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Migration of energy in the hydrogen bonded chain of peptide groups

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Received 16 April 1991, in final form 2 December 1991

Abstract. A theory is proposed for the nonlinear excited states in the hydrogen bonded chain of peptide groups, where the interaction between intramolecular and intermolecular vibrations is taken into account. It is an interpolation between the behaviour in two limiting cases, i.e. the vibron soliton in the subsonic region, and the acoustic soliton in the supersonic region. Using this framework, the mechanism of energy migration in hydrogen bonded systems of peptide groups is analysed.

1. Introduction

In recent years interest has been aroused by attempts to apply solid state theory to the problem of describing biological processes at the molecular level [1, 2]. This approach is based on experimental data on the periodic structure of the protein molecule [3]. The methods of solid state physics are often applied to investigating one of the central issues of bioenergetics—the explanation of the reasons for the high efficiency of the transfer of energy. Theoretical studies of the phenomena of energy transfer in complex biological systems in an aqueous environment inevitably involve considerable simplification and modelling of the main properties of these phenomena.

The relative flexibility of large protein molecules is reflected in the large number of possible conformations which are transformed into one another on changing the external conditions. One of the most important and interesting secondary structures is the alpha-helical structure which is formed as a result of intramolecular hydrogen bonds between the peptide groups of the protein molecule [3]. The potential of the hydrogen-bonding interaction between peptide groups has a remarkable, nonlinear character, which is often described by the Toda-potential [4]. The energy of formation of one hydrogen bond between peptide groups is of the order of 0.21 eV. This hydrogen bond therefore belongs to the weak type. The amide I vibration in peptide groups has an energy equal to 0.21 eV and a large electrical dipole moment.

When the adenosine triphosphate (ATP) molecule is hydrolysed, an energy of about 0.49 eV is released which is insufficient to excite the electronic states of the molecule. It is only possible to excite the intramolecular amide I vibration in the peptide group of a protein molecule. The vibrational dipole moment (0.3 D) is also sufficiently large to provide a strong resonance interaction leading to collective vibrational excitons. If the energy released by the hydrolysis of the ATP molecule is used for the formation of an initial impulsive lattice distortion in the chain of peptide groups, the impulse may break up into a single soliton plus some additional background effect. In this situation the created soliton induces the excitation of intramolecular amide I vibration through

the classical coupling between intramolecular and intermolecular vibrational oscillators [5-7].

Recently Yomosa [4] regarded the one-dimensional hydrogen-bonded chain of peptide groups in the alpha-helical protein molecule, as a Toda nonlinear lattice [8, 9]. It was shown that the local increase in density—the so-called acoustic solitons—can propagate in alpha-helical proteins if higher-order spatial derivatives of the displacements of molecules (dispersion) are taken into account. Their velocity exceeds that of longitudinal sound velocity c_2 in all cases. As the excitation velocity decreases to c_2 , the excitation energy and momentum approach zero. This implies that the longitudinal sound velocity c_2 is in some way special. Such difficulty should be removed by inclusion of the coupling between the vibrational exciton of the intramolecular amide I mode and the intermolecular lattice phonon.

Davydov [5] proposed a quantum theory for alpha-helical protein to construct a molecular theory of muscle contraction. Attempts were later made by Scott and coworkers [6] to generalize the Davydov theory in several directions by performing extensive numerical calculations. The presented soliton is a collective excitation formed as a result of combining amide I excitation with local deformation of the chain. Takeno [7] also considered that the naive model exciton Hamiltonian employed in the Davydov theory does not appear to be equally applicable to vibrational excitons, since the nature of vibrational excitation transfer is not necessarily analogous to that of electronic exciton transfer by exchange interactions. He showed that the classical theory appears to be more appropriate to describe the vibrational energy transfer. In the theories of Davydov and Takeno [5-7], solitary excitation propagates only with velocities which are smaller than the longitudinal sound velocity c_2 appropriate to the chain under study. As the excitation velocity approaches c_2 , the excitation energy and momentum grow infinitely. Thus difficulty also should be removed by the inclusion of anharmonicity into the interaction between molecules.

