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Kink Pair in Hydrogen Bonded Systems with Symmetric Double-Well Potential

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Abstract In hydrogen-bonded systems with a symmetric double-well potential, using the variational method, we study the nonlinear excitations and motion of the solitons in the presence of the optical mode of the heavy ion sublattice, based on a new two-component soliton model. We give the equations of motion and soliton-solutions in such a case. Based on these results we calculate further the energy, the momentum and the effective mass of the kink pair.

Keywords Hydrogen-bonded chains · Two-component model · Optical mode · Kink pair

1 Introduction

There is a large number of hydrogen bonded condensed matter systems, such as solid alcohol, ice, ferroelectric hydrogen bonded crystals, carbon hydrates and proteins, the dynamics of proton transfer along hydrogen bonded chains is an interesting and important subject and has been investigated by a number of authors [1–9]. The hydrogen bonded chains consist of series of hydrogen bonds as follows, $\cdots X{-}H\cdots X{-}H\cdots$, where X is a heavy ion or oxygen atom in ice—indicates a covalent bond, and $\cdots$ represents a hydrogen bond. The proton potential energy in each hydrogen bridge can be written as follows, $U(u_i) = 1/4U_0[1-(u_i/u_0)^2]^2$, it is a symmetric double-well potential. In the transfer process, the proton from one well of the double-well potential to the other well, solitonic defects are excited in the proton sublattice of the hydrogen-bonded chains. Furthermore, some two-component soliton models have been suggested in order to evaluate the influence of the motion of the heavy-ion sublattice on the proton sublattice. The results show that solitonic defects in the proton sublattice and in a heavy-ion sublattice may exist [3–6]. Recently, a new two-component soliton model for proton transport in hydrogen-bonded chains was suggested by Pang [6]. However, the heavy ion sublattice is not an ideal simplex atomic lattice. The heavy ion has an internal vibration, as e.g. the amide-I vibration in the peptide

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group of α-helical protein and the vibration of the oxygen ions in ice [2, 8]. Therefore, in this paper, on the basis of this model, we investigate the nonlinear excitations and motion of the kink pair in the presence of the optical mode of the heavy ion sublattice using variational method. We obtain the equations of motion and the soliton-solutions of a kink pair and calculate the energy, the momentum and the effective mass of the kink pair.

2 Hamiltonian and Equation of Motion

We assume that the coupling between the proton sublattice and acoustic mode of the heavy-ion sublattice is the nonlinear, and a new model Hamiltonian of the hydrogen-bonded systems is expressed by [6]

$$\begin{aligned} H &= H_{\mathrm{p}} + H_{\mathrm{ion}} + H_{\mathrm{int}} \\ &= \sum_i \left\{ \frac{1}{2m} p_i^2 + \frac{1}{2} m\omega_0^2 u_i^2 - \frac{1}{2} m\omega_1^2 u_i u_{i+1} + \frac{1}{4} U_0 \left[1 - \left(\frac{u_i}{u_0} \right)^2 \right]^2 \right\} \\ &\quad + \sum_i \left[\frac{1}{2M} P_i^2 + \frac{1}{2} \beta (\eta_i - \eta_{i-1})^2 \right] \\ &\quad + \sum_i \left[\frac{1}{2} m\chi_1 (\eta_{i+1} - \eta_{i-1})^2 u_i^2 + m\chi_2 (\eta_{i+1} - \eta_i) u_i u_{i+1} \right] \end{aligned} \tag{1}$$

