# COMMENTS

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

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(Received 11 November 1992; revised manuscript received 9 August 1993)

We disagree with the deduction of the equations of motion for the Davydov soliton and of the results in the paper by Jia-Xin Xiao *et al.* [Phys. Rev. A **44**, 8375 (1991)]. The weakness and faults of the Davydov theory are also indicated.

PACS number(s): 87.10.+e, 87.15.He, 65.90.+i, 05.90.+m

### I. INTRODUCTION

Xiao and Yang have investigated in Ref. [1] (hereafter denoted as paper I) thermodynamic properties (the specific heat), of $\alpha$-helix protein and calculated the critical temperature of the Davydov soliton as well. Their method can be summarized as follows (1) They show and prove that the motion of the Davydov soliton based on the equations of motion of the Davydov soliton and its solutions can satisfy the equation of motion of $\phi^4$ chains, and they deal with some of the thermodynamic properties of the $\alpha$-helix protein, such as the critical temperature for the existence of the Davydov soliton and the linear specific heat of a protein, by using classical statistical mechanics of $\phi^4$ chains. (2) They believe that the influence of the thermal fluctuation on the value of parameters in equations of motion of a soliton can be discussed in terms of the equations of motion of operators for the exciton and phonons. Starting from the Davydov Hamiltonian and Heisenberg's equations of motion for the operators, Xiao and Yang study the thermal effect of the Davydov soliton and use a temperature-dependent coefficient for the nonlinear term in a nonlinear Schrödinger equation they obtained. After reading this paper in detail we disagree with the deduction of these equations and in our conclusions we shall indicate the disagreements in Secs. II and III.

### II. THE EQUATIONS OF MOTION OF OPERATORS FOR THE EXCITONS AND PHONONS

It is known that the Hamiltonian of the Davydov theory in protein molecules is of the form [2]

$$H=\sum_{n=1}^{N} B_n^\dagger[\mathscr{E}B_n-J(B_{n+1}+B_{n-1})] +\frac{1}{2}\sum_{n=1}^{N}[(P_n^2/M)+w(u_n-u_{n-1})^2] +\chi\sum_{n=1}^{N}B_n^\dagger B_n(u_{n+1}-u_{n-1}) , \quad (1)$$

or

$$H=\sum_q \hbar\omega_q(b_q^\dagger b_q+\tfrac{1}{2}) +\sum_{n=1}^{N}[\mathscr{E}B_n^\dagger B_n-J(B_n^\dagger B_{n+1}+B_n^\dagger B_{n+1})] +\frac{1}{\sqrt{N}}\sum_{q,n=1}^{N}F(q)B_n^\dagger B_n(b_q+b_{-q}^\dagger)e^{iqna} , \quad (2)$$

where $F(q)=2\chi i(\hbar/2M\Omega q)^{1/2}\sin(qa)$, $\mathscr{E}=E_0-D$, $u_n=\sum_q(\hbar/2MN\Omega q)^{1/2}(b_q+b_{-q}^\dagger)e^{iqna}$. Here $B_n^\dagger$ ($B_n$) and $b_q^\dagger$ ($b_q$) are the creation (annihilation) operators of exciton and phonon, respectively, $u_n$ is this displacement of the nth amino acid molecule, and $P_n$ is the corresponding momentum. $M$ is the molecular mass and $\chi$ is the exciton-phonon coupling constant. $\mathscr{E}$ is the single molecule excitation energy and $J$ is the nearest neighbor resonance interaction and $\hbar\Omega_q$ is the energy of the phonon. Xiao and Yang have deduced the equations of motion for the operator, $B_n$, starting from the above Hamiltonian and Heisenberg's equation,

$$i\hbar\dot{B}_n=[B_n,H]=\mathscr{E}B_n-J(B_{n+1}+B_{n-1}) +\chi B_n(u_{n+1}-u_{n-1}) \quad (3)$$

$$=\mathscr{E}B_n-J(B_{n+1}+B_{n-1}) +\frac{1}{\sqrt{N}}\chi\sum_q F(q)B_n(b_q+b_{-q}^\dagger)e^{inaq} \quad (4)$$

