# Reply to "Comment on 'Thermodynamic properties of $\alpha$-helix protein: A soliton approach'"

Jia-xin Xiao and Jia-tih Lin
*China Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing, 100080, China and Department of Physics, Tianjin University, Tianjin, 300072, China*
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We make some additional remarks in response to Pang's Comment [preceding paper, Phys. Rev. **49**, 4747 (1994)], and indicate some disagreements to his comment. We explain the condition of satisfying the $\Phi^4$ chain for the lattice vibration.

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We have studied the preceding Comment [1] carefully. We would like to make some additional remarks as a reply to Pang's questions.

(1) The thermal stability of the Davydov soliton is determined by the dynamic equations derived from the thermally averaged Hamiltonian $H_T$

$$H_T=\sum_\nu \rho_\nu H_{\nu\nu} , \tag{1}$$

$$\rho_\nu=\frac{\langle \nu|\exp(-H_{\text{ph}}/k_BT)|\nu\rangle}{\sum_\nu \langle \nu|\exp(-H_{\text{ph}}/k_BT)|\nu\rangle} . \tag{2}$$

The $H_{\nu\nu}$ has been given by Davydov [2] as

$$(H_{\nu\nu})_D=\langle \phi_\nu(t)|H_{\text{ex}}+H_{\text{int}}|\phi_\nu(t)\rangle + \sum_n \langle \nu|U_n^\dagger H_{\text{ph}}U_n|\nu\rangle , \tag{3}$$

$$|\phi_\nu(t)\rangle=\sum_n \psi_n B_n^\dagger|0\rangle U_n|\nu\rangle , \tag{4}$$

$$U_n=\exp\left[\sum_q(\tilde\beta_{qn}^* b_q-\tilde\beta_{qn}b_q^\dagger)\right], \quad \tilde\beta_{qn}=\beta_{qn}e^{-iqna} . \tag{5}$$

In Davydov's form, the influence of the exciton state on the "pure" vibration of the lattice is neglected and restricted to a single excitation $\sum|\psi_n|^2=1$. This approximation is reasonable under the lower excited state.

Cruzeiro *et al.* [3] calculated the thermal average Hamiltonian operator based on the following $(H_{\nu\nu})_{C-S}$ in Eq. (6). The only difference between both works is that Cruzeiro *et al.* made no approximation,

$$(H_{\nu\nu})_{C-S}=\langle \phi_\nu(t)|H_{\text{ex}}+H_{\text{ph}}+H_{\text{int}}|\phi_\nu(t)\rangle , \tag{6}$$

$$(H_T)_{C-S}=\sum_N \left[\varepsilon|\psi_n|^2-J(\psi_n^*\psi_{n-1}e^{-\overline{W}}+\psi_n^*\psi_{n+1}e^{-\overline{W}}) -|\psi_n|^2\frac{1}{\sqrt{N}}\sum_q F(q)e^{iqna}(\beta_{qn}+\beta_{-qn}^*)+|\psi_n|^2\sum_q h\omega_q(\bar\nu_q+|\beta_{qn}|^2)\right]+\frac{1}{2}\sum_q h\omega_q . \tag{7}$$

Using (1), (2), and (4)–(7), they obtained the evolution equations of $\psi_n$ and $\beta_{qn}$

$$ih\frac{d\beta_{qn}}{dt}=-J\{\psi_n^*\psi_{n-1}e^{-\overline{W}}[(\bar\nu_q+1)\beta_{qn-1}-(\bar\nu_q+\tfrac{1}{2})\beta_{qn}] +\psi_{n+1}^*\psi_n e^{-\overline{W}}[\bar\nu_q\beta_{qn+1}-(\bar\nu_q+\tfrac{1}{2})\beta_{qn}]+\psi_n^*\psi_{n+1}e^{-\overline{W}}[(\bar\nu_q+1)\beta_{qn+1}-(\bar\nu_q+\tfrac{1}{2})\beta_{qn}] +\psi_{n-1}^*\psi_n e^{-\overline{W}}[\bar\nu_q\beta_{qn-1}-(\bar\nu_q+\tfrac{1}{2})\beta_{qn}]\}-|\psi_n|^2\frac{1}{\sqrt{N}}F^*(q)e^{-iqna}+|\psi_n|^2h\omega_q\beta_{qn} \tag{8}$$

$$ih\frac{d\psi_n}{dt}=\varepsilon_{C-S}\psi_n-J(\psi_{n-1}e^{-\overline{W}}+\psi_{n+1}e^{-\overline{W}})+\psi_n\sum_q F(q)e^{iqna}(\beta_{qn}+\beta_{-qn}^*)+\psi_n\sum_q h\omega_q(\bar\nu_q+|\beta_{qn}|^2) . \tag{9}$$

The above equations (8) and (9) are Eqs. (10) and (11) given by Pang in his comment [1]. As we know, using the above equations, one cannot obtain equations of motion with an analytical soliton solution under the quasicontinuous approximation. The numerical results of Cruzeiro *et al.* have stated clearly that their soliton solution has some main properties similar to the Davydov solitons. According to the above-mentioned reasons we can take Davydov's form to investigate analytically the thermal properties for the Davydov soliton.

