Supersonic Vibron Solitons and Their Possible Existence in Polypeptides

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Abstract. Nonlinear interactions of vibrons with lattice solitons due to the soft cubic nonlinearity in a quasi-one-dimensional lattice yield supersonic vibron solitons. Their binding energy is larger than those of the conventional Davydov solitons and vibron solitons, and their propagation velocity is uniquely determined in contrast to the latter two. Examination of parameters in the model Hamiltonian for polypeptides leads to the result that the supersonic vibron solitons obtained here are more likely to be realizable than the Davydov solitons and the conventional vibron solitons in alpha-helical proteins.

1. Introduction

Extensive studies have been made in recent years to examine the possibility of energy transport via soliton mechanisms in proteins. The so-called Davydov soliton [1, 2] and the vibron soliton [3], which involve the coupling of amide-I (CO-stretching) vibrations of peptide groups to acoustic phonons on alpha-helix, have received particular attention over the past two decades. Recently, attempts have been made to (1) improve the Davydov model using the polaron theory [4], (2) to examine the stability of the Davydov soliton against quantum [5] and thermal fluctuations [6] on the one hand, and (3) to formulate a quantum theory of vibron solitons [7] and to make a more detailed study of their physical characteristics, on the other [8]. In spite of extensive efforts, however, our understanding of the possible existence of solitons in biological systems and their roles in biological functioning has remained far from conclusive.

The conventional Davydov and vibron soliton models are characterized by the nonlinearity in interactions between vibrational excitons or vibrons and acoustic phonons while the excitons, the vibrons and the phonons themselves are taken to be linear. Here, the soft nonlinearity inherent in acoustic phonons on hydrogen-bonded polypeptide chains of alpha helices is overlooked. A numerical study by Pierce using ab-initio SCF-MO calculations [9] has shown that the potential energy for longitudinal phonons, to which the excitons or the vibrons couple in polypeptides, is well described by the Morse potential. It is therefore imperative to re-examine, both analytically and numerically, the soliton dynamics in polypeptides

by including the intrinsic nonlinearity in phonon systems. For the case of Davydov solitons, this point was investigated in recent years by Gaididei, Christiansen and Mingaleev to show the existence of a bound state of Davydov electro-solitons and Boussinesq solitons [10].

It is the purpose of this paper to show a possible existence in alpha-helical proteins of supersonic vibron solitons arising from nonlinear interactions of vibrons with acoustic solitons on hydrogen-bonded chains due to the soft cubic lattice nonlinearity there. The supersonic vibron solitons obtained here have the following characteristics: (1) They can only exist provided the cubic anharmonicity exceeds a certain critical value. (2) They have a unique propagation velocity. (3) Their binding energy is larger than that of subsonic vibron solitons including the conventional vibron solitons (referred to as c-vibron solitons). These properties of the supersonic vibron soliton are to be contrasted with the conventional Davydov and vibron solitons where the soliton velocity can be taken to be arbitrary as it is smaller than the sound velocity and no critical value of soliton parameters so long as given above exists. The present result is different from that of Gaididei et al. in that the result obtained by these workers precludes the existence of a bound state of Davydov solitons and Boussinesq solitons in alpha-helical proteins. It is shown that the supersonic vibron solitons obtained here appear to be much better candidates for solitons realizable in polypeptides than the c-vibron solitons and the Davydov solitons.

2. Model Hamiltonian

The Hamiltonian for a vibron-phonon system that we studied is given by

$$\hat{H} = \hat{H}_{vib} + \hat{H}_{aph} + \hat{H}_{int}, \quad (1)$$

with

$$\hat{H}_{vib} = \sum_n \left[\frac{\hat{p}_n^2}{2\mu} + \hat{v}(\hat{q}_n) \right] - \frac{1}{2} \sum_{nm} L(n, m) \hat{q}_n \hat{q}_m, \quad (2)$$

$$\hat{H}_{aph} = \sum_n \left[\frac{\hat{p}_n^2}{2M} + \hat{U}(\hat{u}_{n+1} - \hat{u}_n) \right], \quad (3)$$

$$\hat{H}_{int} = \sum_n \left[\lambda_+ \hat{V}(\hat{q}_n)(\hat{u}_{n+1} - \hat{u}_n) + \lambda_- \hat{V}(\hat{q}_n)(\hat{u}_n - \hat{u}_{n-1}) \right]. \quad (4)$$

Here, $\hat{H}_{vib}$ is the Hamiltonian of a vibron system simulating vibrations of amide-I oscillators in a polypeptide molecular chain, in which $\hat{q}_n$, $\hat{p}_n$, $\hat{v}(\hat{q}_n)$ and $L(n, m)$ are the displacement of the n th oscillator with the effective mass μ from its equilibrium position, its momentum, its on-site potential energy and the coefficient of the dipole-dipole interaction energy between the n th and m th oscillators, respectively.