 

and

$$i\hbar\frac{d}{dt}|B_n^\dagger B_n|=2\mathcal{E}B_n^\dagger B_n-J[B_n^\dagger(B_{n-1}+B_{n+1})+(B_{n-1}^\dagger+B_{n+1}^\dagger)B_n]+\frac{2}{\sqrt{N}}\sum_q B_n^\dagger B_n(b_q+b_{-q}^\dagger)e^{inaq} . \quad (5)$$

These are just Eqs. (A3)–(A4) in the Appendix of paper I (Ref. [1]). According to Ref. [3] Davydov has suggested that the corresponding collective excitation states of the protein molecule can be described by the ansatz wave function

$$|\phi_\nu(t)\rangle=\sum_n\psi_n(t)B_n^\dagger|0\rangle\hat{U}_n(t)|\nu\rangle ,$$

$$\hat{U}_n(t)=\exp\left[\sum_q(\tilde{\beta}_{qn}^*b_q-\tilde{\beta}_{qn}b_q^\dagger)\right] , \quad (6)$$

$$|\nu\rangle=\prod_q|\nu_q\rangle=\prod_q(\nu_q!)^{-1/2}(b_q^\dagger)^{\nu_q}|0\rangle .$$

Now we calculate the thermal average of every term in Eqs. (3) and (4) in terms of the following formula:

$$\langle\langle O(t)\rangle\rangle=\mathrm{Tr}[\rho_{\mathrm{ph}}O(t)]=\sum_\nu(\rho_{\mathrm{ph}})_{\nu\nu}\langle\phi_\nu|O(t)|\phi_\nu\rangle \quad (7)$$

with

$$\rho_{\mathrm{ph}}=\exp(-H_{\mathrm{ph}}/k_BT)/\mathrm{Tr}[\exp(-H_{\mathrm{ph}}/k_BT)] ;$$

$$H_{\mathrm{ph}}=\frac{1}{2}\sum_n\left[\frac{1}{M}P_n^2+w(u_n-u_{n-1})^2\right] .$$

Substituting Eqs. (6) and (7) in Eq. (4) and making use of the following equalities,

$$\langle\phi_\nu|B_n|\phi_\nu\rangle=\langle\phi_\nu|B_n^\dagger|\phi_\nu\rangle=0 ;$$

and

$$\langle\phi_\nu|B_n^\dagger B_n b_q|\phi_\nu\rangle=|\psi_n|^2\tilde{\beta}_{qn}(t)=|\psi_n|^2\beta_{qn}e^{-iqna} ,$$

$$\langle\phi_\nu|B_n^\dagger B_{n\pm1}|\phi_\nu\rangle=\psi_n^*\psi_{n\pm1}\exp(-W_{nn\pm1}) ,$$

$$\langle\nu|\hat{U}_n^\dagger(b_q+b_q^\dagger)\hat{U}_n|\nu\rangle=-(\tilde{\beta}_{qn}+\tilde{\beta}_{-qn}^*) ,$$

$$\langle\nu|\hat{U}_n^\dagger b_q^\dagger b_q\hat{U}_n|\nu\rangle=(\tilde{\nu}_q+|\tilde{\beta}_{qn}|^2) ,$$

$$\tilde{\nu}_q=[\exp(\hbar\Omega q/k_BT)-1]^{-1} ,$$

$$W_{nn\pm1}=\sum_q[-(\tilde{\nu}_q+1)\tilde{\beta}_{qn}^*\tilde{\beta}_{qn\pm1}-\tilde{\nu}_q\tilde{\beta}_{qn}\tilde{\beta}_{qn\pm1}^*+(\tilde{\nu}_q+1)(|\tilde{\beta}_{qn}|^2+|\tilde{\beta}_{qn\pm1}|^2)] , \quad (8)$$

