PHYSICAL REVIEW E VOLUME 62, NUMBER 5 NOVEMBER 2000

Improvement of the Davydov theory of bioenergy transport in protein molecular systems

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(Received 20 July 1998; revised manuscript received 1 June 2000)

The Hamiltonian and the wave function in the Davydov theory have simultaneously been improved and extended, based on some physical and biological grounds and on results from other models. The equations of motion for the improved Davydov model with a quasicoherent two-quanta state and a new interaction term in the Hamiltonian describe bioenergy transport along the molecular chains in protein molecules by a soliton mechanism. Some elementary properties of the soliton, including the nonlinear coupling energy and greatly increased binding energy of the soliton, are also given. The results obtained suggest that the model could be a candidate for a bioenergy transport mechanism in protein molecules.

PACS number(s): 87.17.Aa, 03.65.−w, 05.40.−a, 71.38.+i

I. INTRODUCTION: THE PHYSICAL AND BIOLOGICAL BACKGROUND TO THE PROBLEM

Many biological processes are associated with bioenergy transport through protein molecules, where energy is released by the hydrolysis of adenosine triphosphate (ATP). This is an important problem in biology. Understanding the mechanism of bioenergy transport in biomacromolecular systems has been a long-standing problem that remains of great interest today. As an alternative to electronic mechanisms [1], one can assume that the energy is stored as vibrational energy in the $C=0$ stretching mode (amide-I) of a polypeptide chain. Following Davydov's idea [2], one can take into account the coupling between the amide-I vibrational quantum (exciton) and the acoustic phonon (molecular displacements) in the lattice. Through the coupling, nonlinear interaction appears in the motion of the vibrational quanta, which could lead to a self-trapped state of the vibrational quantum. The latter plus the deformational lattice together can travel over macroscopic distances along the molecular chains, retaining the wave shape, energy, momentum, and other properties of the quasiparticle. In this way, the bioenergy can be transported as a localized ''wave packet'' or soliton. This is just the Davydov model for the bioenergy transport, which was first proposed by Davydov in the 1970s [2].

Davydov's idea yields a compelling picture for the mechanism of bioenergy transport in protein molecules and consequently has been the subject of a large number of works [3–23]. Problems related to the Davydov model, including the foundation and the accuracy of the theory, the quantum and classical properties, and the thermal stability and lifetimes of the Davydov soliton, have been extensively studied by many scientists [3–23]. However, considerable controversy has arisen in recent years over whether the Davydov soliton is sufficiently stable in the region of biological temperature to provide a viable explanation for bioenergy transport. Many numerical simulations [7–11] have been based essentially on classical equations of motion and are subject to the criticism that they are likely to yield unreliable estimates for the stability of the soliton since the dynamics of the soliton is not being determined by the Schrödinger equation [3]. The simulations based on the $|D_2\rangle$ state [2] (i.e., $|D_2\rangle=\Sigma_n\varphi_n(t)B_n^\dagger|0\rangle_{\rm ex}\exp\{-(i/\hbar)\Sigma_n[\beta_n(t)P_n-\pi_n(t)u_n]\}|0\rangle_{\rm ph}$, where $B_n^\dagger(B_n)$ is the creation (annihilation) operator of an amide-I quantum excitation (exciton) in the site n; u_n is the displacement operator of lattice oscillator in site n; P_n is its conjugate momentum operator; $|0\rangle_{\rm ex}$ and $|0\rangle_{\rm ph}$ are the ground states of the exciton and phonon, respectively; and $\varphi_n(t)$, $\beta_n(t)$, and $\pi_n(t)$ are undetermined functions) generally agree that the stability of the soliton decreases with increasing temperatures and that the soliton is not sufficiently stable in the region of biological temperature. Since the dynamical equations used in the simulations are not equivalent to the Schrödinger equation, the stability of the soliton obtained by these numerical simulations is unavailable or unreliable. The simulations [9] based on the $|D_1\rangle$ state (i.e., $|D_1\rangle=\Sigma_n\varphi_n(t)B_n^\dagger(t)\exp\{\Sigma_q[\alpha_{nq}(t)a_q^\dagger-\alpha_{nq}^*(t)a_q]\}0\rangle$, where $|0\rangle=|0\rangle_{\rm ex}|0\rangle_{\rm ph}$, $a_q^\dagger(a_q)$ is the creation (annihilation) operator of the lattice phonon, and $\alpha_{nq}(t)$ and $\alpha_{nq}^*(t)$ are some undetermined functions) with the thermal treatment of Davydov [8], where the equations of motion are derived from a thermally averaged Hamiltonian, yield the surprising result that the stability of the soliton can be enhanced with increasing temperature. Evidently, this conclusion is not reliable because the Davydov procedure in which one constructs an equation of motion for an average dynamical state from an average Hamiltonian, corresponding to the Hamiltonian averaged over a thermal distribution of phonons, is inconsistent with standard concepts of quantum-statistical mechanics in which a density matrix must be used to describe the system. Therefore, there exists no exact fully quantum-mechanical treatment for the numerical simulation

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1063-651X/2000/62(5)/6989(10)/$15.00

of the Davydov soliton. However, for the thermal equilibrium properties of the Davydov soliton, there is a quantum Monte Carlo simulation [13]. In the simulation, correlations characteristic of solitonlike quasiparticles occur only at low temperatures, about $T < 10\,\mathrm{K}$, for widely accepted parameter values. This is consistent at a qualitative level with the result of Cottingham *et al.* [14]. The latter is a straightforward quantum-mechanical perturbation calculation. The lifetime of the Davydov soliton obtained by using this method is too small (about 10^{-12}–10^{-13} sec) to be useful in biological processes. This shows clearly that the Davydov solution is not a true wave function of the systems. A thorough study in terms of parameter values, different types of disorder, different thermalization schemes, different wave functions, and different associated dynamics leads to a very complicated picture for the Davydov model [10–12]. These results do not completely rule out the Davydov theory, however they do not eliminate the possibility of another wave function and a more sophisticated Hamiltonian of the system having a soliton with longer lifetimes and good thermal stability.