The quantity $\hat{H}_{aph}$ is the Hamiltonian for an anharmonic phonon system simulating longitudinal acoustic phonons on the hydrogen-bonded polypeptide chain, where $\hat{u}_n$ and $\hat{P}_n$ are the displacement of an n th molecule (peptide unit) with mass M from its equilibrium position and its momentum, respectively, and the quantity $\hat{U}(u_{n+1} - u_n)$ is the intermolecular potential energy between the n th molecule and the $(n + 1)$ th molecule. The quantity $\hat{H}_{int}$ is the Hamiltonian for vibron-phonon interactions, where $\lambda_{\pm} \hat{V}(\hat{q}_n)$ describes fluctuations of the on-site potential energy due to interactions of the n th oscillator with acoustic phonons, where $\lambda_{\pm}$ are constants. Explicit expressions for $\hat{v} \equiv \hat{v}(x)$, $\hat{U} \equiv \hat{U}(x)$, and $\hat{V} \equiv V(x)$ as functions of x will be specified later on.

It is understood that a pair of the quantities $\hat{q}_n$ and $\hat{p}_n$ and the corresponding $\hat{u}_n$ and $\hat{P}_n$ for the vibron system and the phonon system, respectively, are written in terms of the boson operators as

$$\hat{q}_n = \sqrt{\frac{\hbar}{2\mu\omega_0}}(\hat{a}_n + \hat{a}_n^\dagger), \quad \hat{p}_n = \frac{1}{i}\sqrt{\frac{\mu\hbar\omega_0}{2}}(\hat{a}_n - \hat{a}_n^\dagger), \quad (5)$$

$$\begin{aligned} \hat{u}_n &= \sum_q \sqrt{\frac{\hbar}{2N_1 M \omega(q)}} \exp(iqna) (\hat{b}_q + \hat{b}_{-q}^\dagger), \\ \hat{P}_n &= \sum_q \sqrt{\frac{M\hbar\omega(q)}{2N_1}} \exp(iqna) \frac{1}{i} (\hat{b}_q - \hat{b}_{-q}^\dagger), \end{aligned} \quad (6)$$

where

$$\omega(q)^2 = \frac{2K_2}{M} [1 - \cos(ka)] \quad (7)$$

is the square of the eigenfrequency of harmonic phonons characterized by the wave number q . In the above equations, $\hat{a}_n$ and $\hat{a}_n^\dagger$ are the annihilation and creation operators, respectively, of vibrons at the site n , while $\hat{b}_q$ and $\hat{b}_q^\dagger$ are annihilation and creation operators, respectively, of harmonic phonons with wavenumber q . The quantities a and N_1 are the lattice constant of the acoustic phonon system and the total number of peptide units, respectively.

3. Large-amplitude Collective Modes and Coherent-state Path Integral Formulation

We are concerned with large-amplitude, soliton-like collective modes in the vibron-phonon system governed by the Hamiltonian, Equation (1). Two basic questions arise: (1) What are solitons in a general sense in such a quantum system? and (2) what is the nature of their eigenstates? The characteristic key point of the present model, in contrast to the Davydov model and its versions, is the existence of anharmonicity in the acoustic phonon system and the inclusion of terms representing

simultaneous excitations and de-excitations of two vibrons not only in H_{vib} itself but also in H_{int} (cf. Equations (5) and (39)). We note that solitons in quantum many-particle systems have been recognized to be exact classical solutions to equations in quantum field theory [11]. One physically acceptable working method with which we can perform exact, non-perturbative calculations, here, is to resort to the use of the functional-integral method in the coherent-state basis with stationary phase approximation [12]. As is well known, such an approach is equivalent to the time-dependent Hartree-Fock approximation or the time-dependent mean-field approximation [12], successfully applied, for example, to studying large-amplitude collective modes in nuclear physics [13]. Our answer to the above question is therefore in line with the abovementioned approach. Namely, our basic assumption is that solitons in our vibron-anharmonic-phonon model may be obtained by applying the stationary-phase approximation or the quasi-classical approximation in the coherent-state-based path-integral formulation to Equation (1).

