Temperature effects on vibron solitons

1994 J. Phys. A: Math. Gen. 27 6005

(http://iopscience.iop.org/0305-4470/27/17/031)

J. Phys. A: Math. Gen. 27 (1994) 6005–6013. Printed in the UK

Temperature effects on vibron solitons

Hai-Jun Yu and Yi Xiao†

Department of Physics, Huazhong University of Science and Technology, Wuhan 430074, People's Republic of China

Received 1 December 1993

Abstract. An analytical study of the temperature effects on the vibron soliton of the Takeno model for energy transport in protein is presented, using Davydov's thermally averaged Hamiltonian method. The conditions of the existence of vibron solitons in the model system are found and ideal protein parameters are used to show whether these conditions can be satisfied.

1. Introduction

In recent years interest has been aroused by attempts to apply solid state theory to describe biological processes at the molecular level [1,2]. The problem of the storage and transport of energy in the alpha-helical structure of the protein molecule has been studied by many authors [3–5]. Davydov and his coworkers have shown that the energy of Amide-I($C = 0$) vibration in alpha-helical proteins could be transported in the form of solitons and that this might be responsible for the mechanism of muscle contraction [6]. In the Davydov theory, the solitons are formed through the coupling of molecular vibration exciton nonlinearly with longitudinal phonons. Takeno modified Davydov's theory and proposed a coupled oscillator lattice model in which a relevant mode of molecular vibrations of a given molecule in a one-dimensional molecular crystal is taken to be coupled linearly with the others and nonlinearly coupled with lattice vibrations. The soliton formed in such an oscillator system was called a vibron soliton [4]. Takeno considered that a vibron soliton would be more appropriate to describe vibrational energy transfer in α-helical proteins. Recently many related studies of temperature effects on Davydov solitons [6–9] have been made by Davydov and others. However, the study of temperature effects on vibron solitons is still lacking. In this paper, we will investigate the temperature effects on the vibron solitons by using Davydov's thermally averaged Hamiltonian method [6,9].

This paper is organized as follows: in section 2 the model Hamiltonian of the system is presented and the corresponding temperature-dependent equations of motion are derived. In section 3, two types of soliton solutions are presented. Finally section 4 is discussion and conclusion.

2. Hamiltonian and basic equations of motion

The total Hamiltonian of the one-dimensional Takeno model is composed of three parts:

† To whom all correspondence should be addressed.

0305-4470/94/176005+09$19.50

$$\begin{aligned}
\hat{H} &= \hat{H}_{\mathrm{L}} + \hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{I}} \\
\hat{H}_{\mathrm{L}} &= \sum_n \left[\tfrac{1}{2} M \hat{u}_n^2 + \tfrac{1}{2} K (\hat{u}_n - \hat{u}_{n-1})^2 + \tfrac{1}{3} K_1 (\hat{u}_n - \hat{u}_{n-1})^3 \right] \\
\hat{H}_{\mathrm{A}} &= \tfrac{1}{2} \sum_n (m \hat{\dot{q}}_n^2 + m\omega_0^2 \hat{q}_n^2) - \tfrac{1}{2} L \sum_n (\hat{q}_n \hat{q}_{n-1} + \hat{q}_n \hat{q}_{n+1}) \\
\hat{H}_{\mathrm{I}} &= \tfrac{1}{2} \sum_n \frac{m\chi}{R_0} (\hat{u}_{n+1} - \hat{u}_{n-1}) \hat{q}_n^2
\end{aligned} \tag{2.1}$$

where H_{L} is the phonon operator. $\hat{u}_n$, M, K and K_1 are the displacement operator of the nth molecule from its equilibrium position, the molecule mass, the longitudinal elastic constant of the harmonic lattice and the anharmonicity parameter, respectively. H_{A} is the operator for the intramolecular Amide-I vibration. $\hat{q}_n$, m and ω_0 are normal coordinate operator, effective mass and frequency, respectively, of the relevant intramolecular Amide-I vibration of the nth molecule, and L is a force constant giving vibrational exciton transfer between the nearest-neighbour peptide molecules. H_{I} describes the couplings between the intramolecular Amide-I vibration and the lattice vibration of peptide groups. R_0 is the lattice constant and χ is the coupling constant.

