and dashed lines are the results in the new model in equation (62) and in the Davydov model, respectively.

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. Modifying the wave function and the Hamiltonian of the model, however, we could produce a soliton stable at biological temperatures. This result was obtained considering a new coupled interaction between the acoustic and amide-I vibration modes and a wave function with quasi-coherent two-quanta state. In such a way, the quasi-coherent soliton is a viable mechanism for the bio- energy transport in living systems.

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Appendix A

Utilizing equation (13) and in a semiclassical approximation, we can get [2,27,28]

$$\mathrm{i}\hbar\dot{\varphi}_n = 2\varepsilon_0\varphi_n - 2J(\varphi_{n+1}+\varphi_{n-1}) + \frac{2}{\sqrt{N}}\sum_q [g_1(q)(a_q + a^*_{-q}) \times \varphi_n + g_2(q)((a_q + a^*_{-q})\varphi_{n+1} + q(a_q + a^*_{-q})\varphi_{n-1})]\mathrm{e}^{\mathrm{i}nr_0q}, \tag{A.1}$$

$$\mathrm{i}\hbar\dot{\alpha}_q = \hbar\omega_q\alpha_q + \frac{1}{\sqrt{N}}\sum_n 2[g_1(q)|\varphi_n|^2 + g_2(q)\varphi^*_n\varphi_{n-1} + \varphi^*_n\varphi_{n-1})]\mathrm{e}^{-\mathrm{i}nr_0q} \tag{A.2}$$

$$\mathrm{i}\hbar\dot{\alpha}^*_{-q} = -\hbar\omega_q\alpha^*_{-q} - \frac{1}{\sqrt{N}}\sum_n 2[g_1(q)|\varphi_n|^2 + g_2(q)(\varphi^*_n\varphi_{n-1} + \varphi^*_n\varphi_{n-1})]\mathrm{e}^{-\mathrm{i}nr_0q} \tag{A.3}$$

from the generalized Hamilton's equations:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\varphi_n(t) = \frac{\partial}{\partial\varphi^*_n(t)}\langle\Phi|H|\Phi\rangle$$

and

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\alpha_q(t) = \frac{\partial}{\partial\alpha^*_q(t)}\langle\Phi|H|\Phi\rangle$$

where $\alpha_q(t) = \langle\Phi|a_q|\Phi\rangle$,

$$\langle\Phi|H|\Phi\rangle = \sum_n 2\{\varepsilon_0|\varphi_n|^2 - J\varphi^*_n(\varphi_{n+1}+\varphi_{n-1}) + \frac{1}{\sqrt{N}}\sum_q [g_1(q)(\alpha^*_{-q}+\alpha_q)|\varphi_n|^2 + g_2(q) \times (\alpha^*_{-q}+\alpha_q)(\varphi^*_n\varphi_{n+1} + \varphi^*_n\varphi_{n-1})]\mathrm{e}^{\mathrm{i}nr_0q}\} + \sum_q(\hbar\omega_q|\alpha_q|^2 + \frac{1}{2}\hbar\omega_q).$$

In the above calculation we utilized equations (10, 11) and [24]

$$\langle\Phi(t)|\sum_n(B^+_nB_{n+1} + B_nB^+_{n+1})|\Phi(t)\rangle = 2\sum_n(\varphi^*_n\varphi_{n+1} + \varphi^*_{n+1}\varphi_n)$$

$$\langle\Phi(t)|\sum_n(u_{n+1} - u_{n-1})B^+_nB_n|\Phi(t)\rangle = 2\sum_{n,q} g_1(q)(\alpha_q + \alpha^*_{-q})|\varphi_n|^2\,\mathrm{e}^{\mathrm{i}nqr_0}$$

We can also get a nonlinear Schrödiger equation for $\varphi_n(t)$ in the continuum approximation from equations (A1–A3) [2,27,28]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\varphi(x,t) = 2(\varepsilon_0 - 2J)\varphi(x,t) - 2Jr_0^2\frac{\partial^2\varphi(x,t)}{\partial x^2} - 2G_\mathrm{p}|\varphi(x,t)|^2\varphi(x,t) \tag{A.4}$$