Indeed, the question of the lifetime of the soliton in protein molecules is twofold. In Langevin dynamics, the problem consists of uncontrolled effects arising from the semiclassical approximation. In quantum treatments, the problem has been the lack of an exact wave function for the soliton. The exact wave function of the fully quantum Davydov model has not been known up to now. Different wave functions have been used to describe the states of the fully quantum-mechanical systems [4,5]. Although some of these wave functions lead to exact quantum states and exact quantum dynamics in the $J=0$ state, they also share a problem with the original Davydov wave function, namely that the degree of approximation included when $J\neq 0$ is not known. Therefore, it is necessary to reform Davydov's wave function. Scientists had thought that the soliton with a multiquantum state $(n\geqslant 2)$, for example, the coherent state of Brown *et al.* [4], the quantum state of Kerr *et al.* [12] and Schweitzer *et al.* [14], the two-quantum state of Cruzeiro-Hansson [10] and Förner [21], and so on, would be thermally stable in the region of biological temperature and could provide a realistic mechanism for bioenergy transport in protein molecules. However, the assumption of the standard coherent state is unsuitable or impossible for biological protein molecules because there are innumerable particles in this state and one could not retain conservation of the number of particles of the system. The assumption of a multiquantum state $(n>2)$ along with a coherent state is also inconsistent with the fact that the energy released in ATP hydrolysis (about 0.43 eV) can excite only two quanta of amide-I vibration. On the other hand, the numerical result of the two-quantum model by Förner [21] reveals remarkable differences from one-quantum dynamics, i.e., the soliton with a two-quantum state is more stable than that with a one-quantum state.

Cruzeiro-Hansson [10] had thought that Förner's two-quantum state in the semiclassical case was not exact. Therefore, he constructed a so-called exactly two-quantum state of the semiclassical Davydov system as follows [10]:

$$I\varphi(t)\rangle=\sum_{n,m=1}^{N}\varphi_{nm}(\{u_l\},\{P_l\},t)B_n^{\dagger}B_m^{\dagger}|0\rangle_{\mathrm{ex}}, \tag{1}$$

where B_n $(B_n^{\dagger})$ is the annihilation (creation) operator for an amide-I vibrational quantum (exciton), u_1 is the displacement of the lattice molecules, P_1 is its conjugate momenta, and $|0\rangle_{\mathrm{ex}}$ is the ground state of the exciton. He calculated the average probability distribution of the exciton per site, the average displacement difference per site, and the thermodynamics average of the variable, $P=B_1^{\dagger}B_1-B_2^{\dagger}B_2$, as a measure of localization of the exciton, versus quantity $\nu=Jw/\chi_1^2$ and $\ln\beta(\beta=1/k_BT)$ in the so-called two-quantum state, Eq. (1), where χ_1 is a nonlinear coupling parameter related to the interaction of the exciton-phonon in the Davydov model. Their energies and stability are compared with that of the one-quantum state. From the results of above-thermal averages, he drew the conclusion that the wave function with a two-quantum state can lead to more stable soliton solutions than the wave function with a one-quantum state, and that the usual Langevin dynamics, whereby the thermal lifetime of the Davydov soliton is estimated, must be viewed as underestimating the soliton lifetime.

However, by checking carefully Eq. (1) [10], we can find that the Cruzeiro-Hansson wave function does not represent exactly the two-quantum state. To find out how many quanta the state, Eq. (1), indeed contains, we have to compute the expectation value of the exciton number operator, $\hat{N}=\Sigma_n B_n^{\dagger}B_n$, in this state, Eq. (1), and sum over the sites, i.e., the exciton numbers N are

$$\begin{aligned}N&=\left\langle\varphi\left|\sum_n B_n^{\dagger}B_n\right|\varphi\right\rangle\\&=\sum_{ijlmn}\varphi_{im}^{*}\varphi_{jl}\ {}_{\mathrm{ex}}\langle 0|B_iB_mB_n^{\dagger}B_nB_j^{\dagger}B_l^{\dagger}|0\rangle_{\mathrm{ex}}\\&=\sum_{nj}(\varphi_{nj}^{*}\varphi_{jn}+\varphi_{jn}^{*}\varphi_{jn})+\sum_{nl}(\varphi_{nl}^{*}\varphi_{nl}+\varphi_{ln}^{*}\varphi_{nl})=4,\end{aligned} \tag{2}$$

where we use the relations

$$[B_n,B_j^{\dagger}]=\delta_{nj},\quad \sum_{nl}|\varphi_{nl}|^2=1, \tag{3}$$

$${}_{\mathrm{ex}}\langle 0|B_n^{\dagger}|0\rangle_{\mathrm{ex}}={}_{\mathrm{ex}}\langle 0|B_n^{\dagger}B_n|0\rangle_{\mathrm{ex}}={}_{\mathrm{ex}}\langle 0|B_n^{\dagger}B_mB_l|0\rangle_{\mathrm{ex}}=\cdots=0. \tag{4}$$

Therefore, the state Eq. (1), as it is put forward in [10], deals, in contradiction to the author's statements, with four excitons (quanta) instead of two excitons. Obviously, it is not possible to create the four excitons by the energy released in the ATP hydrolysis (about 0.43 eV). Thus the author's wave function is still not relevant for protein molecules, and his discussion and conclusion are all unreliable and implausible in that paper [10].

We think that the physical significance of the wave function, Eq. (1), is also unclear, or at least is very difficult to understand. As far as the physical meaning of Eq. (1) is concerned, it represents only a combinational state of single-particle excitation with two quanta created at sites n and m; $\varphi_{nm}(\{u_1\},\{P_1\},t)$ is the probability amplitude of particles occurring at the sites n and m simultaneously. In general, n

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

On the basis of the work of Cruzeiro-Hansson, Förner, and others, we improve and extend the Davydov model by changing simultaneously the Hamiltonian and the wave function of the systems. We add new coupling interaction between the acoustic phonons and the amide-I vibrational modes in the original Davydov Hamiltonian, and we replace the one-quantum exciton state in Davydov's wave function by a quasicoherent two-quantum state. Thus, the equation of motion and the properties of the soliton occurring in the new model are completely different from that in the Davydov model. I believe that this model might resolve the controversy regarding the thermal stability and lifetime of the soliton excited in protein molecules. In this paper, we derive the equation of motion of the improved model and give some elementary properties of the new soliton that predict that the new model could be a candidate for a bioenergy transport mechanism in protein molecules. The organization of this paper is as follows. In Sec. II, 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 Sec. III. In Sec. IV, we discuss the properties and thermal stability of the new soliton, and we predict the possibility of the soliton being a suitable candidate for the mechanism of bioenergy transport in protein molecules on the basis of results obtained in this paper.