we can obtain that the thermal average of Eq. (4) is zero, instead of Eq. (A16) as in paper I, i.e.,

$$i\hbar\dot{\psi}_n=\mathcal{E}\psi_n-Je^{-\overline{W}}(\psi_{n-1}+\psi_{n+1})+\chi\psi_n(\beta_{n+1}-\beta_{n-1}) , \quad (9)$$

we cannot obtain any equations of motion of $\psi_n$ as noted above from the Davydov theory and Heisenberg's equation. This shows clearly that the equation of motion of the Davydov soliton at a finite temperature cannot be obtained from Heisenberg's equation in the Davydov theory. This result exposes the weakness and fault of the Davydov theory, more precisely, the Davydov wave function. However, Eq. (9) or Eq. (A16) in paper I is the basis of paper I from which Xiao and Yang obtained the critical temperature of the Davydov soliton and the linear specific heat of a protein.

For obtaining this equation, Xiao and Yang have to calculate the thermal average of every term in Eq. (5) or Eq. (A4) in paper I by utilizing Eqs. (7) and (8). In this approximation of $\overline{W}_{nn\pm1}\approx\overline{W}$, they get for the thermal average of Eq. (5),

$$i\hbar\frac{d}{dt}|\psi_n|^2=2\mathcal{E}|\psi_n|^2-Je^{-\overline{W}}[\psi_n^*(\psi_{n+1}+\psi_{n-1})+(\psi_{n+1}^*+\psi_{n-1}^*)\psi_n]+2\chi\psi_n^*\psi_n(\beta_{n+1}-\beta_{n-1}) . \quad (10)$$

This is Eq. (A12) in paper I. By comparing Eq. (10) with Eq. (A14) in paper I,

$$i\hbar\frac{d}{dt}|\psi_n|^2=2\mathcal{E}|\psi_n|^2-J[\psi_n^*(\psi_{n-1}+\psi_{n+1})+(\psi_{n-1}^*+\psi_{n+1}^*\psi_n]+2\chi\psi_n^*(\beta_{N+1}-\beta_{n-1}) , \quad (11)$$

they obtain the corresponding relation

$$J\to J'=Je^{-\overline{W}} . \quad (12)$$

Therefore, again from Eq. (A13) in paper I, i.e.,

$$i\hbar\dot{\psi}_n=\mathcal{E}\psi_n-J(\psi_{n-1}+\psi_{n+1})+\chi\psi_n(\beta_{n+1}-\beta_{n-1}) , \quad (13)$$

and making use of this corresponding relation, they obtain Eq. (9) or Eq. (A16) in paper I.

In Xiao and Yang's deduction, there are at least three problems:

(1) Xiao and Yang attempt to get the equation of $\psi_n$, Eq. (9), from the equation of $|\psi_n|^2$, Eq. (10), but we can only get from Eq. (10) in the continuum limit,

$$i\hbar\frac{\partial}{\partial t}|\psi|^2=(2\mathcal{E}-4Je^{-\overline{W}})|\psi|^2-Ja^2e^{-\overline{W}}\frac{\partial^2}{\partial x^2}|\psi|^2+2\chi a\frac{\partial\beta}{\partial x}|\psi|^2 . \quad (14)$$

According to Xiao and Yang's idea, the approximate method, and $\overline{W}=\frac{1}{2}\alpha_0a|\psi_n|^2\overline{H}f(k_BT)$, and inserting the representation of $\partial\beta/\partial x$, i.e., the solution of Eq. (3) in the text of paper I into Eq. (14), the equation becomes

$$i\hbar\frac{\partial}{\partial t}|\psi|^2\approx(2\mathcal{E}-4J)|\psi|^2-Ja^2\frac{\partial^2}{\partial x^2}|\psi|^2+G(T)|\psi|^2|\psi|^2 .$$