It has the envelope soliton solution

$$\varphi(x,t) = \left(\frac{\mu_\mathrm{p}}{2}\right)^{1/2}\mathrm{sech}\left[\frac{\mu_\mathrm{p}}{r_0}(x-vt)\right] \times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{\hbar^2vx}{2Jr_0^2} - E_\mathrm{sol}t\right)\right] \tag{A.5}$$

where

$$\mu_\mathrm{p} = \frac{2(\chi_1+\chi_2)^2}{w(1-s^2)J}, \quad G_\mathrm{p} = \frac{8(\chi_1+\chi_2)^2}{w(1-s^2)J}$$
$$s = v/v_0 \qquad v_0 = r_0(w/M)^{1/2}. \tag{A.6}$$

Appendix B

The partial diagonalization of the Hamiltonian implies the diagonalization of that part of the Hamiltonian in equation (24) which does not involve the creation and annihilation operators of new phonons equation (22). Thus the condition imposed into the functions $C_j(x)$ contained in equation (27) 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

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

For the above expression of $V(x)$ in equation (26) there is only one bound state in equation (B.1)

$$C_s(x) = \left(\frac{\mu_\mathrm{p}}{2r_0}\right)^{1/2}\mathrm{sech}(\mu_\mathrm{p}x/r_0)\exp\left[\mathrm{i}\hbar vx/2Jr_0^2\right] \tag{B.2}$$

with energy

$$E_s = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2v^2}{4Jr_0^2} - J\mu_\mathrm{p}^2\right] \tag{B.3}$$

and unbounded(delocalized) states

$$C_k(x) = \frac{\mu_\mathrm{p}\tanh(\mu_\mathrm{p}x/r_0) - \mathrm{i}kr_0}{\sqrt{Nr_0[\mu_\mathrm{p} - \mathrm{i}kr_0]}}\exp\left[\mathrm{i}kx + \mathrm{i}\hbar vx/2Jr_0^2\right] \tag{B.4}$$

with energy

$$E_k = 2\left[\varepsilon_0 - 2J - \frac{\hbar^2v^2}{2Jr_0^2} + J(kr_0)^2\right]. \tag{B.5}$$

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:

$$\int_{-\infty}^{\infty}\mathrm{d}x\,C^*_k(x)C_{k'}(x) = \delta(kr_0 - k'r_0),$$
$$\int_{-\infty}^{\infty}\mathrm{d}x|C_k(x)|^2 = 1, \quad \int_{-\infty}^{\infty}\mathrm{d}x\,C^*_s(x)C_k(x) = 0$$

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

In getting equation (B.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 we mainly use a discrete description. The continuous description is transformed into a discrete one according to the rules

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

Utilizing equations (24, 25, 27) and (28), then the partially diagonalized Hamiltonian in the new representation is just equation (29).

Appendix C

We now calculate $U(k, k'', t)$ in equation (46) utilizing the coherent state $|u\rangle$ [14,30] defined by $b_q|u\rangle = u_q|u\rangle$ with

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

Utilizing the coherent state $|u\rangle$, the $U(k, k'', t)$ in equation (46) can be represented by

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

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 we can show 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 equation (C.1) equals

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

The second matrix element in equation (C.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:

$$\langle u_k''|\exp[-\mathrm{i}\omega(b_k^+ b_k + \tau^* b_k + b_k^+\tau + \tau^*\tau)]|u_k\rangle =$$
$$\exp\left[-\frac{1}{2}(|u_k''|^2 + |u_k|^2 - \mathrm{i}\omega|\tau|^2 t\right]$$
$$\times\int_{y^*(t)=u''^*}^{y(0)=u_q} D(y^*, y)\exp[\mathrm{i}T(y^*, y)] \qquad \text{(C.2)}$$

where

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

We can evaluate the path integral by standard techniques. The result for equation (C.2) is

$$\exp\left\{-\frac{1}{2}(|u_k''|^2 + |u_k|^2 + u_k''^* u_k \mathrm{e}^{-\mathrm{i}\omega t}\right.$$
$$\left.-(1 - \mathrm{e}^{-\mathrm{i}\omega t})(u_t''^*\tau + \tau^* u_k + |\tau|^2)\right\}. \qquad \text{(C.3)}$$