It would thus be interesting to reinvestigate how the nonlinearity of the hydrogen-bonds generates both a self-trapping mechanism for amide I excitations and an acoustic soliton formation for lattice vibrations. As a model, we now consider a one-dimensional chain with an exponential interaction potential, formed by the same molecules which are spaced from each other by a distance l as shown in figure 1. These molecules possess rather large dipole moments directed along the chain of peptide groups. The vibrational energy of carbon monoxide (CO), incorporated into the peptide groups of the chain, is transferred along the hydrogen-bonded chain. The local contraction of the chain, formed by nonlinear lattice distortion, may serve as a potential well for amide I excitations.

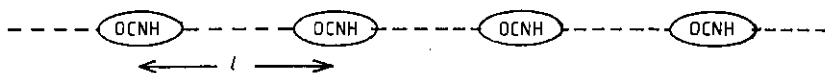


Figure 1. Schematic representation of the system. OCNH denotes a peptide group and the dashed line segments indicate a hydrogen bond.

From these observations we try to calculate the energy and momentum of the solitary excitation moving with velocity V . After presenting our model and giving a brief review (to make the paper self-contained) of basic equations of a model protein system (section 2), we calculate the energy and momentum of the excitation based on the continuum approximation (section 3). The final section provides conclusions and proposals for further work.

2. Model system and basic equations

We describe without of generality the one-dimensional hydrogen-bonded chain of peptide groups, $\cdots\text{OCNH}\cdots\text{OCNH}\cdots$, as a Toda lattice [4, 8, 9]. Then the Hamiltonian of the lattice system is given by

$$H_L = \sum_n \left[\frac{1}{2} M \dot{u}_n^2 + \kappa b^{-1} \{ -(u_{n-1} - u_n) + b^{-1} [\exp(b(u_{n-1} - u_n)) - 1] \} \right] \quad (2.1)$$

where u_n , M , κ and b are the displacement of the n th molecule from its equilibrium position n , the molecular mass, a coefficient of longitudinal elasticity of the harmonic lattice and the parameter of anharmonicity, respectively. The value of the parameters κ and b can be estimated from the results of the *ab initio* SCF MO calculation for a hydrogen-bond in a model dimer system.

The dipole moment of the intramolecular amide I vibration is large enough to provide a strong resonance interaction leading to collective vibrational excitons. The Hamiltonian for the intramolecular amide I vibration is given by

$$H_A = \frac{1}{2} \sum_n (\mu q_n^2 + \mu \varepsilon^2 q_n^2) - \frac{1}{2} L \sum_n (q_n q_{n+1} + q_n q_{n-1}) \quad (2.2)$$

which is derived from the Takeno model [7]. q_n , μ and ε are normal coordinate, effective mass, and frequency, respectively, of the relevant intramolecular amide I vibration of the n th molecule, and L is a force constant giving vibrational exciton transfer between the nearest-neighbour peptide molecules. We note that only the ground state and one of the excited states of the peptide group are considered.

As shown in previous theories [5-7], there always exist some couplings between the intramolecular amide I vibration and the lattice vibration of peptide groups. The energy (ε) of the relevant amide I vibration and the resonance interaction (L) of neighbouring peptide groups depend on the instantaneous position $x_n = nl + u_n$ of the molecules. Two types of interaction constants χ_1 , and χ_2 are obtained by expanding $\varepsilon(x_n)$ and $L(x_n - x_m)$ to first order with respect to the u . Then the Hamiltonian of such types of interaction is described by the following function

$$H_I = \frac{1}{2} \sum_n \left[\frac{\mu \chi_1}{l} (u_{n+1} - u_{n-1}) q_n^2 - \frac{\chi_2}{l} \{ (u_{n+1} - u_n) q_{n+1} + (u_n - u_{n-1}) q_{n-1} \} q_n \right]. \quad (2.3)$$