In the second quantization representation, the system Hamiltonian (2.1) can be rewritten as

$$\begin{aligned}
\hat{H} = {} & \sum_q \hbar\omega(q)(\hat{b}_q^+ \hat{b}_q + \tfrac{1}{2}) + \sum_{q_1 q_2} F(q_1, q_2)(\hat{b}_{q_1} + \hat{b}_{-q_1}^+)(\hat{b}_{q_2} + \hat{b}_{-q_2}^+)(\hat{b}_{-q_1-q_2} + \hat{b}_{q_1+q_2}^+) \\
& + \sum_n \hbar\omega_0 \hat{a}_n^+ \hat{a}_n \frac{\hbar L}{4m\omega_0} \sum_{\substack{nm \\ m=n\pm 1}} (\hat{a}_n^+ \hat{a}_m + \hat{a}_m^+ \hat{a}_n + \hat{a}_n^+ \hat{a}_m^+ + \hat{a}_n \hat{a}_m) \\
& + \sum_n \frac{\hbar\chi}{4R_0\omega_0} \left[\frac{\hbar}{2M\omega(q)N} \right]^{1/2} (\hat{b}_q + \hat{b}_{-q}^+) \exp(\mathrm{i}qnR_0)[2\mathrm{i}\sin(qR_0)](\hat{a}_n + \hat{a}_n^+)^2
\end{aligned} \tag{2.2}$$

where

$$F(q_1, q_2) = \frac{K_1}{3} N \left(\frac{\hbar}{2MN} \right)^{3/2} [1 - \exp(-\mathrm{i}q_1 R_0)][1 - \exp(-\mathrm{i}q_2 R_0)][1 - \exp(\mathrm{i}(q_1 + q_2)R_0)] \times \left(\frac{1}{\omega(q_1)\omega(q_2)\omega(q_1 + q_2)} \right)^{1/2}$$

$$\hat{q}_n = \left(\frac{\hbar}{2m\omega_0} \right)^{1/2} (\hat{a}_n + \hat{a}_n^+)$$

$$\hat{u}_n = \sum_q \left(\frac{\hbar}{2MN\omega} \right)^{1/2} \exp(\mathrm{i}qnR_0)(\hat{b}_q + \hat{b}_{-q}^+)$$

$\hat{a}_n$, $\hat{a}_n^+$ and $\hat{b}_q$, $\hat{b}_q^+$ are boson operators and

$$\omega(q) = 2 \left(\frac{K}{M} \right)^{1/2} \sin(qR_0/2)$$

is the eigenfrequency of acoustic phonons characterized by wave number q.

In this paper, we employ the product of vibron and phonon-coherent states as an ansatz for the eigenstate $\psi(t)$ of the system Hamiltonian

$$|\psi(t)\rangle = \exp\left[\sum_n (\alpha_{nq}^* \hat{a}_n - \alpha_{nq}\hat{a}_n^+)\right]|0\rangle_A \exp\left[\sum_n (\beta_{nq}^* \hat{b}_q - \beta_{nq}\hat{b}_q^+)\right]|\nu\rangle_L \tag{2.3}$$

$$|\nu\rangle_L = \prod_q \frac{(b_q)^{\nu_q}}{(\nu_q)^{1/2}}|0\rangle_L$$

where $|0\rangle_A$ and $|0\rangle_L$ are the vibron and phonon vacuum states, respectively.

