PHYSICAL REVIEW E **66**, 023901 (2002)

Comment on "Improvement of the Davydov theory of bioenergy transport in protein molecular systems"

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(Received 2 January 2001; published 14 August 2002)

It is shown that a certain wave function represents a two quanta state of the Davydov-Scott model, contrary to the claims of Pang. Furthermore, Pang's choice of wave function and derivation of equation of motions are criticized. Directions for future work in this area are indicated.

DOI: 10.1103/PhysRevE.66.023901 PACS number(s): 87.17.Aa, 03.65.−w, 87.15.−v, 71.38.−k

Pang [1] criticizes the following wave function that was used in a previous study [2] of the Davydov-Scott model [3]:

$$|\Psi\rangle=\sum_{n,m=1}^{N}\varphi_{nm}(\{u_l\},\{p_l\},t)\hat{B}_n^\dagger\hat{B}_m^\dagger|0\rangle, \tag{1}$$

where $\hat{B}_n^\dagger$ $(\hat{B}_n)$ are the creation (annihilation) operators for amide I excitations in one dimensional chains in proteins and u_l and p_l are, respectively, the displacements and momenta of the sites. Pang claims that Eq. (1) represents a wave function for a state with four quanta. As in biological processes the energy available from the hydrolysis of ATP is only enough for the creation of two quanta, Pang claims that Eq. (1) is not useful and the "discussion and conclusion are all unreliable and implausible in that paper" [2] and that the two quanta states of the Davydov-Scott model are yet to be explored. The number operator for the total number of excitations, $\hat{N}$, is $\hat{N}=\Sigma_{n=1}^{N}\hat{B}_n^\dagger\hat{B}_n$ and it is trivial to show that

$$\hat{N}|\Psi\rangle=2|\Psi\rangle, \tag{2}$$

which demonstrates that Eq. (1) is an eigenvector of the number operator with eigenvalue 2. In Ref. [1], Pang calculates the average $\langle\Psi|\hat{N}|\Psi\rangle$ and finds that this average is equal to 4. However, this is due to the fact that with $\Sigma_{n,m=1}^{N}|\varphi_{nm}|^2=1$, the wave function, as written in Eq. (1), is not normalized and we have $\langle\Psi|\Psi\rangle=2$. Taking the normalization factor into account, the average number of amide I vibrations is 2. So, Eq. (1) is a two quanta state after all.

On an erroneous assumption, Pang proceeds to propose another wave function of the following form (see Eq. (5) in Ref. [1]):

$$|\Phi(t)\rangle=\frac{1}{\lambda}\left[1+\sum_n\varphi_n\hat{B}_n^\dagger+\frac{1}{2!}\left(\sum_n\varphi_n(t)\hat{B}_n^\dagger\right)^2\right]|0\rangle_{\text{ex}}\times\exp\left\{-\frac{\iota}{\hbar}\sum_n[\beta_n(t)\hat{P}_n-\pi_n(t)\hat{u}_n]\right\}|0\rangle_{\text{ph}}. \tag{3}$$

Pang also includes a term in the Hamiltonian that is not taken into account in Ref. [2]: $\chi_2\Sigma_n(u_{n+1}-u_n)(\hat{B}_{n+1}^\dagger\hat{B}_n+\hat{B}_n^\dagger\hat{B}_{n+1})$, but as Pang acknowledges, other authors have considered such a term and it does not change very much the stability of the soliton solution. Thus, the real original contribution by Pang is the proposed form of the wave function (3). This state is a superposition of three states: one with zero amide I excitations (first term), a second with one amide I excitation (second term), and a third with two amide I excitations (third term) and not a superposition of "an excitonic state with two quanta and the ground state of the exciton," as stated in Pang's paper. Depending on the normalization factor λ (or the values of φ_n) it can be anything from a zero excitation state to a two quanta state.

Pang also states that the physical meaning of φ_{nm} in Eq. (1) is unclear. But the meaning is clear: it is the probability amplitude for one excitation to be in site *n* and another excitation to be in site *m*, and the probabilities of finding excitations in each site can be trivially calculated from them. On the other hand, in Pang's state (3) the variable φ_n appears both as the probability amplitude for one excitation and as a parameter in a state with two excitations.

Using Eq. (3), Pang then proceeds to derive equations of motion. The derivation is completely unclear to me. Since the three terms in Pang's wave function are orthogonal, Pang should have got two *different* sets of equations of motion for the probability amplitudes φ_n, one coming from the second term and another from the third term in the wave function (3), which would indicate clearly that another wave function should have been considered.

The aim of the paper seems to be to determine soliton solutions that have binding energies much larger than those of the Davydov soliton [3]. In that respect, Pang's paper is a complete success. However, using more orthodox wave functions, and derivations, it has been found previously that the binding energy of the Davydov soliton grows roughly as the square of the number of amide I excitations, so that states with two quanta have binding energies that are four times those of states with one quantum. This increase still leads to the conclusion that the Davydov soliton is unstable at biological temperatures. However, this thermal instability of the soliton solution means only that at biological temperatures other states take over and the Davydov-Scott model remains a viable mechanism to transport small amounts of energy in proteins. In previous papers [4,5], it was argued that at biological temperatures, the states of the amide I are localized and jump from site to site in a Brownian-like trajectory. Such

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a stochastic mechanism for energy transfer in proteins is an equally, and indeed more robust, form of energy transfer in proteins.

In the light of the recent experimental evidence of Xie *et al.* [6], which shows that the lifetime of amide I vibration in myoglobin is 15 ps, it is fundamental to make experiments that test the role of amide I vibrations in protein function in a more direct way. A theoretical challenge, on the other hand, is to integrate the Davydov-Scott model in the full protein cycle and find out how vibrational energy transfer may eventually lead to a conformational change, the well-known way in which proteins work.

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