The excited states of a soft molecular chain, which contains vibrational excitons, can be characterized by the Hamiltonian

$$H = H_L + H_A + H_I. \quad (2.4)$$

From the above model Hamiltonian it is straightforward to derive the following self-consistent equations for w_n and q_n ,

$$l \frac{d^2 w_n}{dt^2} - \frac{\kappa b^{-1}}{M} \left(2 \sinh \frac{1}{2} \frac{\partial}{\partial n} \right)^2 \exp(blw_n) - \frac{\mu}{2Ml} \left(\chi_1 - \frac{\chi_2}{\mu} \right) (q_{n-1}^2 - q_{n+1}^2) = 0 \quad (2.5)$$

$$\frac{d^2 q_n}{dt^2} + \varepsilon^2 q_n - \frac{L}{\mu} (q_{n+1} + q_{n-1}) + \frac{1}{l} \left(\chi_1 - \frac{\chi_2}{\mu} \right) (u_{n+1} - u_{n-1}) q_n = 0 \quad (2.6)$$

where $lw_n = u_{n-1} - u_n$. We substitute into these equations the expression

$$q_n(t) = \phi_n(t) \exp[im^*nlV - i\omega t] + \text{cc} \quad (2.7)$$

where m^* is the effective mass of the vibrational amide I exciton and ω is the energy of the bound state of the vibrational exciton in the field of the local deformation moving with velocity V along the chain. Then we obtain the set of equations for the envelope $\phi_n(t)$ of the function (2.7)

$$l \frac{d^2 w_n}{dt^2} - \frac{\kappa b^{-1}}{M} \left(2 \sinh \frac{1}{2} \frac{\partial}{\partial n} \right)^2 \exp(blw_n) - \frac{2\mu}{Ml} \left(\chi_1 - \frac{\chi_2}{\mu} \right) (|\phi_{n-1}|^2 - |\phi_{n+1}|^2) = 0 \quad (2.8)$$

$$\frac{d\phi_n}{dt} = \frac{L}{2\omega\mu} (\phi_{n-1} - \phi_{n+1}) \sin(m^*lV) \quad (2.9)$$

$$(-\omega^2 + \varepsilon^2)\phi_n - \frac{L}{\mu} (\phi_{n+1} + \phi_{n-1}) \cos(m^*lV) + \frac{1}{l} \left(\chi_1 - \frac{\chi_2}{\mu} \right) (u_{n+1} - u_{n-1})\phi_n = 0 \quad (2.10)$$

where $m^* = \mu\omega/Ll^2$.

When the displacement fields $\{\phi_n, w_n\}$ change slowly with n we can employ the so-called continuum approximation under the assumption that the velocity of excitation V satisfies the inequality

$$m^*lV \ll 1. \quad (2.11)$$

Keeping fourth-order derivatives with respect to the coordinate x , we can transform (2.8) to the form

$$w_{tt} - c_2^2 w_{xx} - \frac{(lc_2)^2}{12} w_{xxxx} - \gamma\kappa^{-1} c_2^2 (w^2)_{xx} + \frac{2\mu A'}{M} (\phi^2)_{xx} = 0 \quad (2.12)$$

where $A' = 2(\chi_1 - \chi_2/\mu)$. In the absence of coupling ($A' = 0$), (2.12) is called the Boussinesq equation. The solution of such an equation was studied by Toda and Wadati [9]. Then (2.9) and (2.10) are transformed to equations involving partial derivatives which are denoted below by indexes of the corresponding variables

$$\phi_t = -V\phi_x \quad (2.13)$$

$$-\frac{Ll^2}{\mu} \phi_{xx} + A' u_x \phi = [\omega^2 - \omega_0(V)^2] \quad (2.14)$$

where

$$\omega_0(V)^2 = \omega_0^2 + \frac{L}{2\mu} (m^*)^2 V^2 \quad \text{with } \omega_0^2 = \varepsilon^2 - \frac{L}{\mu}.$$

To study stationary solutions belonging to the class of rapidly decreasing functions, we introduce the following dimensionless variable

$$\xi = \frac{x - Vt}{l}$$

and assume that $\phi(x, t) = \phi(\xi)$, $w(x, t) = w(\xi)$. Then equation (2.13) becomes an identity, and (2.12) and (2.14) are transformed as follows

$$\frac{1}{12} \frac{d^2 w}{d\xi^2} + (1 - s^2)w + \tilde{\gamma}w^2 = \frac{A'}{Mc_2^2} \tilde{\phi}^2 \quad (2.15)$$

$$\tilde{L} \frac{d^2 \tilde{\phi}}{d\xi^2} + A' w \tilde{\phi} + \Omega \tilde{\phi} = 0 \quad (2.16)$$

where $\Omega = \omega^2 - \omega_0(V)^2$, $s = V/c_2$, $\tilde{\gamma} = \gamma\kappa^{-1}$, $\tilde{L} = L/\mu$, $\tilde{\phi} = \phi\sqrt{2\mu}$.