(2) The influence of temperature on excitons can be estimated using the method of statistical summation to

 

compute the energy of excitons and the transfer energy of excitons with different states. According to the above idea based on (1) and (2) we calculated the thermal average of $\psi_n^\dagger\psi_n, \psi_n^\dagger\psi_{n\pm1}, \ldots$, in (7) and analyzed the relations between them. It is the thermal average of every term that is given by Pang's Eqs. (5) in [1].

According to the method of the temperature Green function we have known that the thermal average of the product of the operators will be nonzero only when they have the net effect of not creating or destroying any particles [5]. So we can say that the thermal average of a single creation or destruction operator must be zero and it is incorrect that Pang calculates the average of a single operator in his Eq. (4) [1].

(3) Pang believes that he cannot obtain Eqs. (A16)–(A18) in our paper [4] from his Eqs. (16) and (17) in the comment [1]. In [4] we calculated the thermal average of $u_n$ using Davydov's form,

$$\langle \phi_v | u_n | \phi_v \rangle = \beta_n(t) \tag{10}$$

i.e., (2.11) in [2], and Pang used Eq. (2.17) given by Cruzeiro *et al.* in [3].

$$\langle \psi_v(t) | u_n | \psi_v(t) \rangle = -\sum_q \sum \left[ \frac{h}{2MN\Omega_q} \right]^{1/2} |\phi_m|^2 e^{iqna}(\beta_{qn} + \beta^*_{-qn}) \, . \tag{11}$$

The above difference between (10) and (11) influences neither the equations of motion nor the properties of $\psi_n$, if we change the zero point of the energy using following relation:

$$\varepsilon_{\text{Xiao}} = \varepsilon_{C-S} - \sum_q [h\Omega_q(\bar{v}_q + |\beta_{qn}|^2)] \, . \tag{12}$$

Under the above substitution, Eq. (16) in Pang's paper [1] can be rewritten as

$$ih\frac{d\psi_n}{dt} = \varepsilon_{C-S}\psi_n + Je^{-\overline{W}}(\psi_{n-1} + \psi_{n+1}) + \chi\psi_n(\beta_{n+1} - \beta_{n-1}) \, , \tag{13}$$

and Eq. (A13) in our paper [4] can also be rewritten as

$$ih\frac{d\psi_n}{dt} = \varepsilon_{Xiao}\psi_n + Je^{-\overline{W}}(\psi_{n-1} + \psi_{n+1}) + \chi\psi_n(\beta_{n+1} - \beta_{n-1}) \, . \tag{14}$$

(4) It is common knowledge that the probability amplitude of the excitons obeys the nonlinear Schroedinger (NLS) equation under the quasicontinuous approximations for Davydov theory,

$$ih\frac{\partial}{\partial t}\psi(x,t) = \varepsilon\psi(x,t) - Ja^2\frac{\partial^2}{\partial t^2}\psi(x,t) - G|\psi(x,t)|^2\psi(x,t) \, . \tag{15}$$

But we do not have any reason to require that the square of the probability amplitude, $\Phi = \psi^\dagger(x,t)\psi(x,t)$, also obey the same equation as Pang claims. This is because $\psi$ satisfies the NLS equation but $\psi^\dagger\psi$ does not.

(5) We have proved that the vibration of the lattice can be satisfied by the motion equation of a $\Phi^4$ chain only if the Davydov soliton exists. We can also investigate some properties of the Davydov soliton. This results from the interaction between excitons and phonons under given conditions. According to our comprehension, Davydov solitons include both $\psi(x,t)$ and $\beta(x,t)$. In our paper [4], we obtain that $\beta(x,t)$ satisfies the $\Phi^4$ equation but $\psi(x,t)$ does not:

$$\frac{d^2}{dt^2}Y - v_0^2 Y_{xx} - \omega_0^2\frac{dV}{dY} = 0 \, , \tag{16}$$

where

$$Y(x,t) = \beta(x,t)/a \, , \quad V = \frac{b}{4}\left[Y^2 - \frac{1}{b}\right]^2 - \frac{1}{4b}$$
$$b = a^2w^2(1-s^2)^2/\chi^2 \, , \quad \omega_0^2 = 2\chi^4/MwJ^2(1-s^2) \, . \tag{17}$$

Only with an existing soliton solution can the influence of an exciton on the vibration of a lattice be replaced by an effective double-well potential. Thus $\beta(x,t)$ obeys the $\Phi^4$ equation. But the Hamiltonian corresponding to Eq. (14), namely, the effective Hamiltonian $H'$

$$H' = \sum_n \left[ M\left|\frac{\partial\beta_n}{\partial t}\right|^2 - w(\beta_n - \beta_{n-1})^2 - \tfrac{1}{2}\lambda\beta_n^4 + \gamma\beta_n^2 \right] , \tag{18}$$

does not need to be the Davydov Hamiltonian or part of it. For example, the influence of phonons on excitons can be replaced by a self-action effective potential, thus $\psi(x,t)$ obeys the NLS equation (15) and its effective Hamiltonian $H''$ is

$$H'' = \sum_n [\varepsilon B_n^\dagger B_n - JB_n^\dagger(B_{n+1} + B_{n-1})] - G\sum_n |B_n|^2|B_n|^2 \, . \tag{19}$$

This is obviously not the original Hamiltonian (10).

Additionally, the method given in the paper [4] has been used to discuss some problems about condensed matter, and we have obtained reasonable results [6].


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