With the abovementioned facts in mind, we introduce a set $|\Gamma\rangle$ of boson coherent states $|\alpha_n\rangle$ and $|\beta_q\rangle$ for the vibron system and the phonon system, respectively, by the equations

$$|\Gamma\rangle = \prod_n |\alpha_n\rangle \pi \prod_q |\beta_q\rangle, \quad (8)$$

where

$$|\alpha_n\rangle = \exp\left(-\frac{1}{2}|\alpha_n|^2\right) \exp(\alpha_n \hat{a}_n^\dagger) |0\rangle_v, \quad |\beta_q\rangle = \exp\left(-\frac{1}{2}|\beta_q|^2\right) \exp(\beta_q \hat{b}_q^\dagger) |0\rangle_p. \quad (9)$$

In the above equations the quantities α_n and β_q are complex variables, and $|0\rangle_v$ and $|0\rangle_p$ are the ground state of the vibron system and that of the phonon system, respectively. Then, the functional integral representation in the boson coherent state basis for the matrix element of the evolution operator $\exp(-i\hat{H}t/\hbar)$ between the initial state $|\Gamma_i\rangle$ at time t_i and the final state $|\Gamma_f\rangle$ at time t_f is written in the form

$$\begin{aligned} \langle \Gamma_i | \exp\left[\frac{-i\hat{H}(t_f - t_i)}{\hbar}\right] | \Gamma_f \rangle &= \int D(\Gamma) \exp\left[\frac{1}{\hbar} \int L dt\right] \\ &\equiv \int D(\Gamma) \exp\left(\frac{iS}{\hbar}\right), \end{aligned} \quad (10)$$

where

$$L = \frac{i\hbar}{2} \sum_n \left[\alpha_n^* \frac{d\alpha_n}{dt} - \alpha_n \frac{d\alpha_n^*}{dt} \right] + \frac{i\hbar}{2} \sum_q \left[\beta_q^* \frac{d\beta_q}{dt} - \beta_q \frac{d\beta_q^*}{dt} \right] - \langle \Gamma | \hat{H} | \Gamma \rangle, \quad (11)$$

in which L and S are the Lagrangian and the action, respectively. An explicit expression for $\langle \Gamma | \hat{H} | \Gamma \rangle$ in Equation (11) can be obtained by taking the normal ordered form of $\hat{H}$. This amounts to putting all $\hat{a}_n$'s and $\hat{b}_q$'s in every term there to the right of all $\hat{a}_n^\dagger$'s and $\hat{b}_q^\dagger$'s and using the relations

$$\hat{a}_n|\alpha_n\rangle = \alpha_n|\alpha_n\rangle \text{ and h.c., } \hat{b}_q|\beta_q\rangle = \beta_q|\beta_q\rangle \text{ and h.c.} \quad (12)$$

where the symbol h.c. denotes the Hermite conjugate. In what follows, we rewrite the diagonal coherent state representation $\langle \Gamma | \hat{A} | \Gamma \rangle$ or a c-number-counterpart of a $\hat{A}$ simply as A , i.e.

$$A = \langle \Gamma | \hat{A} | \Gamma \rangle. \quad (13)$$

Equation (10) poses a quantum many-body problem. A working approximation to the formally exact expression for the matrix element of the time-evolution operator is to resort to the use of the stationary-phase approximation

$$\delta S = 0, \quad (14)$$

leading to the Lagrangian equations,

$$\frac{d}{dt} \left[\frac{\partial L}{\partial \dot{\alpha}_n} \right] - \frac{\partial L}{\partial \alpha_n} = 0 \text{ and c.c., } \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{\beta}_q} \right] - \frac{\partial L}{\partial \beta_q} = 0 \text{ and c.c.} \quad (15)$$

Their explicit expressions are written as

$$i\hbar \frac{d\alpha_n}{dt} = \frac{\partial H}{\partial \alpha_n^*} \text{ and c.c., } i\hbar \frac{d\beta_q}{dt} = \frac{\partial H}{\partial \beta_q^*} \text{ and c.c.} \quad (16)$$