It is convenient to replace the set of equations (2.15) and (2.16) by an integral equation. Let us multiply (2.15) by $dw/d\xi$ and (2.16) by $d\tilde{\phi}/d\xi$. Integrating them and taking account of the boundary conditions (the functions ϕ and w and their derivatives vanish at $|\xi| \rightarrow \infty$) and using the replacement $\xi \rightarrow \phi(\xi)$ in the integrands, we obtain the following equations

$$\frac{1}{12} \left(\frac{dw}{d\xi} \right)^2 = (s^2 - 1)w^2 - \frac{2}{3} \tilde{\gamma} w^3 + \frac{2A'}{Mc_2^2} w \tilde{\phi}^2 - \frac{A'}{Mc_2^2} \int_0^{\tilde{\phi}} w(\tau) \tau \, d\tau \tag{2.17}$$

$$\tilde{L} \left(\frac{d\tilde{\phi}}{d\xi} \right)^2 + 2A' \int_0^{\tilde{\phi}} w(\tau) \tau \, d\tau + \Omega \tilde{\phi}^2 = 0. \tag{2.18}$$

In the case of bell-like solitons with centres at $\xi = 0$ the equality

$$\left(\frac{d\tilde{\phi}}{d\xi} \right)_{\xi=0} = 0 \tag{2.19}$$

holds. Using this equality, we find the magnitude of the spectral parameter from (2.18)

$$\Omega = -\frac{2A'}{\tilde{\phi}_0^2} \int_0^{\tilde{\phi}_0} w(\tau) \tau \, d\tau \quad \tilde{\phi}_0 = \tilde{\phi}(0). \tag{2.20}$$

Substituting this value into equation (2.18), we find the measure

$$|d\xi(\tilde{\phi})| = \left(\frac{\tilde{L}}{2A'} \right)^{1/2} \left[\left(\frac{\tilde{\phi}}{\tilde{\phi}_0} \right)^2 \int_0^{\tilde{\phi}_0} w(\tau) \tau \, d\tau - \int_0^{\tilde{\phi}} w(\tau) \tau \, d\tau \right]^{-1/2} d\tilde{\phi}. \tag{2.21}$$

The desired amplitude $\tilde{\phi}_0$ is determined from the normalization condition for the function $\phi(\xi)$. On replacing ξ by $\phi(\xi)$ this condition becomes

$$\int_0^{\tilde{\phi}_0} \tilde{\phi}^2 |d\xi(\tilde{\phi})| = \frac{1}{2} C$$

where C is a constant. Substituting (2.21) into this equation, we obtain

$$\int_0^{\tilde{\phi}_0} \tau^2 \left[\left(\frac{\tau}{\tilde{\phi}_0} \right)^2 \int_0^{\tilde{\phi}_0} w(y) y \, dy - \int_0^{\tau} w(y) y \, dy \right]^{-1/2} d\tau = \left(\frac{A'}{2\tilde{L}} \right)^{1/2} C \tag{2.22}$$

which allows us to evaluate the maximum value ϕ_0 of the envelope $\phi(\xi)$. Finally, integrating (2.17), we obtain the required integral equation

$$w(\tilde{\phi}) = 12 \int_0^{\tilde{\phi}} \left\{ (s^2 - 1)w(\tau)^2 - \frac{2}{3} \tilde{\gamma} w(\tau)^3 + \frac{2A'}{Mc_2^2} \left[\tau^2 w(\tau) - 2 \int_0^{\tau} w(y) y \, dy \right]^{1/2} \right\} |d\xi(\tau)|. \tag{2.23}$$

We note that this integral equation is exactly equivalent to the set of differential equations (2.17) and (2.18). If the norm of the corresponding integral operator is less than unity, the solution of (2.23) can be sought by the method of successive approximations.