where m and M are the masses of the proton and heavy ion, respectively. The proton displacement and momentum are u_i and $p_i = m\dot{u}_i$, respectively. u_0 is the distance between the central maximum and one of the minima of the double-well, U_0 is the height of the barrier of the double-well potential. The quantity $\frac{1}{2} m\omega_1^2 u_i u_{i+1}$ shows the correlation interaction between neighboring protons caused by the dipole-dipole interaction, ω_0 and ω_1 are diagonal and nondiagonal elements of the dynamic matrix of the proton, respectively. Similarly, η_i and $P_i = M\dot{\eta}_i$ are the displacement of the heavy ion from its equilibrium position and its conjugate momentum, respectively. l is the lattice constant and $c_0 = l(\beta/M)^{1/2}$ is the velocity of sound in the heavy ionic sublattice. χ_1 and χ_2 are coupling constants between the proton and the heavy ion sublattices. The part H_{p} of H is the Hamiltonian of the protonic sublattice with symmetric double-well potential $U(u_i)$, H_{ion} being the Hamiltonian of the heavy ionic sublattice and H_{int} is the interaction Hamiltonian between the protonic and the heavy ionic sublattice. In the continuum approximation with the long-wavelength limit [10], the Hamiltonian (1) can be replaced by a continuum representation

$$\begin{aligned} H = \frac{1}{l} \int_{-\infty}^{\infty} \Bigg\{ & \frac{1}{2} m u_t^2 + \frac{1}{2} m\omega_0^2 u^2 - \frac{1}{2} m\omega_1^2 u (u + l u_x + l^2 u_{xx}) \\ & + \frac{1}{4} U_0 \left[1 - \left(\frac{u}{u_0} \right)^2 \right]^2 + \left(\frac{1}{2} M\eta_t^2 + \frac{1}{2} \beta l^2 \eta_x^2 \right) + m(\chi_1 + \chi_2) l \eta_x u^2 \Bigg\} dx \end{aligned} \tag{2}$$

The Euler-Lagrange equations of motion corresponding to (2) are

$$u_{tt} = \upsilon_1^2 u_{xx} - 2(\chi_1 + \chi_2) l \eta_x u + \frac{u U_0}{m u_0^2} \left[1 - \frac{m u_0^2 (\omega_0^2 - \omega_1^2)}{U_0} - \left(\frac{u}{u_0} \right)^2 \right] \tag{3}$$

$$\eta_{tt} = c_0^2 \eta_{xx} + \frac{2m}{M} (\chi_1 + \chi_2) l u_x u \tag{4}$$

where $\upsilon_1^2 = \frac{1}{2} l^2 \omega_1^2$, υ_1 is the characteristic velocity of the proton.

When $G > 0, \alpha > 0$ and $0 < \upsilon < \upsilon_1$, $0 < \upsilon < c_0$, (3) and (4) have kink soliton solutions

$$u = \sigma u_0 \tanh\left[\sqrt{\frac{\varepsilon}{2}}(x - \upsilon t)\right] \tag{5}$$

$$\eta = Du \tag{6}$$

where $\sigma = \pm 1$ is the polarity of the soliton, and $u_0 = (\frac{\alpha}{G})^{1/2}$,

$$\alpha = \frac{U_0}{mu_0^2} + \omega_1^2 - \omega_0^2 - 2g(\chi_1 + \chi_2)l, \quad g = \frac{ml(\chi_1 + \chi_2)u_0^2}{M(c_0^2 - \upsilon^2)}$$

$$G = \frac{U_0}{mu_0^4} - \frac{2(\chi_1 + \chi_2)^2 ml^2}{M(c_0^2 - \upsilon^2)}, \quad \varepsilon = \frac{\alpha}{\upsilon_1^2 - \upsilon^2}$$

and

$$D = -\frac{\sqrt{2}(\chi_1 + \chi_2)ml}{M(c_0^2 - \upsilon^2)}\left(\frac{\upsilon_1^2 - \upsilon^2}{G}\right)^{1/2} \tag{7}$$

υ is the velocity of the soliton. Equations (5) and (6) show that, in the case $\upsilon < \upsilon_1$ and $\upsilon < c_0$, if the nonlinear excitation in the proton sublattice is the kink (antikink), then the nonlinear excitation in the heavy ion sublattice is the antikink (kink). They propagate along the hydrogen bonded chains in pairs with the same velocity. The kink soliton is an ion-type nonlinear defect. According to the theory of charge transport by solitons [11, 12], the kink defect can capture and carry the electron, i.e. it transports charge and energy in hydrogen bonded chains.