Let q_n , p_n , u_n and P_n be a c-number counterpart of $\hat{q}_n$, $\hat{p}_n$, $\hat{u}_n$ and $\hat{P}_n$, respectively, defined by Equations (A.1), (A.2), (A.3) and (A.4) in the Appendix A. Equations (8) and (9) can be re-expressed in terms of the q_n 's, p_n 's, u_n 's and the P_n 's as

$$|\Gamma\rangle = \prod_n |q_n, p_n\rangle \prod_n |u_n, P_n\rangle, \quad (17)$$

where

$$|q_n, p_n\rangle = \exp\left[\frac{1}{i\hbar}[q_n \hat{p}_n - p_n \hat{q}_n]|0\rangle_v, \quad |u_n, P_n\rangle = \exp\left[\frac{1}{i\hbar}[u_n \hat{P}_n - P_n \hat{u}_n]|0\rangle_p. \quad (18)$$

Here, equations corresponding to the first and the second of Equations (16) take the form

$$\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}, \quad \frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n}, \quad (19)$$

and

$$\frac{du_n}{dt} = \frac{\partial H}{\partial P_n}, \quad \frac{dP_n}{dt} = -\frac{\partial H}{\partial u_n}, \quad (20)$$

respectively. Then, in terms of

$$w_n = u_{n+1} - u_n, \quad (21)$$

equations for the q'_n s and the w'_n s are written as

$$\mu \ddot{q}_n + v'(q_n) - \sum_m L(n, m) q_m + \lambda_+ V'(q_n) w_n + \lambda_- V'(q_n) w_{n-1} = 0, \quad (22)$$

$$\begin{aligned} M \ddot{w}_n - [U'(w_{n+1}) + U'(w_{n-1}) - 2U'(w_n)] \\ - \lambda_+ [V(q_{n+1}) + V(q_{n-1}) - 2V(q_n)] \\ - \lambda_- [V(q_{n+2}) + V(q_n) - 2V(q_{n+1})] = 0, \end{aligned} \quad (23)$$

where $f'(x) = (d/dx)f(x)$.

4. Continuum Approximation and Rotating Wave Approximation

Let us assume that the spatial extension of nonlinear modes associated with solutions to Equations (22) and (23) is much larger than the lattice constant a of the system. Then, we can employ the continuum approximation to reduce these two equations to

$$c_1^2 \frac{\partial^2 q}{\partial x^2} - \frac{\partial^2 q}{\partial t^2} - \omega^{*2} q - \frac{1}{\mu} [v^{(a)'}(q) + \lambda V'(q)w] = 0, \quad (24)$$

$$c_0^2 \frac{\partial^2 w}{\partial x^2} - \frac{\partial^2 w}{\partial t^2} + \frac{c_0^2 a^2}{12} \frac{\partial^4 w}{\partial t^4} + \frac{a^2}{M} \frac{\partial^2}{\partial x^2} [U^{(a)'}(w) + \lambda V(q)] = 0, \quad (25)$$

where

$$\lambda = \lambda_+ + \lambda_-, \quad (26)$$

and $v^{(a)}(q)$ and $U^{(a)}(w)$ are an anharmonic part of $v(q)$ and $U(w)$, respectively. The quantities c_1 , c_0 and ω^* are the velocity of phonon-free linear vibrons, that of vibron-free linear phonons and the (renormalized) eigenfrequency of the linear vibrons, respectively. Explicit expressions for these quantities are given in the Appendix B.

We separate the quantity q_n into a negative frequency part ψ_n and a positive frequency part ψ_n^* , i.e.

$$q_n = \psi_n + \psi_n^*, \quad (27)$$

where ψ_n^* is the complex conjugate of ψ_n . Let us assume for simplicity that both of the vibron potential function $v(q)$ and its fluctuation, $V(q)$, are even functions of q . Then, inserting Equation (27) into Equations (24) and (25) and paying attention solely to the negative frequency part of the equations, which is equivalent to using the rotating-wave approximation (RWA), we can reduce these two equations to the form

$$c_1^2 \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial t^2} - \omega^{*2} \psi - \frac{1}{\mu} \left[f(|\psi|^2) \psi + \lambda' \frac{dF(|\psi|^2)}{d|\psi|^2} \psi w \right] = 0, \quad (28)$$

$$c_0^2 \frac{\partial^2 w}{\partial x^2} - \frac{\partial^2 w}{\partial t^2} + \frac{c_0^2 a^2}{12} \frac{\partial^4 w}{\partial t^4} + \frac{a^2}{M} \frac{\partial^2}{\partial x^2} \left[U^{(a)'}(w) + \lambda F(|\psi|^2) \right] = 0, \quad (29)$$

where

$$\begin{aligned} v^{(a)'}(\psi + \psi^*) &\xrightarrow{RWA} f(|\psi|^2) \psi, \quad V(\psi + \psi^*) \xrightarrow{RWA} F(|\psi|^2), \\ V'(\psi + \psi^*) &\xrightarrow{RWA} \gamma \frac{dF(|\psi|^2)}{d|\psi|^2} \psi, \end{aligned} \quad (30)$$