If we let

$$\Phi=|\psi|^2,\quad G(T)=\frac{4a^2\chi^2}{MV_0^2(1-S^2)}[1-\tfrac{1}{4}\overline{H}f(k_BT)] ,$$

we can only get

$$i\hbar\frac{\partial}{\partial t}\Phi(x,t)\approx(2\mathcal{E}-4J)\Phi(x,t)-Ja^2\frac{\partial^2}{\partial x^2}\Phi(x,t)+G(T)\Phi(x,t)^2 .$$

Obviously, this is not the Eq. (9) devised by Xiao and Yang. At the same time, it also is not a standard nonlinear Schrödinger equation, which is not the desired result for Xiao and Yang and us.

(2) On the other hand, due to the fact that

$$U_n(t)=\langle\phi_v|u_n|\phi_v\rangle=-\sum_q\sum_n\left[\frac{\hbar}{2MN\Omega q}\right]^{1/2}|\psi_n|^2e^{iqna}(\tilde{\beta}_{qn}+\tilde{\beta}^*_{-qn}) ,$$

instead of $\langle\phi_v|u_n|\phi_v\rangle=\beta_n(t)$, which is devised by Xiao and Yang, and making use of Eq. (8), we can only get for the thermal average of Eq. (5),

$$i\hbar\frac{d}{dt}|\psi_n|^2=2\mathcal{E}|\psi_n|^2-J[\psi^*_n(\psi_{n+1}e^{-\overline{W}_{nn+1}}+\psi_{n-1}e^{-\overline{W}_{nn-1}})+(\psi^*_{n+1}e^{-\overline{W}_{n+1n}}+\psi^*_{n-1}e^{-\overline{W}_{n-1n}})\psi_n]-\frac{2}{\sqrt{N}}\sum_q F(q)|\psi_n|^2(\tilde{\beta}_{qn}+\beta^*_{-qn})e^{iqna}$$

instead of Eq. (10). Therefore, Eq. (A12) in paper I is also incorrect.

(3) The origin of Eq. (A14) in paper I is ambiguous. Xiao and Yang do not explain clearly this equation. On the other hand, the corresponding relation, $J\to J'=Je^{-\overline{W}}$ for Eq. (13), is also incorrect, that is to say, the equation of motion of $\psi_n(t)$ at finite temperature is not Eq. (9). In practice, the equations of motion of the Davydov soliton at finite temperature can be obtained from the Hamilton equation in the quantum soliton problem through utilizing Eqs. (2), (6), (7), (8), and

$$\langle H\rangle=\overline{\langle\phi_v|H|\phi_v\rangle}\sum_v\rho_{vv}\langle\phi_v|H_{\rm ex}+H_{\rm ph}+H_{\rm int}|\phi_v\rangle$$
$$=\sum_n\left\{\mathcal{E}|\psi_n|^2-J(\psi^*_n\psi_{n-1}e^{-\overline{W}_{nn-1}}+\psi^*_n\psi_{n+1}e^{-\overline{W}_{nn+1}})-|\psi_n|^2\left[\sum_q\frac{1}{\sqrt{N}}F(q)e^{iqna}(\tilde{\beta}_{qn}+\tilde{\beta}^*_{qn})-\sum_q\hbar\Omega_q(\tilde{\nu}_q+|\tilde{\beta}_{qn}|^2)\right]\right\}+\sum_q\tfrac{1}{2}\hbar\Omega_q \tag{15}$$