II. CONSTRUCTION OF THE IMPROVED DAVYDOV MODEL AND THE EXTENDED HAMILTONIAN AND WAVE FUNCTION OF THE SYSTEMS

The results obtained by many scientists over the years show that the Davydov model, whether it be the wave function or the Hamiltonian, is indeed too simple, i.e., it does not denote elementary properties of the collective excitations occurring in protein molecules, and many improvements to it have been unsuccessful, as mentioned above. What is the source of this problem? It is well known that the Davydov theory on bioenergy transport was introduced into protein molecules from an exciton-soliton model in generally one-dimensional molecular chains [24]. Although the molecular structure of the alpha-helix protein is analogous to some molecular crystals, for example acetanilide (ACN) (in fact, both are polypeptides; the alpha -helix protein molecule is the structure of three peptide channels, ACN is the structure of two peptide channels. If comparing the structure of alpha-helix protein with ACN, we find that hydrogen-bonded peptide channels with the atomic structure along the longitudinal direction are the same except for the side group), a lot of properties and functions of the protein molecules are completely different from that of the latter. The protein molecules are both a 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 effects, and mutual correlation are very important in bio-self-organization, including the protein molecules when compared with generally molecular systems [25,26]. Therefore, it is worth studying how we can physically describe these properties. We note that Davydov operation is not strictly correct. Therefore, we think that a basic reason for the failure of the Davydov model is just that it ignores completely the above important properties of the protein molecules.

Let us consider the Davydov model with the present viewpoint. First, as far as the Davydov wave functions, both $|D_1\rangle$ and $|D_2\rangle$, are concerned, they are not true solutions of the protein molecules. On the one hand, there is obviously asymmetry in the Davydov wave function since the phononic part is a coherent state while the excitonic part is only an excitation state of a single particle. It is not reasonable that the same nonlinear interaction generated by the coupling between the excitons and phonons produces different states for the phonon and exciton. Thus, Davydov's wave function should be modified [23], 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 [4] and large-n excitation states [12] are not appropriate for the protein molecules due to the reasons mentioned above. Similarly, Förner's and Cruzeiro-Hansson's two-quantum states do not fulfill the above request. In view of the above discussion, we propose the following wave function of the protein molecular systems:

$$\begin{aligned}|\Phi(t)\rangle &= |\varphi(t)\rangle|\beta(t)\rangle\\ &= \frac{1}{\lambda}\left[I+\sum_n \varphi_n(t)B_n^\dagger+\frac{I}{2!}\left(\sum_n \varphi_n(t)B_n^\dagger\right)^2\right]|0\rangle_{\rm ex}\\ &\quad\times\exp\left\{-\frac{i}{\hbar}\sum_n [\beta_n(t)P_n-\pi_n(t)u_n]\right\}|0\rangle_{\rm ph},\end{aligned} \tag{5}$$

where $B_n^\dagger$ and B_n are boson creation and annihilation operators for the exciton, and $|O\rangle_{\rm ex}$ and $|O\rangle_{\rm ph}$ are the ground states of the exciton and phonon, respectively. u_n and P_n are the displacement and momentum operators of the lattice oscillator at site n, respectively. The $\varphi_n(t)$, $\beta_n(t) = \langle\Phi(t)|u_n|\Phi(t)\rangle$ and $\pi_n(t)=\langle\Phi(t)|P_n|\Phi(t)\rangle$ are three sets of unknown functions, and λ is a normalization constant. We assume hereafter that $\lambda=1$ for convenience of calculation, except when explicitly mentioned.

A second problem arises for the Davydov Hamiltonian [23]. The Davydov Hamiltonian takes into account the resonant or dipole-dipole interaction of the neighboring amide-I vibrational quanta in neighboring peptide groups with an electrical moment of about 3.5 D, but why do we not consider the changes of relative displacement of the neighboring peptide groups arising from this interaction? Therefore, it is reasonable to add the new interaction term $\chi_2(u_{n+1} - u_n)(B_{n+1}^\dagger B_n + B_m^\dagger B_{n+1})$ to Davydov's Hamiltonian to represent 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 change of relative displacement of neighboring peptide groups resulting from this interaction cannot be ignored due to the sensitive dependence of dipole-dipole interaction on the distance between amino acids in the protein molecules, which is a kind of soft condensed matter and bio-self-organization. Thus, we replace Davydov's Hamiltonian by

$$\begin{aligned}H&=H_{\mathrm{ex}}+H_{\mathrm{ph}}+H_{\mathrm{int}}\\&=\sum_n\,[\varepsilon_0B_n^\dagger B_n-J(B_n^\dagger B_{n+1}+B_nB_{n+1}^\dagger)]\\&\quad+\sum_n\left(\frac{P_n^2}{2M}+\tfrac{1}{2}w(u_n-u_{n-1})^2\right)\\&\quad+\sum_n\,[\chi_1(u_{n+1}-n_{n-1})B_n^\dagger B_n+\chi_2(u_{n+1}-u_n)\\&\quad\times(B_{n+1}^\dagger B_n+B_n^\dagger B_{n+1})],\end{aligned}\tag{6}$$

where $\varepsilon_0=\hbar\omega_0=1665\,\mathrm{cm}^{-1}$ is the energy of the exciton (the $C=0$ streching 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 the excitons caused by the molecular displacements, respectively. M is the mass of an amino acid molcule and w is the elasticity constant of the protein molecular chains. J is the dipole-dipole interaction energy 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. (5) and (6) are different from Davydov's. We add a new interaction term, $\Sigma_n\chi_2(u_{n+1}-u_n)(B_{n+1}^\dagger B_n+B_n^\dagger B_{n+1})$, into the original Davydov Hamiltonian. Thus the Hamiltonian now has better symmetry and can also represent the features of mutual correlations of the collective excitations and of collective motions in the protein molecules. We should point out here that the different coupling between the relevant modes was also considered by Takeno *et al.* [22,27,28] and Pang [23] in the Hamiltonian of the vibron-soliton model for one-dimensional oscillator-lattice and protein systems, respectively, but the wave functions of the system they used are different from Eq. (5).