In Equation (28), we have set $\lambda' = \gamma \lambda$, where γ is a constant. We seek solutions to Equations (28) and (29) in the form

$$\psi \equiv \psi(x, t) = \phi(x - vt) e^{i(kx - \omega t)} \equiv \phi(\xi) e^{i(kx - \omega t)}, \quad (31)$$

$$w \equiv w(x, t) = w(x - vt) \equiv w(\xi), \quad (32)$$

to arrive at a pair of equations

$$A_1 \frac{d^2 \phi}{d\xi^2} = A_2 \phi + \frac{1}{\mu} \left[f(\phi^2) \phi + \lambda' \frac{dF(\phi^2)}{d\phi^2} \phi w \right], \quad (33)$$

$$B_1 \frac{d^2 w}{d\xi^2} = B_2 w - \frac{a^2}{M} \left[U_N^{(a)'}(w) + \lambda F(\phi^2) \right], \quad (34)$$

with

$$k = \frac{\omega}{c_1^2} v. \quad (35)$$

where

$$\begin{aligned} A_1 &= c_1^2 - v^2, \quad A_2 = \omega^{*2} + c_1^2 k^2 - \omega^2, \\ B_1 &= \frac{c_0^2 a^2}{12}, \quad B_2 = v^2 - c_0^2. \end{aligned} \quad (36)$$

Here, v in Equations (31) and (32) is the velocity of nonlinear modes with which we are concerned.

5. Exact One-soliton Solutions

The simplest, yet physically interesting and non-trivial, solutions to Equations (33) and (34) are provided by the case (cf. Appendix B),

$$f(\phi^2) = b\phi^2, \quad F(\phi^2) = \phi^2, \quad \lambda' = \lambda, \quad (37)$$

$$U'^{(a)}(w) = -K_3 w^2. \quad (38)$$

This corresponds to the vibron-phonon system described by Equations (1)–(4) with

$$\hat{v}(\hat{q}) = \frac{\mu\omega_0^2}{2}\hat{q}^2 + \frac{b}{4}\hat{q}^4, \quad \hat{V}(\hat{q}) = \frac{1}{2}\hat{q}^2. \quad (39)$$

$$\hat{U}(\hat{w}) = \frac{K^2}{2}\hat{w}^2 - \frac{K_3}{3}\hat{w}^3, \quad K_2 > 0, \quad K_3 > 0. \quad (40)$$

It is a straightforward matter to show that Equations (33) and (34) with Equations (35) and (36) exhibit exact non-soliton solutions

$$\phi = \frac{A}{\cosh(K\xi)}, \quad (41)$$

$$w = -\frac{B}{\cosh^2(K\xi)}, \quad (42)$$

where

$$\omega^2 \equiv \omega(k)^2 = \omega^{(0)}(k)^2 - \Delta\omega_B^2, \quad (43)$$

with

$$\omega^{(0)}(k) = \sqrt{\omega^{*2} + c_1^2 k^2}, \quad (44)$$

$$\Delta\omega_B^2 = \frac{\lambda B - bA^2}{2\mu}, \quad (45)$$

$$K = \sqrt{\frac{\Delta\omega_B^2}{c_1^2 - v^2}}, \quad v = \sqrt{c_1^2 - \frac{M}{4\mu} \frac{\lambda - [bA^2/B]}{2K_3} c_0^2} < \left[1 + \frac{2K_3 B}{3K_2}\right] c_2 \equiv v_0^2, \quad (46)$$

$$B = \frac{3M(v^2 - c_0^2)}{4K_3 a^2} + \sqrt{\left(\frac{3M(v^2 - c_0^2)}{4K_3 a^2}\right)^2 + \frac{3\lambda}{2K_3} A^2}, \quad K_3 > K_{3c} \text{ for } v > c_0,$$

$$B = -\frac{3M(c_0^2 - v^2)}{4K_3 a^2} + \sqrt{\left(\frac{3M(c_0^2 - v^2)}{4K_3 a^2}\right)^2 + \frac{3\lambda}{2K_3} A^2}, \quad K_3 < K_{3c} \text{ for } v < c_0, \quad (47)$$

with

$$K_{3c} = \frac{M\Delta\omega_B^2}{2B} \frac{c_0^2}{c_1^2 - c_0^2}. \quad (48)$$