Following Davydov [6], the evolutions of α_{nq} and β_{nq} are determined from dynamical equations derived from the thermally averaged Hamiltonian $\langle H\rangle$ in the state (2.3)

$$\begin{aligned}\langle H\rangle = \sum_\nu \rho_{\nu\nu}\langle\psi(t)|\hat{H}|\psi(t)\rangle &= \sum_q \hbar\omega_q(|\beta_{nq}|^2 + \bar{\nu}_q) \\ &- \sum_{qk} F(q,k)(\beta_{q,n} + \beta_{-q,n}^*)(\beta_{k,n} + \beta_{-k,n}^*)(\beta_{-q-k,n} + \beta_{q+k,n}^+) \\ &+ \sum_n \hbar\omega_0(\delta_n + |\alpha_{nq}|^2) - \frac{\hbar L}{4\mu\omega_0}\sum_n [(\alpha_{q,n}^*\alpha_{q,n+1} + \alpha_{q,n}\alpha_{q,n+1}^*) \\ &\times (\alpha_{q,n}^*\alpha_{q,n-1} + \alpha_{q,n}\alpha_{q,n-1}^*)]e^{-W_n} - \sum \frac{\chi}{4\omega_0 R_0}\left[\frac{\hbar^3}{2MN\omega(q)}\right]^{1/2} \\ &\times (2i\sin(qR_0))e^{iqnR_0}(\beta_{q,n} + \beta_{q,n}^*)(\alpha_{q,n}^*\alpha_{q,n} + \alpha_{q,n}\alpha_{q,n}^*)\end{aligned} \tag{2.4}$$

where the temperature-dependent density matrix is given by

$$\begin{aligned}\rho_{\nu\nu} &= \frac{\langle\nu|\exp(-\hat{H}_{ph}/(k_B T))|\nu\rangle}{\sum_\nu\langle\nu|\exp(-\hat{H}_{ph}/(k_B T))|\nu\rangle} \\ \hat{H}_{ph} &= \sum_q \hbar\omega_q \hat{b}_q^+\hat{b}_q \\ \bar{\nu}_q &= (\exp(\hbar\omega_q/k_B T) - 1)^{-1} \\ W_n &= \tfrac{1}{2}\sum_q |\beta_{n,q}|^2(1 + 2\bar{\nu}_q)(R_0 q)^2\end{aligned} \tag{2.5}$$

with k_B being Boltzmann's constant and T the absolute temperature.

From $\langle H\rangle$, we derive the dynamical equations for α_{nq} and β_{nq} by using the Hamilton equations

$$\begin{aligned}i\hbar\dot{\alpha}_{q,n} &= \hbar\omega_0\alpha_{q,n} - \frac{\hbar L}{2m\omega_0}(\alpha_{q,n+1} + \alpha_{q,n-1})e^{-W_n} \\ &- \sum_q \frac{\chi}{2\omega_0 R_0}\left(\frac{\hbar^3}{2MN\omega(q)}\right)^{1/2}(2i\sin(qR_0))\alpha_{q,n}(\beta_{q,n} + \beta_{q,n}^*)\end{aligned} \tag{2.6}$$

$$\begin{aligned}-(\dot{\beta}_{q,n} + \dot{\beta}_{-q,n}^*) &= \omega^2(q)(\beta_{q,n} + \beta_{-q,n}^*) - \sum \frac{2\omega(q)K_1}{3N^{1/2}}\left(\frac{\hbar^{2/3}}{2M\omega(q)}\right)^3 \\ &\times F(k,-q)(\beta_{k,n} + \beta_{-k,n}^*)(\beta_{q-k,n} + \beta_{k-q,n}^*) \\ &- i\frac{2\chi\omega(q)}{\omega_0 R_0}\left(\frac{\hbar}{2MN\omega(q)}\right)^{1/2} e^{-inR_0 q}\sin(qR_0)|\alpha_{q,n}|^2\end{aligned} \tag{2.7}$$

where the dots denote the derivative with respect to time.