3. Solitary excitations

As mentioned in the previous section, the solution of the integral equation (2.13) can be obtained using the method of successive approximations. Integrating (2.21), we

find the envelope $\tilde{\phi}(\xi) = \tilde{\phi}(-\xi)$ in the implicit form

$$|\xi| = \left(\frac{\tilde{L}}{2A'}\right)^{1/2} \int_{\tilde{\phi}(\xi)}^{\tilde{\phi}_0} \left[\left(\frac{\tau}{\tilde{\phi}_0}\right)^2 w(y)y \, dy - \int_0^\tau w(y)y \, dy \right]^{-1/2} d\tau. \quad (3.1)$$

As the zeroth approximation we choose the function

$$w^{(0)}(\tilde{\phi}) = \alpha \tilde{\phi}^2 \quad (3.2)$$

where α is a positive number which is to be determined. Equation (2.22), taking into account (3.2), defines the amplitude $\tilde{\phi}_0$ of the function

$$\tilde{\phi}_0^{(0)} = \sqrt{\frac{A'\alpha}{8\tilde{L}}}. \quad (3.3)$$

Substituting (3.2) and (3.3) into (2.21) and the right-hand side of (2.23), we obtain for the first-order approximation

$$|d\xi^{(1)}(\tilde{\phi})| = \frac{\sqrt{2\tilde{L}}}{[\alpha A'(\alpha A'/8\tilde{L} - \tilde{\phi}^2)]^{1/2}} \frac{d\tilde{\phi}}{\tilde{\phi}} \quad (3.4)$$

$$w^{(1)}(\tilde{\phi}) = \left(\frac{24\tilde{L}}{A'}\right)^{1/2} \int_0^{\tilde{\phi}} \left[\frac{A'}{Mc_2^2} + \alpha(s^2 - 1) - \frac{2}{3}\tilde{\gamma}\alpha^2\tau^2 \right]^{1/2} \frac{\tau \, d\tau}{(A'\alpha/8\tilde{L} - \tau^2)^{1/2}}. \quad (3.5)$$

Unfortunately, the evaluation of this integral leads, in general, to a complicated expression. If α is, however, a positive root of the following cubic equation

$$\frac{\tilde{\gamma}A'}{12\tilde{L}} z^3 + (1 - s^2)z - \frac{A'}{Mc_2^2} = 0 \quad (3.6)$$

the integral is simplified and becomes easily evaluated. Then the first-order approximation function takes the following form

$$w^{(1)}(\tilde{\phi}) = \alpha g \tilde{\phi}^2 \quad (3.7)$$

where $g = \sqrt{\tilde{L}\tilde{\gamma}/3\nu A'}$ with $\nu = \frac{1}{12}$. Substituting (3.7) into (2.22), we find the amplitude of the function $\tilde{\phi}(\xi)$ to the first-order approximation

$$\tilde{\phi}_0^{(1)} = \sqrt{\frac{A'g\alpha}{8\tilde{L}}}. \quad (3.8)$$

Now we can write the solutions of the set of equations (2.17) and (2.18) explicitly to the first-order approximation. Let us substitute (3.7) and (3.8) into (3.1) and (2.20). Then we obtain

$$\tilde{\phi}^{(1)}(\xi) = \sqrt{\frac{\tilde{\mu}}{2}} \operatorname{sech}(\tilde{\mu}\xi) \quad \Omega^{(1)} = -\tilde{L}\tilde{\mu}^2 \quad (3.9)$$

and it follows from (3.7) that

$$w^{(1)}(\xi) = \frac{2\tilde{L}\tilde{\mu}^2}{A'} \operatorname{sech}^2(\tilde{\mu}\xi). \quad (3.10)$$