In Equations (43) and (44), $\omega^{(0)}(k)$ is the eigenfrequency of phonon-free vibrons characterized by the wave number k . The quantity v_0 in Equation (46) is the velocity of Boussinesq solitons in a system of vibron-free anharmonic phonons. Here, physically acceptable solutions must satisfy the condition

$$\lambda B - bA^2 > 0, \quad (49)$$

because in order for vibron solitons arising from interactions of vibrons with non-linear phonons to be stable, they should appear outside (below) the lower ω_1^* of the frequency band $\omega^{(0)}(k)$ of phonon-free vibrons. Five independent equations obtained above, Equation (35) and (43)–(46), determine six unknown factors k , K , ω , v , A and B characterizing the properties of vibron solitons provided one of these quantities are taken as a parameter. Namely, taking one of k , K , ω , v , A and B as a parameter, all the other quantities are uniquely determined by a set of these equations.

Let us study the physical properties of the obtained solutions. (1) We note, first of all, that there exist two types of vibron solitons, one being supersonic $v > c_0$ and the other subsonic $v < c_0$ in accordance with $K_3 > K_{3c}$ and $K_3 < K_{3c}$, respectively. (2) Lowering of the energy of vibrons is due to (i) their interactions with phonons and (ii) the soft nonlinearity,

$$b < 0, \quad (50)$$

of the vibron potential $\hat{v}(\hat{q})$ which favors more the existence of vibron solitons. (3) These two types of solitons are realizable for

$$\lambda > 0. \quad (51)$$

as seen from Equation (45). It is worth noticing that no such restriction exists for c-vibron solitons [3] to which subsonic vibron solitons reduce in the limit

$$K_3 \rightarrow 0, \quad (52)$$

because the quantity B here is connected with the quantity A by

$$B = \frac{\lambda a^2}{M(c_0^2 - v^2)} A^2. \quad (53)$$

It goes without saying that in the c-vibron soliton theory, Equation (53) is derived by setting $U^{(a)'}(w) \rightarrow 0$ and $c_0^2 a^2 / 12 \partial^4 w / \partial t^4 \rightarrow 0$ from the outset. (4) The binding energy E_B of vibron solitons is defined by

$$E_B = \hbar[\omega^{(0)}(k) - \omega(k)] \simeq \frac{\hbar \Delta \omega_B^2}{2\omega^{(0)}(k)}. \quad (54)$$

Then, obviously, supersonic vibron solitons existing for $K_{3c} > K_3$ have binding energy larger than that of subsonic vibron solitons for $K_{3c} < K_3$. (5) The existence of the anharmonicity constant K_3 in the denominator in Equation (47) clearly

Figure 1. A schematic feature of the alpha-helicals structure in proteins.

Figure 2. The valence-bond and hydrogen-bond sequences in the polypeptide.

Figure 3. A one-dimensional lattice model of the polypeptide.

shows that the supersonic vibron solitons obtained here cannot be attained by a perturbation procedure.

6. Application to Polypeptides

Let us apply the result obtained in the preceding sections to amide-I vibrations of peptide groups coupled to acoustic phonons on alpha-helix (see Figure 1). To appreciate Equation (1) as a model dynamical system of the alpha-helicals, the valence-bond sequence and a single spine of the hydrogen-bonded sequence are taken up as a basic frame for studying the nonlinear dynamical properties of the alpha helix (see Figure 2). Namely, the oscillator of the vibron system stands for the C=O stretching vibration with eigenfrequency ω_0 in the amide-I unit, while the phonon system represents the hydrogen-bonded stretching vibrations, where M is the mass of a peptide unit. Each of the amide-I oscillators and that of the peptide unit are assumed to be arranged on 1d periodic lattices (see Figure 3). The evaluation of the parameters in the Hamiltonian is made by making a one-to-one correspondence of Equation (1) to the model Hamiltonian in the standard form of the Davydov soliton theory. Assuming that the $L(n, m)$'s in Equation (2) are non-vanishing only for nearest-neighbor pairs and writing the nearest-neighbor interaction constant as L , we obtain

$$\frac{\hbar}{2\mu\omega_0}L \equiv \Lambda_0^2 L = J, \quad \lambda_i = \frac{\chi_i}{\Lambda_0^2} \frac{2n_p}{2n_p + 1}, \quad i = 1, 2, \quad (55)$$