If we introduce new functions

$$u_{q,n} = \left(\frac{\hbar}{2M\omega(q)}\right)^{1/2}(1 - e^{-iR_0q})(\beta_{q,n} + \beta^*_{-q,n})$$

$$u(x,t) = u_n(t) = N^{-1/2}\sum_q u_{q,n}e^{inR_0q} \qquad x = nR_0$$

$$\alpha_{q,n} = \alpha(x,t)$$

and use the long wavelength approximation

$$\alpha_{q,n\mp1}(x,t) - \alpha_{q,n}(x,t) = \mp\frac{\partial\alpha}{\partial x}R_0 + \frac{R_0^2}{2!}\frac{\partial^2\alpha}{\partial x^2}$$

$$\sin(R_0q) \simeq R_0q \qquad \exp(\pm R_0q) = 1 \pm R_0q$$

$$\omega^2(q) = v_0^2q^2 - \frac{v_0^2R_0^2}{12}q^4$$

the dynamical equations can be reduced to

$$\ddot{\rho} - v_0^2\left[\frac{\partial^2\rho}{\partial x^2} + \frac{R_0^2\partial^4\rho}{12\partial x^4} + \frac{K_1\partial^2}{3K\partial x^2}(\rho^2)\right] = \frac{\chi\hbar R_0}{\omega_0 M}\frac{\partial^2}{\partial x^2}|\alpha(x,t)|^2 \tag{2.8}$$

$$i\hbar\dot{\alpha}(x,t) = \left(\hbar\omega_0 - \frac{\hbar L}{2m\omega_0}e^{-W_n}\right)\alpha(x,t) - \frac{\hbar Le^{-W_n}}{4\omega_0 m}\frac{\partial^2}{\partial x^2}\alpha(x,t) + \frac{\chi\hbar}{4\omega_0R_0}\rho(x,t)\alpha(x,t) \tag{2.9}$$

where $v_0^2 = R_0^2K/M$ and $\rho(x,t) = -u_x$. Equations (2.8) and (2.9) are the basic equations we want to study in this paper.

To study solitary wave solutions with constant velocity V, we introduce the following dimensionless variable

$$\xi = \frac{x - Vt}{R_0} \qquad \alpha(x,t) = \phi(x,t)e^{i(kx-\omega t)} \tag{2.10}$$

and assume that $\phi(x,t) = \phi(\xi)$, $\rho(x,t) = \rho(\xi)$. Then (2.8) and (2.9) are transformed into

$$\bar{L}\frac{d^2\phi}{d\xi^2} + \bar{\chi}\rho\phi + \lambda\phi = 0 \tag{2.11}$$

$$\frac{1}{12}\frac{d^2\rho}{d\xi^2} + (1 - s^2)\rho + \gamma\rho^2 = \varepsilon\phi^2 \tag{2.12}$$

where

$$\int \phi^2\,d\xi = C \qquad (C \text{ is an arbitrary constant})$$

$$\lambda = \frac{\hbar L}{2m\omega_0}e^{-W_n} + \frac{\hbar Lk^2}{4m\omega_0}e^{-W_n} + \hbar(\omega_0 - \omega)$$

$$s = \frac{V}{v_0} \qquad \bar{L} = \frac{\hbar Le^{-W_n}}{4m\omega_0R_0^2} \qquad \bar{\chi} = \frac{\hbar\chi}{4\omega_0R_0}$$

$$\varepsilon = \frac{\chi\hbar}{K\omega_0R_0} \qquad k = \frac{2m\omega_0V}{L}e^{W_n} \qquad \gamma = K_1/(3K).$$

3. Soliton excitations of the model system

The solitary wave solutions of equations (11) and (12) have been studied by Davydov and Zolotariuk [10, 12]. They have shown that two types of approximate solitary wave solutions can be found by using iterative method.

(1) *Solitary waves of the first type.* Following Davydov's derivation, the nth order approximation of the solitary wave solutions of the first type of (11) and (12) is

$$\rho^{(n)}(\xi) = Ag^n \mu_n C^2 \operatorname{sech}^2(C\mu_n \xi) \tag{3.1}$$

$$\phi_0^{(n)}(\xi) = (\mu_n)^{1/2} C \operatorname{sech}(C\mu_n \xi) \tag{3.2}$$