(note: We cannot adopt $(H_{vv})_D=\langle\phi_v|H_{\rm ex}+H_{\rm int}|\phi_v\rangle+\sum_n\langle v|U^+_nH_{\rm ph}U_n|v\rangle$ for the wave function (6), strictly speaking). They are of the form [5]

$$i\hbar\frac{d\psi_n}{dt}=\frac{\partial\langle H\rangle}{\partial\psi^*_n}=\mathcal{E}\psi_n-J(e^{-\overline{W}_{nn-1}}\psi_{n-1}+e^{-\overline{W}_{nn+1}}\psi_{n+1})-\psi_n\left[\frac{1}{\sqrt{N}}\right]\sum_q F(q)e^{iqna}(\tilde{\beta}_{qn}+\tilde{\beta}^*_{-qn})+\psi_n\sum_q[\hbar\Omega_q(\tilde{\nu}+|\tilde{\beta}_{qn}|^2)] , \tag{16}$$

$$i\hbar\frac{d\tilde{\beta}_{qn}}{dt}=\frac{\partial\langle H\rangle}{\partial\tilde{\beta}^*_{qn}}=-J\Big\{\psi^*_n\psi_{n-1}e^{-\overline{W}_{nn-1}}[(\tilde{\nu}_q+1)\tilde{\beta}_{qn-1}-(\tilde{\nu}_q+\tfrac{1}{2})\tilde{\beta}_{qn}]+\psi^*_n\psi_{n+1}e^{-\overline{W}_{nn+1}}[(\tilde{\nu}_q+1)\tilde{\beta}_{qn+1}-(\tilde{\nu}_q+\tfrac{1}{2})\tilde{\beta}_{qn}]+\psi^*_{n-1}\psi_ne^{-\overline{W}_{n-1n}}[\tilde{\nu}_q\tilde{\beta}_{qn-1}-(\tilde{\nu}_q+\tfrac{1}{2})\tilde{\beta}_{qn}]+\psi^*_{n+1}\psi_ne^{-\overline{W}_{n+1n}}[\tilde{\nu}_q\tilde{\beta}_{qn+1}-(\tilde{\nu}_q+\tfrac{1}{2})\tilde{\beta}_{qn}]\Big\}-|\psi_n|^2\left[\frac{1}{\sqrt{N}}F^*(q)e^{-iqna}+\hbar\Omega_q\tilde{\beta}_{qn}\right] . \tag{17}$$

Adopting Xiao and Yang's or Davydov's approximation,

$$\overline{W}_{nn\pm1}\approx\overline{W}=\tfrac{1}{2}a\alpha_0|\psi_n|^2\overline{H}f(k_BT) ,$$

we also cannot obtain Eqs. (A16)–(A18) in paper I from Eqs. (16) and (17).

Thus, the corresponding relation, Eq. (12), and the equations of motion of the Davydov soliton at finite temperature in paper I, are invalid. Therefore, the results of the critical temperature, $T_c$, of the Davydov soliton and the linear specific heat of a protein obtained from these equations (A16)–(A18) in paper I are also unreliable.

In addition, from the above-mentioned study, we also find a weakness in the Davydov theory. Now we discuss this problem. It is known that the equation of motion of the soliton in the protein molecules can be found out by using the following four methods. Hamilton's equations [2–5,8,9]

$$i\hbar\frac{\partial\psi_n}{\partial t}=\frac{\sigma\langle H\rangle}{\delta\psi^*_n}$$

and

$$i\hbar\frac{\partial\beta_{qn}}{\partial t}=\frac{\delta\langle H\rangle}{\delta\beta^*_{qn}} ,$$

where

$$\langle H\rangle=\sum_{v}(\rho_{\rm ph})_{vv}\langle\phi_v|H|\phi_v\rangle$$

and the Euler-Lagrange equation [6,10]

$$\frac{\partial\mathcal{L}}{\partial\psi_n^*}=\frac{\partial}{\partial t}\frac{\delta\mathcal{L}}{\delta\dot{\psi}_n^*}+\frac{\partial}{\partial x}\frac{\delta\mathcal{L}}{\delta(\partial\psi^*/\partial x)}\ ,$$