Obviously, the present wave function of the exciton in Eq. (5) is not an excitation state of a single particle, but rather a coherent state, or more accurately, a quasicoherent state. To see this, we can represent the $|\varphi(t)\rangle$ by

$$\begin{aligned}|\varphi(t)\rangle&=\frac{1}{\lambda}\left[1+\sum_n\,\varphi_n(t)B_n^\dagger+\frac{1}{2!}\left(\sum_n\,\varphi_n(t)B_n^\dagger\right)^2\right]|0\rangle_{\mathrm{ex}}\\&\sim\frac{1}{\lambda}\exp\left\{\sum_n\,\varphi(t)B_n^\dagger\right\}|0\rangle_{\mathrm{ex}}\\&=\frac{1}{\lambda}\exp\left\{\sum_n\,[\varphi_n(t)B_n^\dagger-\varphi_n^*(t)B_n]\right\}|0\rangle_{\mathrm{ex}}.\end{aligned}\tag{7}$$

The last representation in Eq. (7) is a standard coherent state. More precisely, the new wave function retains only three terms of the expansion of a standard coherent state, which mathematically is 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, we call $|\varphi(t)\rangle$ a quasicoherent state. However, it is not an eigenstate of the number operator, $\hat{N}=\Sigma_nB_n^\dagger B_n$, since

$$\begin{aligned}\hat{N}|\varphi(t)\rangle&=\sum_n\,B_n^\dagger B_n|\varphi(t)\rangle\\&=\left\{\sum_n\,\varphi_n(t)B_n^\dagger+\left(\sum_n\,\varphi_n\varphi_n(t)B_n^\dagger\right)^2\right\}|0\rangle_{\mathrm{ex}}\\&=2|\varphi(t)\rangle-\left(2+\sum_n\,\varphi_n(t)B_n^\dagger\right)|0\rangle_{\mathrm{ex}}.\end{aligned}\tag{8}$$

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

$$\begin{aligned}N&=\langle\varphi(t)|\hat{N}|\varphi(t)\rangle\\&=\sum_n\,\langle\varphi(t)|B_n^\dagger B_n|\varphi(t)\rangle\\&=\left\{\sum_n\,|\varphi_n(t)|^2+\left(\sum_n\,|\varphi_n(t)|^2\right)\left(\sum_m\,|\varphi_m(t)|^2\right)\right\}\\&=\left(\sum_n\,|\varphi_n(t)|^2\right)\left(1+\sum_m\,|\varphi_m(t)|^2\right)=2,\end{aligned}\tag{9}$$

where we utilize Eq. (4) and the following relations:

$$\sum_n\,|\varphi_n(t)|^2=1,\quad\sum_m\,|\varphi_m(t)|^2=1,\quad[B_n,\;B_m^\dagger]=\delta_{nm}.\tag{10}$$

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. (5), in which each term contributes only an exciton, but it is not an excitation state of two single particles. Hence, as far as the form and meanings of the new wave function are concerned, they are either two-quanta states proposed by Förner [21] and Cruzeiro-Hansson [10] or a standard coherent state proposed by Brown *et al.* [4,2] and Kerr *et al.*'s [12] and Schweitzer *et al.*'s [14] multiquanta states. Therefore, the wave function, Eq. (5), is new for the protein molecular systems. It not only exhibits coherent features of collective excitations of the excitons and phonons caused by the nonlinear interaction generated by the exciton-phonon interaction, which, thus, also makes the wave function of the states of the system symmetrical, but it also agrees with the fact that the energy released in the ATP hydrolysis (about 0.43 eV) may only create two amide-I vibrational quanta which, thus, can also make the numbers of excitons maintain conservation in the Hamiltonian, Eq. (6). 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. (5) and (6), but the wave function of the states of the system in other models, including the one-quantum state [2] and the two-quanta state [10–12] could not. Therefore, the above Hamitonian and wave function, Eqs. (5) and (6), are reasonable and appropriate to the protein molecules.

III. THE EQUATIONS OF MOTION AND THE SOLITON SOLUTION

We now derive the equations of motion from the improved Davydov model. First of all, we give the interpretation of $\beta_n(t)$ and $\pi_n(t)$ in Eq. (5). We know that the phonon part of the new wave function in Eq. (5) depending on the displacement and momentum operators is a coherent state of the normal model creation and annihilation operators. A coherent state for the mode with wave vector q is [2,12,23,25]

$$|\alpha(t)\rangle=\exp\left(\sum_q [\alpha_q(t)a_q^\dagger-\alpha_q^*(t)a_q]\right)|0\rangle_{\text{ph}}. \tag{11}$$

Utilizing the standard transformations

$$\begin{aligned}u_n&=\sum_q\left[\frac{\hbar}{2NM\omega_q}\right]^{1/2}e^{iqnr_0}(a_{-q}^\dagger+a_q),\\ P_n&=i\sum_q\left[\frac{M\hbar\omega_q}{2N}\right]^{1/2}e^{iqnr_0}(a_{-q}^\dagger-a_q),\end{aligned} \tag{12}$$

we can get [12,23] $|\alpha(t)\rangle=|\beta(t)\rangle$, where $|\beta(t)\rangle$ is in Eq. (5), and $\omega_q=2(w/M)^{1/2}\sin(r_0q/2)$, r_0 is the distance between neighboring amino acid molecules, and a_q $(a_q^\dagger)$ is the annihilation (creation) operator of the phonon with wave vector q, where

$$\begin{aligned}\langle\alpha(t)|a_q|\alpha(t)\rangle&=\alpha_q(t)\\ &=\left(\frac{M\omega_q}{2\hbar}\right)^{1/2}\beta_q(t)+i\left(\frac{1}{2M\hbar\omega_q}\right)^{1/2}\pi_q(t),\end{aligned}$$

$$\beta_q(t)=\frac{1}{\sqrt{N}}\sum_n e^{-iqnr_0}\beta_n(t), \tag{13}$$

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

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

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

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\langle\Phi(t)|u_n|\Phi(t)\rangle&=\langle\Phi(t)|[u_n,H]|\Phi(t)\rangle,\\ i\hbar\frac{\partial}{\partial t}\langle\Phi(t)|P_n|\Phi(t)\rangle&=\langle\Phi(t)|[P_n,H]|\Phi(t)\rangle,\end{aligned} \tag{14}$$

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

$$\begin{aligned}M\ddot{\beta}_n(t)=&\,w[\beta_{n+1}(t)-2\beta_n(t)+\beta_{n-1}(t)]+2\chi_1[|\varphi_{n+1}(t)|^2\\ &-|\varphi_{n-1}(t)|^2]+2\chi_2\{\varphi_n^*(t)[\varphi_{n+1}(t)-\varphi_{n-1}(t)]\\ &+\varphi_n(t)[\varphi_{n+1}^*(t)-\varphi_{n-1}^*(t)]\}.\end{aligned} \tag{15}$$

From Eq. (15) we see that the presence of two quanta for the oscillators increases the driving force on the phonon field by that factor when compared with the Davydov theory.