where

$$\mu_n = \frac{Ag^n \bar{\chi}}{2\bar{L}} \tag{3.3}$$

$$g = \left(\frac{4\bar{L}\gamma}{\bar{\chi}}\right)^{1/2} \tag{3.4}$$

is a Debye–Waller-factor-like parameter, μ_n (or A) is the amplitude which is a positive root of the cubic equation

$$\frac{C^2}{12} Z^3 + (1 - s^2) g^{2n-2} Z - 2\gamma\varepsilon g^{3n-4} = 0 \tag{3.5}$$

it is clear that when $g = 1$ (or $\gamma = \bar{\chi}/4\bar{L}$) the solutions (3.1) and (3.2) become the exact soliton solution. Near $g = 1$ equations (3.1) and (3.2) represent the nth-order approximate soliton solution.

At a fixed value of s, equation (3.5) has only one positive root, which is an increasing function of velocity ratio s for both subsonic velocity with $s > 1$, including the case $s = 1$, and supersonic velocity with $s > 1$. The only restriction on soliton velocities comes from the long-wavelength approximation which requires $\mu_n \ll R_0$. Thus, we have shown that (at least sufficiently close to $g = 1$) the set of equations (2.11) and (2.12) admits the bell-shaped soliton solutions with both subsonic and supersonic velocities.

Furthermore, the energy and the momentum carried by a solitary excitation of this kind are

$$E(V) = m\frac{V^2}{R_0^2} \int \left[\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right)^2 - \phi \left(\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2}\right) \right] \mathrm{d}\xi + 2m\omega^2 \int \phi^2 \, \mathrm{d}\xi$$
$$+ \frac{1}{2} M c_0^2 \int \left\{ (1 + s^2)\rho^2 \frac{1}{12} \left(\frac{\mathrm{d}\rho}{\mathrm{d}\xi}\right)^2 + \frac{2}{3}\gamma\rho^3 \right\} \mathrm{d}\xi \tag{3.6}$$

$$P(V) = \left(\mu^* + M \int \rho^2 \, \mathrm{d}\xi\right) V \tag{3.7}$$

where μ^* is the effective mass of soliton.

There are two limit cases of the solitary wave solution of the first type. (i) Subsonic case. If the dispersion term and the anharmonicity term in (2.12) are absent and the parameter γ

approaches zero in such a way that the relation $\mu_1 = Ag\bar{\chi}/2\bar{L}(g = 1)$ remains valid and (3.5) has a positive solution only for subsonic travelling velocity:

$$\mu_1^{(D)} = \frac{\varepsilon\bar{\chi}}{4\bar{L}(1-s^2)} \qquad s < 1.$$

The first-order approximation energy and momentum of the subsonic soliton are

$$E^{(D)}(V) = \frac{1}{2}\mu^* V^2 + 2m\omega^2 C^2 + \frac{4}{3}\left(\frac{\bar{L}}{\bar{\chi}}\right)^2 Mc_0^2\left[1 + s^2\frac{1}{15}(\mu_1^{(D)})^2C^2\right](\mu_1^{(D)})^3C^3$$

$$P(V) = \left[\mu^* + \frac{8}{3}M(\mu_1^{(D)})^3\left(\frac{\bar{L}}{\bar{\chi}}\right)^2 C^3\right]V$$

$$\mu^* = \frac{4m\mu_1^2}{3R_0^2}C^3.$$

(ii) Supersonic case. In the subsonic solitary excitation, coupling between the intramolecular amide-I vibration and the intermolecular lattice vibration is essential. This is a high-order mechanism for soliton formation. There also exists a mechanism of soliton formation through the anharmonicity of the hydrogen-bond. This occurs when (3.5) holds as the ratio $\bar{\chi}/\bar{L}$ approaches zero. In this case, only the supersonic acoustic soliton is excited with

$$\mu_1^{(B)} = [3(s-1)]^{1/2}/(2C) \qquad s > 1.$$

The first-order approximation energy and momentum of the supersonic soliton are

$$E(V) = \tfrac{1}{2}\mu^* V^2 + 2m\omega^2 C$$

$$P(V) = \mu^* V.$$

(2) *Soliton excitations of the second type.* In a similar way to the first type of solution, the nth-order approximation solution of the second type is found to be