Here, J , χ_i ($i = 1, 2$) and n_p are the nearest neighbor interaction constant for vibrational excitons, exciton-phonon interaction constants and the occupation number of harmonic phonons, respectively, when the exciton transfer term from site n to site m and the exciton-phonon interaction are written as

$$J(n, m)a_n^\dagger a_m$$

and

$$\sum_n \left[\chi_1 a_n^\dagger a_n (u_{n+1} - u_n) + \chi_2 a_n^\dagger (u_n - u_{n-1}) \right].$$

Here, $a_n^\dagger$ and a_n are exciton creation and annihilation operators, respectively, at the site n , and $J(n, m)$ is a constant. The quantity Λ_0^2 and n are the mean square displacement of the amide-I oscillator in its zero-point motion and the vibron quantum number, respectively.

Then, using the result obtained by Pierce,

$$\mu = 1.1 \times 10^{-26} \text{ kg}, \omega_0 = 3.7 \times 10^{-10} \text{ J}, J = 1.8 \times 10^{-22} \text{ J}, \quad (56)$$

$$M = 1.9 \times 10^{-25} \text{ kg}, K_2 = 2.0 \times 10 \text{ N m}^{-1}, K_3 = 5.5 \times 10^{11} \text{ N m}^{-2}, \quad (57)$$

$$\chi_1 + \chi_2 = 2.6 \times 10^{-11} \text{ N}, a = 4.5 \times 10^{-10} \text{ m}, \quad (58)$$

and setting $n_p = 1$ in Equation (55), we obtain

$$c_1 = 1.6 \times 10^4 \text{ m s}^{-1}, c_2 = 4.6 \times 10^3 \text{ m s}^{-1}, \Lambda_0 = 3.7 \times 10^{-12} \text{ m}, \quad (59)$$

$$v = 5.7 \times 10^3 \text{ m s}^{-1}, k = 8.2 \times 9 \text{ m}^{-1}, B_c = 3.1 \times 10^{-11} \text{ m}, \quad (60)$$

$$aK = 5.5 \times 10^{-2}. \quad (61)$$

It is therefore seen that solitons here derived are supersonic. We choose B as a parameter, writing it in terms of a dimensionless constant b as

$$B = (3.2 + b) \times 10^{-11} \text{ m}. \quad (62)$$

Here, the case $b = 0$ corresponds to taking $A^2 = \Lambda_0^2$ in Equation (18). The quantum-number indefiniteness inherent in coherent states of the vibron-phonon system yields a finite, but presumably small, value of b . The quantities E_B , a_α and v_0 are then given by

$$\frac{E_B}{J} = 1.5(1 + 0.3b), \quad aK = 1.3(1 + 0.3b)^{\frac{1}{2}}, \quad v_0 = 1.2(1 + 0.3b)^{\frac{1}{2}} \times 10^4 \text{ m s}^{-1}. \quad (63)$$

It is seen that even in the case $b = 0$, the numerical values of the relevant physical quantities obtained here favor the existence of supersonic vibron solitons in polypeptides. It is seen that the obtained soliton binding energy is much larger than those obtained previously.

7. Concluding Remarks

In summary, we have shown the existence in a one-dimensional vibron-anharmonic phonon system of supersonic vibron solitons as a dynamical bound state of vibrons by intrinsic lattice solitons due to the soft cubic anharmonicity. The supersonic

solitons obtained here possess larger binding energy than that of conventional vibron solitons and also subsonic vibron solitons, and their unique propagation velocity is slightly smaller than the lattice soliton velocity. Examination of the numerical values of the parameters in the Hamiltonian for alpha-helics leads to the conclusion that the supersonic vibron solitons are realizable in polypeptides in contrast to the case of Gaididei et al. [10] and that they are more likely to exist in alpha-helical proteins than conventional, subsonic vibron solitons.