etc., where

$$\mathcal{L}=\langle\phi_v|\tfrac{1}{2}i\hbar\frac{\overleftrightarrow{\partial}}{\partial t}-H|\phi_v\rangle$$
$$=\frac{i\hbar}{2}\sum_n(\dot{\psi}_n\psi_n^*-\dot{\psi}_n^*\psi_n)+\tfrac{1}{2}i\hbar\sum_{nq}(\dot{\tilde{\beta}}_{qn}\tilde{\beta}_{qn}^*-\dot{\tilde{\beta}}_{qn}^*\tilde{\beta}_{qn})$$
$$-\langle\phi_v|H|\phi_v\rangle\ ,$$

with

$$\langle\phi_v|i\hbar\frac{\overleftrightarrow{\partial}}{\partial t}|\phi_v\rangle=i\hbar\langle\phi_v|\left[\frac{\partial}{\partial t}|\phi_v\rangle\right]-i\hbar\left[\frac{\partial}{\partial t}\langle\phi_v|\right]|\phi_v\rangle$$

and the Schrödinger equation [7,10,12] is

$$\langle\phi_v|\left[i\hbar\frac{\partial}{\partial t}|\phi_v\rangle\right]=\langle\phi_v|[H|\phi_v\rangle] \tag{18}$$

and the Heisenberg equation [8–13] is

$$i\hbar\frac{\partial}{\partial t}\langle\phi_v|B_n|\phi_v\rangle=\langle\phi_v|[B_n,H]|\phi_v\rangle\ ,$$

and

$$t\hbar\frac{\partial}{\partial t}\langle\phi_v|b_q|\phi_v\rangle=\langle\phi_v|[b_q,H]|\phi_v\rangle\ ,$$

and so on, where $H$ is a Hamiltonian of the system. In the general case, the equation of motion of the soliton obtained from the four methods above should be basically the same and consistent for the same Hamiltonian or theory. (Certainly, the equations of motion of the soliton can also be obtained from the variational method.) However, this conclusion is contrary to the Davydov theory; for example, the equations of motion of the Davydov soliton cannot be obtained at all from Heisenberg's equation in the Davydov theory as stated above. This is a weakness or fault of the Davydov theory. This shows that the Davydov theory is not self-consistent. The crucial reason for the fault of the inconsistency mentioned above is that the Davydov wave function, Eq. (6), is imperfect and improper for the protein molecules. According to the results from our studies [14], the protein molecules are a biological self-organization in which a collective excitation results from a localized fluctuation and the deformation of the structure caused by the energy released by ATP (adenosine tripohosphate molecules) hydrolysis has coherent features, that is to say, the state of both excitons and phonons is a coherent state [14]. Therefore, the excitons and the phonons should be described by a coherent wave function. However, the Davydov wave function, Eq. (6), is not symmetric: part of wave function of the phonon is coherent, but that of the exciton is not in Eq. (6). The latter is an eigenstate of the number operator $N=\sum_n B_n^\dagger B_n$; this describes the state of a single (collective) exciton, i.e., the Davydov wave function is restricted to the subspace of a single (collective) excitation, $N=1$. Therefore, in the Davydov theory a soliton is exactly one exciton (spread out over several sites) plus the resulting acoustic deformation, just so the Davydov theory exhibits the above difficulty.

However, if we adopt the following quasicoherent wave function [8–19],

$$|\phi_v\rangle=\frac{1}{\Lambda}\left[1+\sum_n\psi_n(t)B_n\right]^\dagger|0\rangle_{\rm ex}\hat{U}_n(t)|v\rangle\ ,$$

in our theory to describe the collective excitation and the collective motion resulting from the energy released by ATP hydrolysis in the protein molecules, we may avoid the above-mentioned difficulty in the Davydov theory, i.e., the equations of motion of the soliton can also be deduced from Heisenberg's equation for the operators now, and it is basically the same as the one obtained from the other three methods mentioned above. The thermal average of the equation of motion of the soliton is not zero now in our theory. In fact our wave function, Eq. (18), is not an eigenstate of the number operator $N_n=\sum_n B_n^\dagger B_n$. It belongs to a large space with $N=0,1$. It represents rather a superposition of a state with no exciton and a state with one exciton. If it is represented as