$$\phi_0^{(n)}(\xi) = \tfrac{1}{2}(3\bar{\mu}_n)^{1/2}C^{2/3}\operatorname{sech}^2(\tfrac{1}{2}C^{1/3}\bar{\mu}_n\xi) \tag{3.8}$$

$$\rho^{(n)}(\xi) = \tfrac{1}{2}Bh^n(3\bar{\mu}_n)^{1/2}C^{2/3}\operatorname{sech}^2(\tfrac{1}{2}C^{1/3}\bar{\mu}_n\xi) \tag{3.9}$$

where the amplitude B is a positive root of the equation

$$\frac{1}{3}C^{2/3}\left(\frac{3Z\bar{\chi}}{\bar{L}}\right)^{1/3}(\gamma Z^2 - \varepsilon) + (1-s^2)Z = 0 \tag{3.10}$$

and

$$\bar{\mu}_n = \frac{1}{3}\left(\frac{3Bh^n\bar{\chi}}{\bar{L}}\right)^{2/3} \tag{3.11}$$

$$h = \left(\frac{\gamma - \varepsilon B^{-2}}{\bar{\chi}/(12\bar{L})}\right)^{1/2} \tag{3.12}$$

where h is a Debye–Waller-factor-like parameter, but now (3.8) and (3.9) are well defined only for $s > 1$, i.e. the solitary wave of the second type can only travel at supersonic velocity. When $h = 1$, the solution (3.8) and (3.9) becomes the exact one. It follows from (3.12) and constraint $h = 1$ that B must be given by

$$B_* = \left(\frac{\varepsilon}{\gamma - (\bar{\chi}/12\bar{L})}\right)^{1/2}. \tag{3.13}$$

The first-order approximation energy and momentum of the soliton of the second type are

$$E(V) = \frac{1}{2}\bar{\mu}^* V^2 + 2m\omega^2 C + \frac{3}{2}Mc_0^2\bar{\mu}_1^3 C\left(\frac{\bar{L}}{\bar{\chi}}\right)^2\left\{1 + s^2\frac{1}{15}\bar{\mu}_1^2 C^{2/3} + \frac{4}{45}\gamma C^{2/3}\bar{\mu}_1^2\left(\frac{\bar{L}}{\bar{\chi}}\right)\right\} \tag{3.14}$$

$$P(V) = \left[\bar{\mu}^* + 3C\left(\frac{\bar{L}}{\bar{\chi}}\right)^2 Mc_0^2\bar{\mu}_1^3\right]V \tag{3.15}$$

where

$$\bar{\mu}^* = \frac{4m\bar{\mu}_1^2}{5R_0^2}.$$

The main differences between the solitary waves of the first and second type are: (i) the velocity of the former goes from zero to infinite while the latter must be larger than that of sound; (ii) $\rho \propto \phi^2$ for the former while $\rho \propto \phi$ for the latter; and (iii) the energy of the former is lower than that of the latter for the same wave velocities. Therefore, we only discuss the solitary wave of the first type in the following.

4. Discussion and conclusions

The differences between the Davydov model and the Takeno model have already been discussed by Takeno [4]. The aim of the present paper is to show whether the Takeno model can support solitary waves at physiological temperature. It is clear from the results above that the condition of the existence of solitary waves is that the Debye–Waller-factor-like parameter g (or h) must be near 1 for the first (or second) type solutions and at the same time that the amplitude of the solitary wave must be smaller than the lattice constant (R_0). From the expressions (3.4) and (3.12), it can be seen that g and h are determined by the protein parameters and temperature. The widely used protein parameters are [5]

$$\chi_D = 35\text{–}62 \text{ (pN)} \qquad L_D = 1.55 \times 10^{-22} \text{ (J)} \qquad K = 13 \text{ (N m}^{-1}\text{)}$$

$$K_1 = 17 \text{ (N m}^{-1}\text{)} \qquad m = 30M_P \qquad M = 114M_P \qquad R_0 = 4.5 \text{ (Å)}$$