The dimensionless parameter

$$\tilde{\mu} = \frac{\alpha g A'}{4\tilde{L}} \quad (3.11)$$

depending on the velocity, characterizes the inverse width of the solitary excitations. Substituting the expressions (3.7) and (3.8) into (2.21) and the right-hand side of (2.23), we find the solution to the second-order approximation. However, it is easily proved that if the relation

$$g = 1 \quad \text{or} \quad \tilde{L}\tilde{\gamma} = 3\nu A' \tag{3.12}$$

holds, the first-order approximation coincides with the zeroth one as shown in figure 2. Actually, Scott and coworkers [10] have already demonstrated that the interaction constant (A') represents the anharmonicity (γ) in the longitudinal hydrogen bonds. Therefore, if the relation (3.12) is satisfied, the solution

$$\tilde{\phi}(\xi) = \sqrt{\frac{\mu_0}{2}} \operatorname{sech}(\mu_0 \xi) \quad \Omega = -\tilde{L}\mu_0^2 \tag{3.13}$$

$$w(\xi) = \frac{2\tilde{L}\mu_0^2}{A'} \operatorname{sech}^2(\mu_0 \xi) \tag{3.14}$$

becomes the exact one, if μ_0 is defined by the expression

$$\mu_0 = \frac{\alpha A'}{4\tilde{L}} \tag{3.15}$$

where α is a positive root of (3.6). Using (3.15), we can transform (3.6) to the following:

$$4\nu\mu_0^3 + (1 - s^2)\mu_0 - \frac{A'^2}{4\tilde{L}M c_2^2} = 0. \tag{3.16}$$

It involves directly μ_0 , which enters into the exact solutions.

At a fixed value of s , (3.16) has the single positive root $\mu_0 = \mu_0(s)$ if $s^2 < 1$ and $s^2 > 1$. This is shown in figure 3. It follows from figure 3 that the sound velocity $c_2(s = 1)$ is not in any way special. The solutions have meaning for subsonic ($s^2 < 1$) and for supersonic ($s^2 > 1$) velocities. When $\tilde{\phi}(\xi)$ is known, we can determine the displacement field

$$w(\xi) = w[\tilde{\phi}(\xi)] \tag{3.17}$$

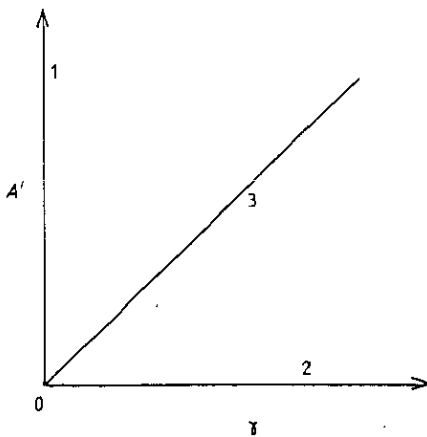


Figure 2. The A' - γ relation. Numbers attached to each curve denote (1) the subsonic case, (2) the supersonic case, (3) the general case, respectively.

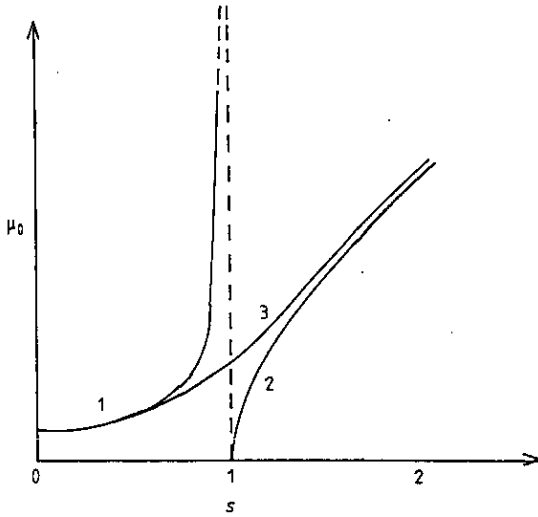


Figure 3. The dependence of μ_0 on the velocity. Numbers attached to each curve denote (1) the subsonic case, (2) the supersonic case, (3) the general case, respectively.

and with its help we can obtain the energy and momentum of the solitary excitation moving with velocity V

$$\begin{aligned}
 E(V) &= \frac{1}{2}m^*V^2 + \Omega + \omega_0(V) + \frac{1}{2}Mc_2^2 \int d\xi \left[(1+s^2)w^2 + \frac{1}{12} \left(\frac{dw}{d\xi} \right)^2 + \frac{2}{3}\tilde{\gamma}w^3 \right] \\
 &= \frac{1}{2}m^*V^2 + \omega_0(V)^2 - \tilde{L}\mu_0^2 + \frac{8}{3}Mc_2^2 \left(\frac{\tilde{L}}{A'} \right)^2 [1+s^2 + \frac{1}{3}\mu_0^2]\mu_0^3 \tag{3.18}
 \end{aligned}$$

$$P(V) = \left(m^* + M \int w^2 d\xi \right) V = \left[m^* + \frac{16}{3}M\mu_0^3 \left(\frac{\tilde{L}}{A'} \right)^2 \right] V. \tag{3.19}$$

Such a solitary excitation is stable if its energy is less than that of the bottom of the energy band of free amide I excitation, i.e. if $E(V) < \omega_0(V)^2$.