We now derive the equation of motion for the $\varphi(t)$. A basic assumption in the derivation is that $|\Phi(t)\rangle$ in Eq. (5) is a solution of the time-dependent Schrödinger equation [12,23]:

$$i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle=H|\Phi(t)\rangle. \tag{16}$$

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

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle=&\left\{i\hbar\left(\sum_n\dot{\varphi}_n(t)B_n^\dagger\right.\right.\\ &\left.\left.+\sum_n\dot{\varphi}_n(t)\varphi_n(t)B_n^\dagger B_n^\dagger\right)|0\rangle_{\text{ex}}\right\}|\beta(t)\rangle\\ &+|\varphi(t)\rangle\left\{\sum_n\{\dot{\beta}_n(t)P_n-\dot{\pi}_n(t)u_n\right.\\ &\left.+\tfrac{1}{2}[\beta_n(t)\dot{\pi}_n(t)-\dot{\beta}_n(t)\pi_n(t)]\}|\beta(t)\rangle\right\}.\end{aligned} \tag{17}$$

Now left-multiplying the both sides of Eq. (16) by $\langle\Phi(t)|$, we can yield the left-hand side of Eq. (16) to be

$$\begin{aligned}&i\hbar\langle\Phi(t)|\frac{\partial}{\partial t}|\Phi(t)\rangle\\ &\quad=i\hbar\sum_n\varphi_n^*(t)\dot{\varphi}_n(t)\left(\sum_m\varphi_m^*(t)\varphi_m(t)+1\right)\\ &\qquad+\tfrac{5}{4}\sum_n[\dot{\beta}(t)\pi_n(t)-\dot{\pi}(t)\beta_n(t)]\sum_n|\varphi_n(t)|^2.\end{aligned} \tag{18}$$

Similarly, for the right-hand side of Eq. (16) we have [12,23]

$$
\begin{aligned}
&\langle\Phi(t)|(H_{\mathrm{ex}}+H_{\mathrm{ph}}+H_{\mathrm{int}})|\Phi(t)\rangle\\
&\quad=\Bigg\{\sum_n\{\varepsilon_0|\varphi_n(t)|^2-J\varphi_n^*(t)[\varphi_{n+1}(t)+\varphi_{n-1}(t)]\}\\
&\qquad\times\Big(1+\sum_m|\varphi_m(t)|^2\Big)+\Bigg\{\sum_n\{\chi_1[\beta_{n+1}(t)\\
&\qquad-\beta_{n\text{-}1}(t)]|\varphi_n(t)|^2+\chi_2[\beta_{n+1}(t)-\beta_n(t)]\\
&\qquad\times\varphi^*(t)[\varphi_{n+1}(t)-\varphi_{n-1}(t)]\}\Bigg\}\Big(1+\sum_m|\varphi_m(t)|^2\Big)\\
&\qquad+\tfrac{5}{2}W(t)\sum_n|\varphi_n(t)|^2, \qquad (19)
\end{aligned}
$$

where

$$
\begin{aligned}
W(t)&=\langle\beta(t)|H_{\mathrm{ph}}|\beta(t)\rangle\\
&=\sum_n\Big(\frac{1}{2M}\pi_n^2(t)+\tfrac{1}{2}w[\beta_n(t)-\beta_{n-1}(t)]^2\Big)\\
&\quad+\sum_q\tfrac{1}{2}\hbar\omega_q \qquad (20)
\end{aligned}
$$

and utilizing Eqs. (4) and (8)–(10) and the relations

$$
\begin{aligned}
&\sum_m[\beta_{m+1}(t)-2\beta_m(t)+\beta_{m-1}(t)]\beta_m(t)=-\sum_m[\beta_{m+1}(t)-\beta_m(t)]^2,\\
&\langle\Phi(t)|\sum_n(B_n^\dagger B_{n+1}+B_nB_{n+1}^\dagger)|\Phi(t)\rangle=\sum_n[\varphi_n^*(t)\varphi_{n+1}(t)+\varphi_{n+1}^*(t)\varphi_n(t)]\Big(1+\sum_m|\varphi_m(t)|^2\Big),\\
&\langle\Phi(t)|\sum_n(u_{n+1}-u_{n-1})(B_n^\dagger B_n)|\Phi(t)\rangle=\sum_n\{[\beta_{n+1}(t)-\beta_{n-1}(t)]|\varphi_n(t)|^2\}\Big(1+\sum_m|\varphi_m(t)|^2\Big),\\
&\langle\Phi(t)|\sum_n(u_{n+1}-u_n)(B_n^\dagger B_{n+1}+B_nB_{n+1}^\dagger)|\Phi(t)\rangle=\sum_n\{[\beta_{n+1}(t)-\beta_n(t)][\varphi_n^*(t)\varphi_{n+1}(t)+\varphi_{n+1}^*(t)\varphi_n(t)]\}\\
&\qquad\times\Big(1+\sum_m|\varphi_m(t)|^2\Big). \qquad (21)
\end{aligned}
$$

From Eqs. (16)–(19) we can obtain

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\varphi_n(t)&=\varepsilon_0\varphi_n(t)-J[\varphi_{n+1}(t)+\varphi_{n-1}(t)]+\chi_1[\beta_{n+1}(t)\\
&\quad-\beta_{n-1}(t)]\varphi_n(t)+\chi_2[\beta_{n+1}(t)-\beta_n(t)]\\
&\quad\times[\varphi_{n+1}(t)+\varphi_{n-1}(t)]\\
&\quad+\tfrac{5}{2}\Big(W(t)-\tfrac{1}{2}\sum_m[\dot\beta_m(t)\pi_m(t)\\
&\quad-\dot\pi_m(t)\beta_m(t)]\Big)\varphi_n(t). \qquad (22)
\end{aligned}
$$

In the continuum approximation we get from Eqs. (15) and (22)

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\varphi(x,t)&=R(t)\varphi(x,t)-Jr_0^2\frac{\partial^2\varphi(x,t)}{\partial x^2}\\
&\quad-G_p|\varphi(x,t)|^2\varphi(x,t) \qquad (23)
\end{aligned}
$$

and

$$
\frac{\partial\beta(x,t)}{\partial\zeta}=\frac{\partial\beta(x,t)}{\partial x}=-\frac{4(\chi_1+\chi_2)}{w(1-S^2)r_0}|\varphi(x,t)|^2, \qquad (24)
$$

where $\zeta=x-Vt$, $R(t)=\varepsilon_0-2J+\frac{5}{2}\{W(t)-\frac{1}{2}\Sigma_m[\dot\beta_m(t)\pi_m(t)-\dot\pi_m(t)\beta_m(t)]\}$, and $S=V/V_0$. The soliton solution of Eq. (23) is thus

$$
\begin{aligned}
\varphi(x,t)&=\Big(\frac{\mu_P}{2}\Big)^{1/2}\operatorname{sech}[(\mu_P/r_0)(x-x_0-Vt)]\\
&\quad\times\exp\Big\{i\Big[\frac{\hbar V}{2Jr_0^2}(x-x_0)-E_v\frac{t}{\hbar}\Big]\Big\} \qquad (25)
\end{aligned}
$$

with

$$
\mu_P=\frac{2(\chi_1+\chi_2)^2}{w(1-S^2)J},\quad G_P=\frac{8(\chi_1+\chi_2)^2}{w(1-S^2)}. \qquad (26)
$$