3 Influence of the Optical Mode on the Kink Pair

In this section, we shall consider the influence of the optical mode of the heavy ion sublattice on the kink pair, the Hamiltonian (2) is revised as follows,

$$\begin{aligned} H = \frac{1}{l}\int_{-\infty}^{\infty}\Big\{ & \frac{1}{2}mu_t^2 + \frac{1}{2}m\omega_0^2 u^2 - \frac{1}{2}m\omega_1^2 u(u + lu_x + l^2 u_{xx}) \\ & + \frac{1}{4}U_0\left[1 - \left(\frac{u}{u_0}\right)^2\right]^2 + \left(\frac{1}{2}M\eta_t^2 + \frac{1}{2}\beta l^2 \eta_x^2\right) \\ & + m(\chi_1 + \chi_2)l\eta_x u^2 + \frac{1}{2}M\Omega^2\eta^2\Big\} dx \end{aligned} \tag{8}$$

here Ω is the frequency of the optical mode of the heavy ion sublattice [2, 5]. The Euler-Lagrange equations of motion corresponding to (8) are

$$mu_{tt} = m\upsilon_1^2 u_{xx} - 2m(\chi_1 + \chi_2)lu\eta_x + \frac{uU_0}{u_0^2}\left[1 + \frac{mu_0^2(\omega_1^2 - \omega_0^2)}{U_0} - \left(\frac{u}{u_0}\right)^2\right] \tag{9}$$

$$M\eta_{tt} = Mc_0^2\eta_{xx} + 2m(\chi_1 + \chi_2)luu_x - M\Omega^2\eta \tag{10}$$

The term involving Ω can be regarded as a small perturbation. Supposing that the main effect of the Ω term is to modify the shape of the soliton [13]. We assume that the solutions of (9) and (10) have the following form,

$$u = \sigma u_0 \tanh \frac{S}{\sqrt{2}} y \tag{11}$$

$$\eta = Du \tag{12}$$

where $y = x - \upsilon t$ and S is a variational parameter. Inserting (11) and (12) into (8), we obtain the Lagrangian function

$$\begin{aligned} L(S) = \frac{1}{l}\Bigg[& \frac{2}{3}(m + D^2 M)u_0^2 \upsilon^2 \frac{S}{\sqrt{2}} - m(\omega_0^2 - \omega_1^2)u_0^2 \frac{\sqrt{2}}{S} \\ & - \frac{1}{3} m\omega_1^2 l^2 u_0^2 \frac{S}{\sqrt{2}} - \frac{1}{3} U_0 \frac{\sqrt{2}}{S} - \frac{2}{3} M c_0^2 D^2 u_0^2 \frac{S}{\sqrt{2}} \\ & - \frac{2}{3} m(\chi_1 + \chi_2) l D\sigma u_0^3 + M\Omega^2 D^2 u_0^2 \frac{\sqrt{2}}{S} \Bigg] \end{aligned} \tag{13}$$

According to the variational method, the parameter S is determined by the condition $dL(S)/dS = 0$ [13], and we obtain

$$\begin{aligned} & \frac{\sqrt{2}}{3}(m + D^2 m)u_0^2 \upsilon^2 - \frac{\sqrt{2}}{6} m\omega_1^2 l^2 u_0^2 - \frac{\sqrt{2}}{3} M c_0^2 D^2 u_0^2 \\ & \quad + m(\omega_0^2 - \omega_1^2)\frac{\sqrt{2}}{S^2} + \frac{1}{3} U_0 \frac{\sqrt{2}}{S^2} - M\Omega^2 D^2 u_0^2 \frac{\sqrt{2}}{S^2} = 0 \end{aligned} \tag{14}$$

when $\Omega = 0$, from (14), we get $S^2 = \varepsilon$. Considering the optical mode of the heavy ion sublattice Ω with low frequency, from (14), we can use the first-order approximation to obtain

$$S = \varepsilon^{1/2}(1 - M\Omega^2 D^2 u_0^2 / 2B) \tag{15}$$

where $B = m(\omega_0^2 - \omega_1^2)u_0^2 + \frac{1}{3} U_0$.