$$|\phi_v\rangle\geq\frac{1}{\Lambda}\exp\left[\sum_n\psi_n(t)B_n^\dagger\right]|0\rangle_{\rm ex}\hat{U}_n(t)|v\rangle\ ,$$

then this is a coherent state. Therefore, our wave function can better represent the nature of collective excitation in the protein molecules. Therefore, if we adopt again the following more sophisticated Hamiltonian in our theory, i.e., [8–19]

$$H=\left[\frac{1}{2m}\sum_n p_n^2+\tfrac{1}{2}m\omega_0^2\sum_n r_n^2-\tfrac{1}{2}m\omega_1^2\sum_n r_n r_{n+1}\right]$$
$$+\left[\frac{1}{2M}\sum_n P_n^2+\tfrac{1}{2}w\sum_n(u_n-u_{n-1})^2\right]$$
$$+\left[\tfrac{1}{2}m\chi_1\sum_n(u_{n+1}-u_{n-1})r_n^2\right.$$
$$\left.+m\chi_2\sum_n(u_{n+1}-u_n)r_n r_{n+1}\right]\ , \tag{19}$$

simultaneously, where $r_n$ and $p_n=m\dot{r}_n$ are the normal coordinate of the $n$th oscillator and its canonical conjugate momentum, respectively; $w_0$ and $w_1$ are the diagonal and nondiagonal elements of the dynamic matrix and $w_0$ is also the Einstein frequency. $2\chi_1=\partial w_0^2/\partial u_n$ and $2\chi_2=\partial\omega_1^2/\partial u_n$ are a change of energy of vibration of molecular lattice and the coupling energy between the neighboring molecules by unit extension. Meanwhile, Eq. (19) is also different from Takeno's [20] in content, meaning, form, and terms, then the equations of motion and properties of the soliton in our theory are different from the Davydov soliton. In Eq. (19), our soliton contains more than one exciton, this state being a coherent superposition of zero plus one "inner excitation," which is consistent with the proposition in current research in which it is mostly assumed that the soliton in proteins should contain more than one exciton. Meanwhile, the results, for example, the soliton energy, the specific heat, and the lifetimes of the soliton obtained from our theory are more justifiable compared with the Davydov solution [8–13,15–17], it more closely approaches the experimental data in the protein molecules [8,15–17]. Our theory could possibly address the main problems that the Davydov theory faces, i.e., thermal stability and the lifetime of the soliton. In practice, after studying the influence of the temperature on the soliton, we find that it is still quite stable in the biological temperature range [15,18], and its lifetime can achieve $10^{-9}$–$10^{-8}$ at 310 K [18], which is more than ten thousand times greater than one of the Davydov soliton. The critical temperature of the soliton is about 348–357 K [19].

## III. THE DAVYDOV SOLITON CANNOT SATISFY THE EQUATION OF MOTION OF A $\phi^4$ CHAIN

It is incorrect to say that the Davydov soliton satisfies the equation of motion of a $\phi^4$ chain, which Xiao and Yang do in paper I. It is known that the Davydov soliton is a dynamic self-sustaining entity arising from a self-trapping of amide-I vibrons (excitons) interacting with low-frequency longitudinal phonons, namely, it is a intramolecular excitation (exciton) (spread out over several sites) motion together with the local chain deformation. The Davydov soliton follows a nonlinear Schrödinger equation,

$$\left[i\hbar\frac{\partial}{\partial t}-\Lambda'+a^2J\frac{\partial^2}{\partial x^2}-2\chi a\frac{\partial}{\partial x}\beta(x,t)\right]\psi(x,t)=0 \quad (\Lambda'=\mathcal{E}+W-2J)\,, \tag{20}$$