Although forms of the above equation of motion and the corresponding solution, Eqs. (23)–(26), 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. (23) and (25), including $R(t)$, G_P, and μ_P, have obvious distinctions from that in the Davydov model. A straightforward result of our model is to increase the nonlinear interaction energy G_P ($G_P=2G_D[1+2(\chi_2/\chi_1)+(\chi_2/\chi_1)^2]$) and the amplitude of the new soliton, and decrease its width due to an increase of $\mu_P(\mu_P=2\mu_D[1+2(\chi_2/\chi_1)+(\chi_2/\chi_1)^2])$ when compared with the Davydov soliton, where $\mu_D=\chi_1^2/w(1-S^2)J$ and $G_D=4\chi_1^2/w(1-S^2)$ are the corresponding values in the Davydov model. Thus the localized feature of the new soliton is enhanced, therefore its stability against the quantum fluctuation and thermal perturbations increased considerably as compared with the Davydov soliton.

IV. THE PROPERTIES OF THE NEW SOLITON AND REMARKS

The soliton energy in the improved model becomes

$$E=\langle\Phi(t)|H|\Phi(t)\rangle=\frac{1}{r_0}\int_{-\infty}^{\infty}2\left[Jr_0^2\left(\frac{\partial\varphi(x,t)}{\partial x}\right)^2+R|\varphi(x,t)|^2-G_p|\varphi(x,t)|^4\right]dx+\frac{1}{r_0}\int_{\infty}^{\infty}\tfrac{1}{2}\left[M\left(\frac{\partial\beta(x,t)}{\partial t}\right)^2+wr_0^2\left(\frac{\partial\beta(x,t)}{\partial x}\right)^2\right]dx=E_0+\tfrac{1}{2}M_{\mathrm{sol}}V^2. \tag{27}$$

The rest energy of the new soliton is

$$E_0=2(\varepsilon_0-2J)-\frac{8(\chi_1+\chi_2)^4}{3w^2J}=E_s^0+W, \tag{28}$$

where $W=[2(\chi_1+\chi_2)^4]/3w^2J$ is the energy of deformation of the lattice. The effective mass of the new soliton is

$$M_{\mathrm{sol}}=2m_{\mathrm{ex}}+\frac{8(\chi_1+\chi_2)^4(9S^2+2-3S^4)}{3w^2J(1-S^2)^3V_0^2}. \tag{29}$$

We utilize Eqs. (4) and (8)–(10) in the above calculations.

In such a case, the binding energy of the new soliton is

$$E_{BP}=\frac{-8(\chi_1+\chi_2)^4}{3Jw^2}. \tag{30}$$

The E_{BP} is larger than that of the Davydov soliton. The latter is $E_{BD}=-\chi_1^4/3Jw^2$. They have the following relation:

$$E_{BP}=8E_{BD}\left[1+4\left(\frac{\chi_2}{\chi_1}\right)+6\left(\frac{\chi_2}{\chi_1}\right)^2+4\left(\frac{\chi_2}{\chi_1}\right)^3+\left(\frac{\chi_2}{\chi_1}\right)^4\right]. \tag{31}$$

We can estimate that the binding energy of the new soliton is about several decades larger than that of the Davydov soliton. This is a very interesting result. It is helpful to enhance thermal stability of the new soliton. Obviously, the increase of the binding energy of the new soliton comes from its two-quanta nature and the added interaction, $\Sigma_i\chi_2(u_{n+1}-u_n)(B_{n+1}^+B_n+B_n^+B_{n+1})$, in the Hamiltonian of the systems, Eq. (6). However, we see from Eq. (31) that the former plays the main role in the increase of the binding energy and the enhancement of thermal stability for the new soliton relative to the latter due to $\chi_2<\chi_1$. The increase of the binding energy results in significant changes of properties of the new soliton, which are discussed as follows.

In comparing various correlations to this model, it is helpful to consider them as a function of a composite coupling parameter like that of Young *et al.* [29] and Scott [3] that can be written as

$$4\pi\alpha_P=(\chi_1+\chi_2)^2/2w\hbar\omega_D, \tag{32}$$

where $\omega_D=(w/M)^{1/2}$ is the band edge for acoustic phonons (Debye frequency). If $4\pi\alpha_P\gg1$, the coupling is said to be strong, and if $4\pi\alpha_P\ll1$, it is said to be weak. Using widely accepted values for the physical parameters for the alpha-helix protein molecule [2–23],

$$\begin{gathered}J=1.55\times10^{-22}\ \mathrm{J},\quad w=(13\text{–}19.5)\ \mathrm{N/m},\\ M=(1.17\text{–}1.91)\times10^{-25}\,\mathrm{kg},\\ \chi_1=62\times10^{-12}\,\mathrm{N},\quad \chi_2=(10\text{–}18)\times10^{-12}\ \ \mathrm{N},\\ r_0=4.5\times10^{-10}\,\mathrm{m},\end{gathered} \tag{33}$$

we can estimate that the coupled constant lies in the region of $4\pi\alpha_P=0.11\text{–}0.273$, but $4\pi\alpha_D=0.036\text{–}0.045$ for the Davydov model, which is a weakly coupled model [3]. Therefore, the new model is not said to be a weakly coupled theory as compared with the Davydov model. Using again the notation of Venzel and Fischer [30], Nagy [31], and Wagner and Kongeter [32], it is convenient to define another composite parameter [3]

$$\gamma=J/2\hbar w_D. \tag{34}$$

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

$$E_{BP}/J=8(4\pi\alpha_P/\gamma)^2/3,\quad M_{\mathrm{sol}}=2m_{\mathrm{ex}}[1+32(4\pi\alpha_P)^2/3]. \tag{35}$$

From the above parameter values, we can obtain $\gamma=0.08$. Utilizing these values, the E_{BP}/J versus $4\pi\alpha$ relations in Eq. (35) are plotted in Fig. 1. However, $E_{BD}/J=(4\pi\alpha_D/\gamma)^2/3$ for the Davydov model (here $M'_{\mathrm{sol}}=m_{ex}[1+2(4\pi\alpha_D)^2/3]$, $4\pi\alpha_D=\chi_1^2/2w\hbar\omega_D$); then the E_{BD}/J versus $4\pi\alpha_D$ relation is also plotted in Fig. 1. From this figure we see that the difference of the soliton binding energies between two models becomes larger with increasing $4\pi\alpha$.