Substituting above the matrix elements obtained into equation (C.1) we get

$$U(k,k'',t) = \frac{\mathrm{e}^{R_n(t)}}{Z_{\mathrm{ph}}}\int \mathrm{d}\Omega(u)\int \mathrm{d}\Omega(u'')(u_k''^* + u_{-k}'')$$
$$\times(u_{-k''}^* + u_{k''})\exp\left\{-\sum_q(|u_q|^2 + |u_q''|^2 - u_q^* u_q''\right.$$
$$\times\exp[(\omega_q - qv)(-\beta\hbar + \mathrm{i}t)] - u_q''^* u_q\exp[-\mathrm{i}(\omega_q - qv)t]$$
$$\left.+\frac{1}{n}\frac{1}{\sqrt{N}}(u_q''\alpha_q + u_q^*\alpha_q^*)(1 - \exp[\mathrm{i}(\omega_q - qv)t])\right)\right\}. \qquad \text{(C.4)}$$

where

$$R_n(t) = \frac{-1}{n^2 N}\sum_k |\alpha_k|^2(1 - \exp[-\mathrm{i}(\omega_k - kv)t]). \qquad \text{(C.5)}$$

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

$$U_a(k,k'',t)=\frac{\exp[\mathrm{i}(\omega_k-kv)t+R_n(t)+\xi_n(t)]}{\exp[\beta\hbar(\omega_k-vk)]-1}\left\{\delta_{kk''}-\frac{\frac{1}{n^2}\frac{1}{N}\alpha_k^*\alpha_{k''}(\exp[\mathrm{i}(\omega_{k''}-k''v)t]-1)(\exp[-\mathrm{i}(\omega_k-kv)t]-1)}{\exp\beta\hbar(\omega_k-vk)]-1}\right\}. \tag{C.6}$$

it is associated with the absorption of a phonon, is

see equation (C.6) above

where

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

We note that the breaking of the translational symmetry by the deformation leads to off-diagonal terms corresponding to violation of wavevector conservation. However, we can prove that these terms are proportional to $\frac{1}{N}\alpha_k^*\alpha_{k''}$ which can be neglected when either $|k|$ or $|k''|$ is large as compared to $4\mu_\mathrm{p}/\pi r_0$ as can be seen in the definition of a_k in equation (33). Furthermore when $-\pi\le kr_0\le\pi$ and $\mu_\mathrm{p}<\pi^2$ the off-diagonal terms are negligible except for a small region at the center of the Brillouin zone. Since the small wavevector terms do not significantly contribute to Γ_n due to the k-dependence of $F(q,k)$, we can, thus, neglect the off-diagonal terms in $U_a(k,k'',t)$ in calculating the Γ_n.

The energy of the soliton state is less than that of the unlocalized exciton in the uniform lattice. Therefore, the parts of $U_a(k,k'',t)$ corresponding to the absorption of a phonon make the major contributions to the sum in equation (46) at the temperature and parameter values of interest, and their off-diagonal terms may also be neglected just as above. Using the result of the $U_a(k,k'',t)$ obtained from the above formulae, from equation (46) we get the decay rate equation (48).

Appendix D

If the soliton velocity approaches zero we can get an analytical expression for $R_2(t)$ and $\xi_2(t)$ at $n=2$ defined in equation (49) or equations (C.5) and (C.7) through inserting equation (33) into equations (C.5) and (C.7) and applying the relation of $\frac{1}{N}\sum_q\to\frac{r_0}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}q$, *i.e.*,

$$\lim_{v\to0}R_2(t)=-R_0\int_{-\infty}^{\infty}\frac{y}{\mathrm{sh}^2y}\times\{[1-\cos(\omega_\alpha ty)]+\mathrm{i}\,\sin(\omega_\alpha ty)\}\mathrm{d}y\quad\left(\text{here } y=\frac{\pi qr_0}{2\mu_\mathrm{p}}\right)$$
$$=-R_0[\mathrm{i}x'\Psi'(1+\mathrm{i}x')+\Psi(1+\mathrm{i}x')-\Psi(1)] \tag{D.1}$$