Because the width of the soliton depends directly on S^{-1}, the solutions of (11) and (12) are obtained, obviously, the optical mode of the heavy ion sublattice will increase the width of the kink soliton in the proton and the antikink soliton in the heavy ion sublattices, respectively.

4 Elementary Properties of the Soliton Pair

We now investigate the elementary properties of the above soliton pair, but here we consider only a few physically important quantities concerning the kink and antikink solitons in (11) and (12).

4.1 Energy of the Soliton Pair

We calculate the energy of the kink pair due to influence of the optical mode of the heavy ion sublattice.

Inserting $u_x = u_y, u_t = u_y(-\upsilon), \eta_x = Du_y, \eta_t = Du_y(-\upsilon)$ into Hamilton's equation (8), expression of the energy corresponding to (8) becomes

$$E = \int_{-\infty}^{\infty} \frac{dy}{l} \left\{ \frac{1}{2}(m + D^2 M)\upsilon^2 u_y^2 + \frac{1}{2} m(\omega_0^2 - \omega_1^2)u^2 - \frac{1}{2} m\omega_1^2 luu_y \right.$$
$$- \frac{1}{2} m\omega_1^2 l^2 uu_{yy} + \frac{1}{4} U_0 \left[1 - \left(\frac{u}{u_0} \right)^2 \right]^2 + \frac{1}{2} Mc_0^2 D^2 u_y^2$$
$$\left. + m(\chi_1 + \chi_2) lDu^2 u_y + \frac{1}{2} M\Omega^2 D^2 u^2 \right\} \tag{16}$$

Substituting (11) and (12) into (16), we obtain the energy of the soliton pair

$$E = \frac{1}{l} \left\{ \left[\frac{\sqrt{2}}{3}(m + D^2 M)u_0^2 \upsilon^2 + \frac{\sqrt{2}}{3} Mc_0^2 D^2 u_0^2 + \frac{2\sqrt{2}}{3} m\omega_1^2 l^2 u_0^2 \right] S \right.$$
$$+ \left[\sqrt{2} m(\omega_0^2 - \omega_1^2)u_0^2 + \frac{\sqrt{2}}{3} U_0 + \sqrt{2} M\Omega^2 D^2 u_0^2 \right] S^{-1}$$
$$\left. + \frac{2}{3} m(\chi_1 + \chi_2) lD\sigma u_0^3 \right\} \tag{17}$$

The Hamiltonian of the proton sublattice is

$$H_{\mathrm{p}} = \frac{1}{l} \int_{-\infty}^{\infty} \left\{ \frac{1}{2} m\upsilon^2 u_y^2 + \frac{1}{2} m(\omega_0^2 - \omega_1^2)u^2 - \frac{1}{2} m\omega_1^2 luu_y \right.$$
$$\left. - \frac{1}{2} m\omega_1^2 l^2 uu_{yy} + \frac{1}{4} U_0 \left[1 - \left(\frac{u}{u_0} \right)^2 \right]^2 \right\} dy \tag{18}$$

Thus, combining (18) and (15) we obtain the energy of the proton sublattice

$$E_{\mathrm{p}} = \frac{1}{l} \left\{ \left[\frac{\sqrt{2}}{3} mu_0^2 \upsilon^2 + \frac{\sqrt{2}}{3} m\omega_1^2 l^2 u_0^2 \right] S \right.$$
$$\left. + \left[\sqrt{2} m(\omega_0^2 - \omega_1^2)u_0^2 + \frac{\sqrt{2}}{3} U_0 \right] \right\} S^{-1} \tag{19}$$