$$M_P = 1.67 \times 10^{-27} \text{ (kg)} \qquad K_B = 1.38 \times 10^{-23} \text{ (J K}^{-1}\text{)}$$

$$v_0 = (K/M)^{1/2}R_0 = 3.8 \times 10^3 \text{ (m s}^{-1}\text{)} \qquad \hbar = 1.055 \times 10^{-34} \text{ (J s)}$$

where χ_D and L_D in the Davydov model are related to χ and L in the Takeno model by

$$\chi = (2R_0\omega_0/\hbar)\chi_D \qquad L = (2m\omega_0/\hbar)L_D$$

respectively.

In the following we discuss whether (3.4) is satisfied when $g = 1$ for the protein parameters. When $g = 1$ and $C = 1$ and if $k_BT \gg \hbar\omega_0$, we can approximate $W_n(T)$ by

$$W_n(T) = \frac{M\mu^2(1+s^2)\gamma^2}{2N\hbar^2}(K_BT)$$

as done in [11] where $\mu = \mu_n$ is the amplitude of the solitary wave of the first type. Since $g = 1$, we have from (3.4)

$$4\gamma\bar{L}/\bar{\chi} = 1.$$

Using the protein parameters and the expression for $W_n(T)$ above, we find

$$\mu = 0.35R_0/(1+s^2)^{1/2}$$

at $T = 300$ K. This shows that $\mu \ll R_0$ for all values of wave velocity and so the long-wavelength approximation is also satisfied. Of course, μ approaches zero for larger s. It is clear that the wave velocity can be smaller, equal to and larger than that of sound. This is because we have included the cubic anharmonicity of the hydrogen-bonded interaction. However, since μ must also satisfy (3.5), the velocity of the solitary is very limited. Solving (3.5) for the protein parameters, we find that s must be near 1, i.e. the solitary wave of the first type can exist only when the wave velocity is around that of sound.

In conclusion, Davydov's thermally averaged method has been used to study the temperature effect on the vibron soliton in the Takeno model. The result shows that the Takeno model can support solitary waves at physiological temperature only for a narrow range of values of wave velocity. This is different from the result obtained by Davydov [6]. They have shown that the solitary wave can be realized in the Davydov model for any values of wave velocity smaller than that of sound. Of course, the Takeno model is different from the Davydov model in that the quantum numbers of the former are not conservative. Furthermore, we have considered the anharmonicity of the hydrogen-bonded interaction between amino-acid molecules. This leads to the result that the velocity of the solitary wave can be larger than that of sound and this is also the reason that the amplitudes of the solitary waves must satisfy certain conditions (equation (3.5) and (3.10)). Our results hold only for the long-wavelength approximation and only under this approximation can the dynamical equations be solved analytically. Since the discreteness of the system is important for energy transport in protein molecules, we will study this in the future.

Acknowledgments

The authors are grateful to the referees for their valuable suggestions. This work is supported by the Yong Teacher Foundation of National Educational Committee and the Life and Environment Science Foundation of the HUST.

References

[1] Davydov A S 1982 *Biology and Quantum Mechanics* (New York: Pergamon)
[2] Davydov A S 1985 *Solitons in Molecular Systems* (Dordrecht: Reidel)
[3] Davydov A S 1979 *Phys. Scr.* **20** 387
[4] Takeno S 1984 *Prog. Theor. Phys.* **71** 395
[5] Scott A C 1992 *Phys. Rep.* **217** 1
[6] Davydov A S 1980 *Sov. Phys.–JETP* **51** 397
[7] Scott A C 1988 *Phys. Rev.* A **37** 880
[8] Förner W 1991 *Phys. Rev.* A **44** 2695
[9] Förner W 1992 *J. Phys.: Condens. Matter* **4** 1915
[10] Davydov A S and Zolotariuk A V 1984 *Phys. Scr.* **30** 426
[11] Ivic Z, Sataric M, Shemsedini Z and Zakula R 1988 *Phys. Scr.* **37** 564