Also, we see clearly from Eqs. (24)–(28) and (31) that the localized feature of our soliton is enhanced due to increases of the nonlinear interaction and of the binding energy of the new soliton resulting from the increases of exciton-phonon interaction in the improved model. Thus, the stability of the soliton against quantum and thermal fluctuations is also en-

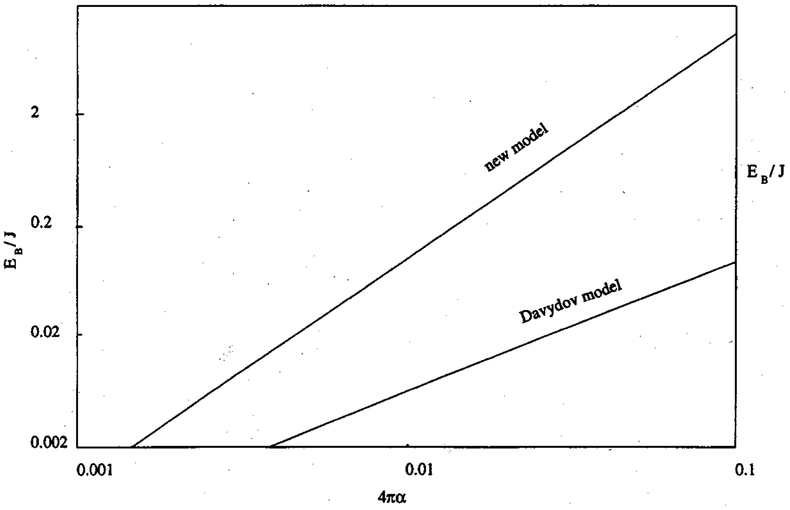

FIG. 1. The binding energy (E_B) of the solitons in our model and the Davydov model in units of dipole-dipole interaction energy (J) vs the coupled constant, $4\pi\alpha$, relations.

hanced considerably. As a matter of fact, the nonlinear interaction energy forming this soliton in the new model is $G_P = 8(\chi_1+\chi_2)^2/(1-S^2)w = 3.8\times10^{-21}$ J, and it is larger than the linear dispersion energy, $J = 1.55\times10^{-22}$ J, i.e., the nonlinear interaction 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 to the soliton theory [2,33]. On the other hand, the nonlinear interaction energy in the Davydov model is only $G_D = 4\chi_1^2/(1-S^2)w = 1.18\times10^{-21}$ J, and it is about three to four times smaller than G_P. Therefore, the stability of the Davydov soliton is weaker as compared with the new soliton. Moreover, the binding energy of the new soliton in the improved model is $E_{BP} = (4.16\text{–}4.3)\times10^{-21}$ J in Eq. (31), which is somewhat larger than the thermal perturbation energy, $k_BT = 4.13\times10^{-21}$ J, at 300 K and about four times larger than the Debye energy, $k_B\Theta = \hbar\omega_D = 1.2\times10^{-21}$ J (here ω_D is the Debye frequency). This shows that transitions of the new soliton to a delocalized state can be suppressed by the large energy difference between the initial (solitonic) state and final (delocalized) state, which is very difficult to compensate for with the energy of the absorbed phonon. Thus, the new soliton is robust against quantum and thermal fluctuations, therefore it has a large lifetime and good thermal stability in the region of biological temperature. In practice, according to Schweitzer *et al.*'s studies (i.e., the lifetime of the soliton increases as μ_P and $T_0 = \hbar V_0 \mu_P / K_B \pi$ increase at a given temperature) [14] and the above obtained results, we could roughly draw an inference that the lifetime of the new soliton will increase considerably as compared with that of the Davydov soliton due to the increases of μ_P and T_0 because the latter are about three times larger than that of the Davydov model. On the other hand, the binding energy of the Davydov soliton $E_{BD} = \chi_1^4/3w^2J = 0.188\times10^{-21}$ J, and it is about 23 times smaller than that of the new soliton, about 22 times smaller than K_BT, and about 6 times smaller than $K_B\Theta$, respectively. Therefore, the Davydov soliton is easily destructed by the thermal perturbation energy and quantum transition effects. Thus we can naturally obtain that the Davydov soliton has a very small lifetime, and it is unstable at the biological temperature 300 K. This conclusion is consistent at a qualitative level with the results of Wang *et al.* [13] and Cottingham *et al.* [14].

However, we do not take into account the influence of the "disorder" in the protein molecules on the stability of the new soliton in the above studies. In practice, the influence actually exists [11,23] because the proteins, strictly speaking, are not a particularly periodic system, and Careri *et al.*'s experiments [34] appear to indicate that even relatively small amounts of disorder in amorphous film of acetanilide (ACN), a proteinlike crystal (i.e., the molecular structure of acetanilide crystal is quite analogic with alpha-helix protein), are enough to destroy the spectral signature of a "soliton." Therefore, it is necessary to investigate the influences of the disorder effects on the stability of the new soliton in the protein. However, this problem is very complicated, and the influences depend also on the concretely molecular structure and the environment conditions of the protein. Therefore, we now discuss briefly this problem by numerical calculation analogous to Förner's method [11] on the basis of Eqs. (15) and (22). Detailed studies on this problem will be discussed in other papers.