The Hamiltonian of the heavy ion sublattice is taken to be

$$H_{\mathrm{h}} = \frac{1}{l} \int_{-\infty}^{\infty} \left(\frac{1}{2} MD^2(\upsilon^2 + c_0^2)u_y^2 + \frac{1}{2} M\Omega^2 D^2 u^2 \right) dy \tag{20}$$

Therefore, combining (20) and (15) we obtain the energy of the heavy ion sublattice

$$E_{\mathrm{h}} = \frac{1}{l} \left[\left(\frac{\sqrt{2}}{3} D^2 Mu_0^2 \upsilon^2 + \frac{\sqrt{2}}{3} Mc_0^2 D^2 u_0^2 \right) S + \sqrt{2} M\Omega^2 D^2 u_0^2 S^{-1} \right] \tag{21}$$

Equations (19) and (21) clearly show that the optical mode of the heavy ion sublattice will decrease the energy of the kink soliton in the proton and the antikink soliton in the heavy ion sublattices, respectively.

4.2 Momentum and Effective Mass of the Soliton Pair

From (11), (12) and (15) we determine the momentum of the kink pair due to influence of the optical mode of the heavy ion sublattice [14],

$$\begin{aligned} P &= -\frac{1}{l}\int_{-\infty}^{\infty}(mu_t u_x + M\eta_t\eta_x)dx \\ &= P_{\mathrm{k}} + P_{\mathrm{ak}} = (m^* + M^*)\upsilon = M^*_{\mathrm{sol}}\upsilon \end{aligned} \tag{22}$$

where P_{k} is the momentum of the protonic kink soliton

$$P_{\mathrm{k}} = -\frac{m}{l}\int_{-\infty}^{\infty} u_t u_x dx = m^*\upsilon \tag{23}$$

$$m^* = mI(S) \tag{24}$$

m^* is the effective mass of the kink in the proton sublattice.

P_{ak} is the momentum of the antikink in the heavy ion sublattice,

$$P_{\mathrm{ak}} = -\frac{M}{l}\int_{-\infty}^{\infty} \eta_t\eta_x dx = M^*\upsilon \tag{25}$$

$$M^* = MD^2 I(S) \tag{26}$$

M^* is the effective mass of the antikink soliton in the heavy ion sublattice.

$$M^*_{\mathrm{sol}} = m^* + M^* = (m + MD^2)I(S) \tag{27}$$

M^*_{sol} represents the effective mass of the kink pair, where

$$I(S) = \frac{2\sqrt{2}\alpha}{3lG}S \tag{28}$$

When $\Omega = 0$, $\upsilon \ll \upsilon_1$ and $\upsilon \ll c_0$, we obtain from (27), (28) and (15)

$$M^{0*}_{\mathrm{sol}} = \frac{2\sqrt{2}(m + D_0^2 M)\alpha_0^{3/2}}{3\upsilon_1 G_0 l} \tag{29}$$

This result agrees with that of the harmonic interaction approximation [10].

From (22)–(28), we can see that the optical mode of the heavy ion sublattice will decrease the momentum and the effective mass of the kink soliton in the proton and the antikink soliton in the heavy ion sublattices, respectively.

5 Conclusions

In conclusion, using variational method, we have studied the nonlinear excitations and the motion of the kink pair in the presence of the optical mode of the heavy ion sublattice, based on a new two-component soliton model. We give also the equations of motion and its corresponding soliton-solutions in such a case. Based on these results we calculate further the energy, the momentum and the effective mass of a kink pair. The optical mode of the heavy ion sublattice will increase the width and decrease the energy, the momentum and the effective mass of the kink soliton in the proton and the antikink soliton in the heavy ion sublattices, respectively.

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