4. Approximation for solitary solution

In this section we examine the behaviour of solitary excitation for various limiting cases.

4.1. Subsonic case

If dispersion and anharmonicity are absent and the parameters ν and γ approach zero simultaneously in such a way that the relation (3.15) remains valid, equation (3.16) has a positive solution only at subsonic travelling velocities

$$\mu_0^{(D)} = \frac{A'^2}{4LM(c_2^2 - V^2)} \quad V^2 < c_2^2. \tag{4.1}$$

Then the functions (3.13) and (3.14) with $\mu_0 = \mu_0^{(D)}$ coincides with those studied in the theories of Davydov and Takeno [5-7]. The existence of the doubly degenerate ground state allows the *topological soliton*, which is a domain wall separating two distinct

ground states. Substituting (4.1) into (3.18) and (3.19) we obtain the energy and the momentum carried by the solitary excitation of this kind

$$E^{(D)}(V) = \frac{1}{2}m^*V^2 + \omega_0(V)^2 - \tilde{L}[\mu_0^{(D)}]^2 + \frac{8}{3}Mc_2^2\left(\frac{\tilde{L}}{A'}\right)^2 [1 + s^2 + \frac{1}{3}\{\mu_0^{(D)}\}^2]\{\mu_0^{(D)}\}^3 \quad (4.2)$$

$$P^{(D)}(V) = \left[m^* + \frac{16}{3}M\{\mu_0^{(D)}\}^3\left(\frac{\tilde{L}}{A'}\right)^2 \right] V. \quad (4.3)$$

As shown in figures 4 and 5, if the excitation velocity approaches c_2 , both the excitation energy and the momentum grow infinitely.

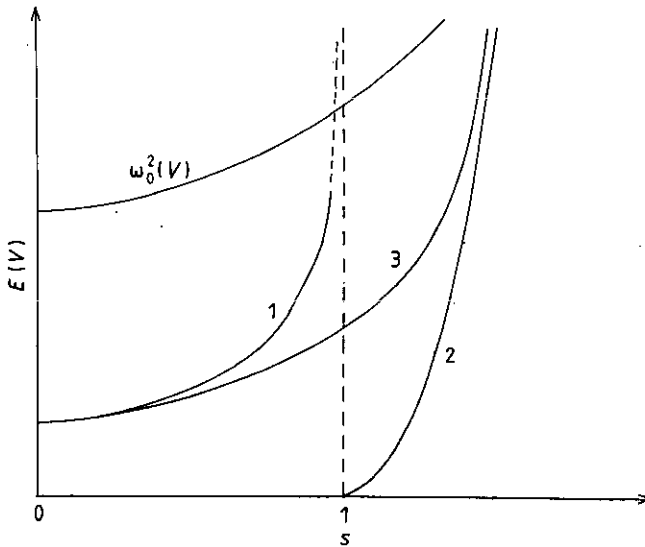


Figure 4. The dependence of the excitation energy on the velocity. Numbers attached to each curve denote (1) the subsonic case, (2) the supersonic case, (3) the general case, respectively.

4.2. Supersonic case

In the theory of subsonic solitary excitation, coupling between the intramolecular amide I vibration and the intermolecular lattice vibration is essential. But before considering such higher-order mechanisms for soliton formation, there exists a more natural and reasonable introduction of a soliton into the hydrogen bonded chain of peptide groups.