We should point out here that an average mass of $\bar{M} = 114m_p = (1.17\text{–}1.91)\times10^{-25}$ kg was used for each amino acid residue in a given site in the above simulation and calculation. However, a real protein molecule is an aperiodic polymer where 20 different amino acid residues occur with molecular weights between $75m_p$ (glycine) and $204m_p$ (tryptophane). This corresponds to a variation between $0.67\bar{M}$ and $1.80\bar{M}$. However, in the improved model only small elongations perpendicular to the protein molecular backbone occur and therefore the influence of the disorder determined by the different masses of the amino acid residues should be much smaller than suggested by the interval given ($0.67\bar{M} \leq M_n \leq 1.80\bar{M}$). To show the stability of the new soliton against the disorder in the sequence of masses in a first series of calculations, we have only increased the mass at site 95. All other masses have been kept equal to $\bar{M}$. Very surprisingly, up to quite large masses of $110\bar{M}$ no obvious perturbations and decays appear in the motion of the new soliton. Meanwhile, the motion of the new soliton does not change much; a quite small fraction of the sound energy is trapped at the impurity and the major fraction is scattered back, and these fractions do not increase up to $M_{95}=950\bar{M}$. From these results one can conclude that an impurity at one site, which may also be some other molecule bound to the protein at this site (like reactive centers such as, e.g., heme groups), does not disturb the soliton at all, unless it does not influence the coupling constants $(\chi_1+\chi_2)$ significantly.

On the other hand, we have also studied the influence of a random series of masses for the whole chain on the soliton. In this study, we introduced here a small parameter α_k which can denote the mass at each point on the molecular chain, i.e., $M_k=\alpha_k\bar{M}$, where the α_k were determined using a random-number generator with equal probability within a prescribed interval. The aperiodicity due to the smaller intervals for α_k, for example $0.67\leqslant\alpha_k\leqslant 100$, does not significantly affect the stability of the new soliton. However, in the case of the large intervals such as $0.67\leqslant\alpha_k\leqslant 260$, the vibrational energy is dispersed. The interval over which the new soliton moves unperturbed $(0.67\leqslant\alpha_k\leqslant 100)$ is evidently larger than the variation of masses of the natural amino acids $(0.67\leqslant\alpha_k\leqslant 1.80)$.

However, the effective perturbation of the changes of mass on the new soliton that we study here is much smaller than the mass interval suggested. This is due to the fact that the amino acide residues in the protein do not move as free particles but are covalently bound in the direction of the main chain, which is perpendicular to the direction of their movement. Thus one can suppose that the effective influence of the mass change in the side groups of the amino acid residues on the soliton should be much smaller than the actual numbers of the masses suggested. Therefore, we can conclude that the aperiodicity or disorder of natural protein molecules should not significantly affect the new soliton formation and stability. In the case of the mass variation of natural amino acid residues $(0.67\bar{M}<M_n<1.80\bar{M})$, virtually no change in the soliton dynamics is found. Thus, the average mass approximation used in the above calculation is certainly justified.

We have also studied the influence of the change of force constant w arising from the disorder of structure on the stability of the new soliton by using numerical calculation. Up to a random variation of $\pm 25\%\ \bar{w}$, we find no change in the dynamics of the new soliton. For $\pm 35\%\ \bar{w}$, the soliton velocity is only somewhat diminished when compared with the case of $\bar{w}$. Finally, for $\pm 45\%\ \bar{w}$, the soliton disperses slowly and the propagation is irregular. In the normal case of force constant $w<30\%\ \bar{w}$, virtually no change in the soliton stability can be obtained. If in addition w is aperiodic, the soliton is stable up to $\pm 15\%\ \bar{w}$, while at $25\%\ \bar{w}$, a slowly dispersive phenomenon of the new soliton occurs.

However, the soliton is more sensitive to the variations in J caused by the disorder of structure when compared with the other parameters, i.e., for variation in J alone or together with the natural mass change, the soliton is stable up to $7\%\ \bar{J}$.

If $(\chi_1+\chi_2)$ alone is aperiodic, which is caused by the disorder of structure, together with the natural mass variation, the $(\chi_1+\chi_2)$ can be varied up to $\pm 25\%\ (\bar{\chi}_1+\bar{\chi}_2)$ without destruction of the soliton. However, if disorder in $\bar{w}$ is also included, $(\chi_1+\chi_2)$ can only be varied up to $\pm 20\%$ and w up to $\pm 32\%\ \bar{w}$. Finally, if all four parameters are randomly varied, the maximal possible disorder that would still occur in the new soliton motion is $\pm 20\%\ \bar{w}$, $\pm 3\%\ \bar{J}$, $\pm 15\%\ (\bar{\chi}_1+\bar{\chi}_2)$, and $0.67\bar{M}\leqslant M\leqslant 1.80\bar{M}$.

In the case of diagonal disorder $\Delta\epsilon_0$ caused by different amino acid side groups and corresponding local geometric distortions due to the imported impurities, we found that for an isolated impurity in the middle of the chain, which causes the change of the energy to be $\Delta\epsilon_{0n}=\epsilon\delta_n$, the soliton can pass the impurity only if $\epsilon<0.6\,\text{meV}$. In other cases it is reflected or dispersed. In the case of a random sequence only for $\epsilon<1.05\,\text{meV}$, the soliton can pass the chain. For higher values of ϵ, the excitation disperses.

However, the actual degree of disorder in protein molecules has been unknown up to now. It is known that protein molecules are a bio-self-organization with high order and coherent features. The order and coherent features of the protein are elementary properties of the protein. These properties are also necessary conditions for the protein to perform its biological functions. Any large disorder appearing in the biological protein means the degeneration of its structure and the disappearance of its biological functions. These phenomena of the protein are not part of the problems discussed in this paper. Therefore, it is not realistic to discuss the influences of large disorder of all physical parameters of the protein on the stability of the new soliton. It is also not possible for large disorder to occur normally in biological protein molecules such as the case of the small amounts of disorder of structure in amorphous films of acetanilide discovered in Careri *et al.*'s experiments [34]. Therefore, for protein molecules it is practical to study the influences of disorder on effective mass and small disorders of other parameters caused by small changes of geometry of the main chain due to the side groups on the stability of the new soliton. However, the results obtained above show that the influences of such disorders on stability of the new soliton are too small to destroy the soliton. Thus, we can conclude that the new soliton with large binding energy is stable in protein molecules. It cannot be destroyed by general or small disorders of the physical parameters in biological protein molecules.

In other words, the new soliton could be thermal stable, because in the improved model increasing the coupling strength of the exciton-phonon interaction and the binding energy of the soliton can suppress influences of the quantum and thermal perturbations in the biological protein molecules. Thus the new soliton is robust and its lifetime could also be larger. Therefore, the improved model could be a likely candidate for bioenergy transport in the protein molecules. The resulting picture is very compelling in living systems since the new soliton with two quasicoherent quanta, which has highly localized features, is a quasiclassical entity which can travel over a macroscopic distance along the molecular chains, retaining wave shape, energy, and momentum.

ACKNOWLEDGMENT

The author would like to acknowledge the National Natural Science Foundation of China for financial support (Grant No. 19974034).

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