where

$$R_0=\frac{4(\chi_1+\chi_2)^2}{\pi\hbar w}\left(\frac{M}{w}\right)^{1/2}=\frac{2J\mu_\mathrm{p}r_0}{\pi\hbar v_0},\quad\omega_\alpha=\frac{2\mu_\mathrm{p}}{\pi}\left(\frac{w}{M}\right)^{1/2}. \tag{D.2}$$

Ψ is the digamma function, Ψ'Å is its derivative and $x'=\omega_\alpha t=K_\mathrm{B}T_0t/\hbar$.

$\xi_2(t)$ can be easily evaluated when $v\approx0$ and $R_0<1$ at sufficiently high temperature $T>T_0(T_0=\hbar\omega_a/K_\mathrm{B})$

$$\xi_2(t)=\frac{-R_0}{\omega_\alpha}\left[\frac{T}{T_0}\right]\int_0^\infty\mathrm{d}\omega_k\frac{\sin^2\left[\frac{1}{2}\omega_kt\right]}{\mathrm{sh}^2(\omega_k/\omega_\alpha)}=\frac{R_0T}{T_0}[1-\pi\omega_\alpha t\coth(\pi\omega_\alpha t)] \tag{D.3}$$

where we use the relation $\exp(\beta\hbar\omega_k)\approx1+\beta\hbar\omega_k$.

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

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

$$\xi_2(t)\approx-\pi R_0k_\mathrm{B}Tt/\hbar \tag{D.5}$$

(where we approximated $\coth\frac{1}{2}\omega_\alpha t\sim1$), *i.e.*,

$$\lim_{t\to\infty}\xi_2(t)=-\eta t,\ \eta=\pi R_0/\beta\hbar=\pi R_0k_\mathrm{B}T/\hbar. \tag{D.6}$$

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 p parameter values of interest and can be neglected. Furthermore, since $R_0<1$ (but it is not very small, about $R_0\approx0.529$) and $T_0<T$ (but it is not too small, about $T_0\approx294$ K) and $R_0T/T_0<1$ for the protein molecules, one can evaluate the integral in equation (48) by using the following approximation and utilizing the above results

$$\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty \mathrm{d}t \exp\left\{-\mathrm{i}[2J(k'r_0)^2+\frac{4}{3}J\mu_\mathrm{p}^2-\hbar\omega_k]t/\hbar+R(t)+\xi(t)\right\} \approx \frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)\times[\eta^2+(\delta(k,k')/\hbar)^2]^{-(1-R_0)/2}$$
$$\times\left\{\cos\left(\frac{\pi R_0}{2}\right)\times\cos\left[(1-R_0)\tan^{-1}\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]-\sin\left(\frac{\pi R_0}{2}\right)\times\sin\left[(1-R_0)\tan^{-1}\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]\right\}$$
$$=\frac{1}{\eta\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)[\eta^2+(\delta(k,k')/\hbar)^2]^{-(1-R_0)/2}\cos(\Phi_1+\Phi_2)\approx\frac{1}{\pi\hbar}(2.43\omega_\alpha)^{-R_0}\Gamma(1-R_0)[\eta^2+(\delta(k,k')/\hbar)^2]^{-(1-R_0)/2}$$
$$\times\left[1-\frac{1}{2}\left[\frac{\pi R_0}{2}+(1-R_0)\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]^2\right], \quad \text{(D.7)}$$

of equations (D.4–D.6)

see equation (D.7) above

where

$$\delta(k,k')=2J(k'r_0)^2+\frac{4}{3}\mu_\mathrm{p}^2J-\hbar\omega_k, \Phi_1=\frac{R_0\pi}{2},$$
$$\Phi_2=\left[(1-R_0)\tan^{-1}\left(\frac{\delta(k,k')}{\eta\hbar}\right)\right]. \quad \text{(D.8)}$$

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