If (3.16) holds as the ratio A^2/\tilde{L} approaches zero, then only the supersonic acoustic soliton (the continuum version of the Toda lattice soliton) is excited, which is described for $\nu = \frac{1}{12}$ by the function [4, 9]

$$\mu_0^{(B)} = \sqrt{3(s^2 - 1)} \quad V = sc_2 \quad s^2 > 1. \quad (4.4)$$

Then the function (3.14) with $\mu_0 = \mu_0^{(B)}$ coincides with that studied in the theory of Toda and Wadati [9]. Unlike phonons, excitations of acoustic solitons do not, in practice, lose energy in collisions with the admixture atoms, because the scattering effect between the supersonic soliton and the intramolecular amide I vibration is neglected.

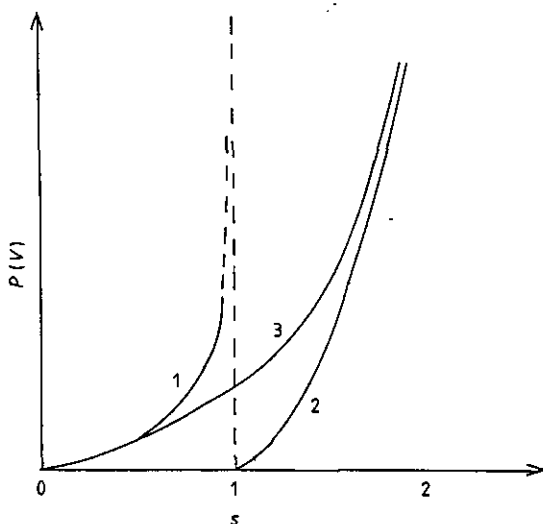


Figure 5. The dependence of the momentum of excitation on the velocity. Numbers attached to each curve denote (1) the subsonic case, (2) the supersonic case, (3) the general case, respectively.

The energy and momentum of the acoustic soliton are given by the analytical expression

$$E^{(B)}(V) = \sqrt{3}\kappa^3(s^2 - 1)^{3/2}(1 + 9s^2)/30\gamma^2 \quad (4.5)$$

$$P^{(B)}(V) = \sqrt{3}\kappa^2(s^2 - 1)^{3/2}\gamma^{-2}MV. \quad (4.6)$$

With a decrease in the velocity V , the soliton energy and momentum are lowered. Hence, in the limit $V \rightarrow c_2$ they vanish as shown in figures 4 and 5.

4.3. General case

We note that the sound velocity $c_2(s = 1)$ is not in any way special as shown in figure 3. In the curve of $\mu_0^{(G)}$, the above-mentioned difficulties have been removed. A restriction on the velocity is determined by the condition of validity of the continuum approach

$$\mu_0 \ll 1 \quad (4.7)$$

and also the requirement that the solitary excitation energy should be below the bottom of the energy band of an intramolecular amide I exciton.

In the *crossover* region $V \sim c_2$, however, the situation is very complicated and we cannot draw a simple picture of the excitation. While in movement, the supersonic soliton may scatter the intramolecular amide I excitons, therefore, it is rapidly decelerated. The problem of the realization of the solitary excitations considered above for the crossover region demands a special study.

5. Discussion

In this paper we proposed an interpolation theory for nonlinear excited states in the hydrogen bonded chain of peptide groups. In this framework, the effect is separated

into the amide I exciton-phonon coupling effect and the effect of anharmonicity of the phonon. Expressions for both effects are taken so that they coincide with theoretical results in limiting cases.

In most previous theories, only one of the two effects has been taken into account. Theories where the effect of amide I exciton-phonon interaction is considered are valid only when $V \ll c_2$. On the other hand, theories where only the anharmonicity of interaction between peptide groups is taken into account are applicable when $V \gg c_2$. In general cases both effects should be taken into account. In particular, the situation is very complicated in the crossover region $V \sim c_2$. Therefore, to examine theoretical results in this region, we should carefully study how the various types of interaction modify the results given in this paper.

From these considerations we can conclude that as the travelling velocity approaches and then exceeds the velocity of sound, the qualitative mechanism of the soliton formation changes and one has an example of a crossover between a topological soliton (vibron soliton) in the subsonic region and a non-topological soliton (acoustic soliton) in the supersonic region.

Throughout this paper we have neglected the effect of discreteness of the lattice. Such an effect will be discussed in forthcoming papers. The calculations described here were carried out on the Nara University ACOS-430/70 computer.

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