In this paper, we confined ourselves to studying the dynamics of the system governed by Equation (1) within the framework of the coherent-state-based path-integral formulation combined with the use of the stationary-phase approximation. This is essentially equivalent to the time-dependent mean-field theory [12]. The obtained result is therefore to be considered as applicable to polypeptides or proteins at low temperatures. Finite-temperature effects may be taken care of to some extent by treating the quantity $B(b)$ in Equation (47) (Equation 63) representing the amplitude of solitons in the phonon system as a temperature-dependent parameter. One of the most important points which has been left untouched in this paper is the stability of the present supersonic vibron solitons against finite temperature effects and environmental fluctuations. This is indispensable for seeking any relevance of the supersonic vibron solitons to biological functioning. This and related problems will be studied in the future.

Appendix A. C-number counterparts of $\hat{q}_n$, $\hat{p}_n$, $\hat{u}_n$ and $\hat{P}_n$

A c-number counterpart of $\hat{q}_n$, $\hat{p}_n$, $\hat{u}_n$ and $\hat{P}_n$ can easily be obtained by replacing $\hat{a}_n$, $\hat{a}_n^\dagger$, $\hat{b}_q$ and $\hat{b}_q^\dagger$ in Equations (5) and (6) by α_n , α_n^* , β_q , and β_q^* , respectively,

$$q_n = \sqrt{\frac{\hbar}{2\mu\omega_0}}(\alpha_n + \alpha_n^*), \quad p_n = \frac{1}{i}\sqrt{\frac{\mu\hbar\omega_0}{2}}(\alpha_n - \alpha_n^*), \quad (\text{A.1})$$

$$u_n = \sum_q \sqrt{\frac{\hbar}{2N_1 M \omega(q)}} \exp(iqna) (\beta_q + \beta_{-q}^*) \quad (\text{A.2.1})$$

$$P_n = \sum_q \sqrt{\frac{\hbar M \omega(q)}{2N_1}} \exp(iqna) \frac{1}{i} (\beta_q - \beta_{-q}^*). \quad (\text{A.2.2})$$

Then, inserting Equations (A.1) and (A.2) into Equation (15) and performing lengthy, though straightforward, calculations, we obtain Equations (18) and (19).

Appendix B. Illustration of normal ordered form

Let us illustrate the normal ordered form by taking $\hat{v}(\hat{q}_n)$, $\hat{V}(\hat{q}_n)$ and $L(n, m)$ in Equation (2) to be of the form

$$\hat{v}(\hat{q}_n) = \frac{\mu\omega_0^2}{2}\hat{q}_n^2 + \frac{b}{4}\hat{q}_n^4, \quad \hat{V}(\hat{q}_n) = \frac{1}{2}\hat{q}_n^2, \quad (\text{B.1})$$

$$L(n, m) = L[\Delta(n, n+1) + \Delta(n, n-1)], \quad (\text{B.2})$$

where ω_0 is the eigenfrequency of the amide-I oscillator. The quantities b and L are constants. For the quantity $\hat{V}(\hat{q}_n)$, retaining solely the first order term which is quadratic with respect to the $\hat{q}_n$'s suffices because it is higher order than $\hat{v}(\hat{q}_n)$. Then, an explicit expression for $v(q_n)$ and $V(q_n)$ are given by

$$v(q_n) = \frac{\mu\omega^{*2}}{2}q_n^2 + \frac{b}{4}q_n^4 + v^{(0)}, \quad V(q_n) = \frac{1}{2}(q_n^2 + q_n^{(0)2}), \quad (\text{B.3})$$

where

$$\omega_0^{*2} = \omega_0^2 + \frac{3b}{\mu}q^{(0)2}, \quad q^{(0)} = \sqrt{\frac{\hbar}{2\mu\omega_0}}, \quad v^{(0)} = \frac{\mu\omega_0}{2}q^{(0)2} + \frac{3b}{2}q^{(0)4}. \quad (\text{B.4})$$

Physically, the quantity $q^{(0)}$ in the above equations denotes the amplitude of the zero-point motion of the amide-I oscillator. From Equations (B.1) and (B.2), explicit expressions for c_1 and ω^{*2} in Equation (23) are given by

$$c_1^2 = \frac{L}{\mu}a^2, \quad \omega^{*2} = \omega_0^2 - \frac{2L}{\mu}. \quad (\text{B.5})$$

Similarly, let $U(x)$ in Equation (3) be of the form

$$U(x) = \frac{K_2}{2}x^2 - \frac{K_3}{3}x^3, \quad (\text{B.6})$$

where $K_2(> 0)$ and $K_3(> 0)$ are constants. Then, the quantity c_0 in Equation (24) is given by

$$c_0^2 = \frac{K_2a^2}{M}. \quad (\text{B.7})$$

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