$$\left[\frac{\partial^2}{\partial t^2}-V_0^2\frac{\partial^2}{\partial x^2}\right]\beta(x,t)-\frac{2xa}{M}\frac{\partial}{\partial x}|\psi(x,t)|^2=0 \quad (V_0^2=a^2w/M) \tag{21}$$

or

$$\left[i\hbar\frac{\partial}{\partial t}-\Lambda'+a^2J\frac{\partial^2}{\partial x^2}+\frac{4\chi^2a^2}{MV_0^2(1-S^2)}|\psi(x,t)|^2\right]\psi(x,t)=0 \quad (S^2=V^2/V_0^2)\,. \tag{22}$$

This is just Eqs. (2)–(3) in paper I, instead of the following $\phi^4$ equation

$$\frac{\partial^2}{\partial t^2}\beta(x,t)-V_0^2\frac{\partial^2}{\partial x^2}\beta(x,t)+b\beta^3(x,t)-c\beta(x,t)=0\,, \tag{23}$$

where $b=2\chi^2(1-S^2)w/MJ^2$, $c=2\chi^4/MwJ(1-S^2)$ [Eq. (7) in paper I]. Therefore, the representation of the Davydov soliton obtained from Eqs. (20)–(22) is

$$\psi(x,t)=\left[\frac{\mu a}{2}\right]^{1/2}\text{sech}[\mu(x-x_0-Vt)]\times\exp\left[\frac{\hbar V}{2Ja^2}(x-x_0)-E_{\rm sol}^t/\hbar\right] \tag{24}$$

instead of

$$\beta(x,t)=-\frac{\chi}{w(1-S^2)}\tanh[\mu(x-x_0-Vt)]\,. \tag{25}$$

The latter is the displacement of an amino acid molecule from the equilibrium in the language of the coherent state. Therefore, the physical content of this solution, Eq. (24), is very clear. It is also known for the physical mechanism and concept of the Davydov soliton. However, Xiao and Yang incorrectly deduce the $\phi^4$ equation of $\beta(x,t)$, Eq. (23), from the solutions of the Davydov soliton equations, Eqs. (20)–(21), and assume that the Davydov soliton satisfies the equation of motion of a $\phi^4$ chain. If Xiao and Yang's idea and result for the Davydov soliton satisfying the $\phi^4$ equation, Eq. (23), were right, then the Hamiltonian of the system corresponding to the Eq. (23) would be the Davydov's Hamiltonian or its parts. However, it is now, in fact, of the form

$$H=\sum_n\left\{M\left|\frac{\partial\beta_n(t)}{\partial t}\right|^2-W(\beta_n(t)-\beta_{n-1}(t))^2-\tfrac{1}{2}b\beta_n^4(t)+C\beta_n^2(t)\right\}.$$

However, this is not Davydov's Hamiltonian or its parts. Simultaneously, the problem now facing us is the following: what are the equations of motion of the Davydov soliton? Equations (3) and (6), or Eqs. (2) and (7) in paper I? In fact, they are neither Eqs. (3) and (6), nor Eqs. (2) and (7). In this context, we feel that the Davydov soliton does not satisfy the equation of motion of a $\phi^4$ chain. Therefore, we can also not use classical statistical mechanics chains to deal with some of thermal properties of the $\alpha$-helix protein. Naturally, the results obtained by this way are also unreliable [21,22].

Certainly, the solution of the Davydov soliton, Eq. (24), has a close relationship with one of the displacements of the molecule or the deformation of a chain, Eq. (25). Due to the existence of deformation of the chain, the exciton can become a self-trapped state or the Davydov soliton through the interaction with deformation. The relation between them has basically an analogy with the SLAC pocket model of the confinement of quark in a hadron, the hadron model, in elementary particle physics [23].

The author would like to acknowledge the ICMP for financial support.

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