International Journal of Theoretical Physics, Vol. 45, No. 2, February 2006 (© 2006)
DOI: 10.1007/s10773-006-9027-1

Motion of Kink in Hydrogen-Bonded Chain with Asymmetric Double-Well Potential

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Received January 31, 2005; accepted January 19, 2006
Published Online: May 23, 2006

We discuss the nonlinear excitations and the motion of kink in hydrogen-bonded chain with asymmetric double-well potential, in presence of an external force and damping using a new two-component soliton model. We obtain the kink soliton solution using the phase-plane method, we study soliton velocity and find the expression of the mobility of the kink soliton.

KEY WORDS: hydrogen bonded chain; two-component model; asymmetric double-well potential; kink.

1. INTRODUCTION

The hydrogen bridge exists in many solid state systems and biological molecular chains. It has two types, namely symmetric, X–H· · ·X, asymmetric, X–H· · ·Y, where –indicates a covalent bond, and · · · indicates a hydrogen bond. For example, the hydrogen bridge in an ice crystal is symmetric, in which proton exists in a symmetric potential with double minima. The conduction mechanism of a soliton have been investigated by a number of author in hydrogen-bonded chain with symmetric double-well potential (Cheng, 2000; Pang and Muller-Kirsten, 2000; Xu, 1992). However, for α-helical proteins and an acctanilide crystal, the hydrogen bridge is asymmetric, in which protons exist in an asymmetric potential with double minima (Xu, 1995). The bell-shape soliton model for proton transport in a hydrogen-bonded chain with an asymmetric double-well potential was suggested by Gordon (1988). The motion of a bell shape soliton pair in a hydrogen-bonded chain with an asymmetric double-well potential has been investigated by Xu and Huang (1995). In this paper, we investigate the nonlinear excitation in a hydrogen-bonded chain with an asymmetric double-well potential, in the presence of an external force and damping, based on the a new two-component soliton model. In Section 2, we present the Hamiltonian of the system and derive the equations of

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motion. In Section 3, we give the kink soliton solution. In Section 4, we investigate soliton velocity and get the expression for the mobility of the kink soliton.

2. MODEL AND THE HAMILTONIAN OF THE SYSTEM

We can consider that the hydrogen-bonded chain is composed of proton sublattice and a heavy ion sublattice. For example, the acctanilide chain $(CH_3CONHC_6H_5)_x$ is composed of a proton sublattice $(H^+)_x$ and heavy ion sublattice $(CH_3CONC_6H_5{}^+)_x$. We take a new two-component model in a hydrogen-bonded chain with asymmetric double-well potential and assume that the coupling between the proton sublattice and the heavy ion sublattice is a linear interaction (Xu and Huang, 1995). The Hamiltonian of the system may be written as a sum of three terms

$$H = H_{\mathrm{p}} + H_{\mathrm{h}} + H_{\mathrm{int}} \tag{1}$$

where

$$H_{\mathrm{p}} = \sum_i \left\{ \frac{1}{2m} P_i^2 + \frac{1}{2} m\omega_0^2 u_i^2 - \frac{1}{2} m\omega_1^2 u_i u_{i+1} + V(u_i) \right\} \tag{2}$$

and

$$V(u_i) = \frac{1}{2} A u_i^2 - \frac{1}{3} B u_i^3 + \frac{1}{4} C u_i^4 \tag{3}$$

$$H_{\mathrm{h}} = \sum_i \left[\frac{1}{2M} p_i^2 + \frac{1}{2} \beta (\rho_i - \rho_{i-1})^2 \right] \tag{4}$$

$$H_{\mathrm{int}} = \sum_i m\chi(\rho_{i+1} - \rho_i)(u_{i+1} - u_i) \tag{5}$$

where H_{p} is the Hamiltonian of the proton sublattice, m the mass of the proton, u_i and $P_i = m\dot{u}_i$ are the proton displacements and momenta respectively, the quantity $\frac{1}{2} m\omega_1^2 u_i u_{i+1}$ shows the correlation interaction between neighbouring protons caused by the dipole–dipole interactions, ω_0 and ω_1 are diagonal and non-diagonal elements of the dynamical matrix of the proton respectively (Cheng, 2002). $V(u_i)$ is an asymmetric potential with double minima. A, B and C are positive (Gordon, 1988). H_{h} is the Hamiltonian of the heavy ionic sublattice with low-frequency harmonic vibration, M the mass of the heavy ion, ρ_i and $p_i = M\dot{\rho}_i$ are the displacement of the heavy ion from its equilibrium position and its conjugate momentum respectively, $c_0 = l(\beta/M)^{1/2}$ is the velocity of sound in the heavy ionic sublattice, and l the lattice constant. H_{int} is the interaction Hamiltonian between the protonic and the heavy ionic sublattices, χ is the coupling constant between the two sublattices (Xu, 1996). In the continuum approximation with the long-wavelength limit (Pang and Muller-Kirsten, 2000), this Hamiltonian can be replaced by a continuum representation

$$H = \int_{-\infty}^{\infty} \frac{dx}{l} \left\{ \left[\frac{1}{2} m u_t^2 + \frac{1}{2} m \omega_0^2 u^2 - \frac{1}{2} m \omega_1^2 u \left(u + l u_x + \frac{1}{2} l^2 u_{xx} \right) + \left(\frac{1}{2} A u^2 - \frac{1}{3} B u^3 + \frac{1}{4} C u^4 \right) + \left(\frac{1}{2} M \rho_t^2 + \frac{1}{2} \beta l^2 \rho_x^2 \right) + m \chi l^2 \rho_x u_x \right] \right\} \tag{6}$$

The Euler–Lagrange equations of motion corresponding to Eq. (6) are

$$m\left(u_{tt} - \upsilon_1^2 u_{xx}\right) - m\chi l^2 \rho_{xx} + \alpha u - B u^2 + C u^3 = 0 \tag{7}$$

$$M\left(\rho_{tt} - c_0^2 \rho_{xx}\right) - m\chi l^2 u_{xx} = 0 \tag{8}$$

where

$$\alpha = A + m\left(\omega_0^2 - \omega_1^2\right), \; \upsilon_1^2 = \frac{1}{4} l^2 \omega_1^2 \tag{9}$$

υ_1 is the characteristic velocity of the proton.

3. THE EQUATIONS OF MOTION AND THEIR SOLITON SOLUTION

In the presence of external force and damping, because of the fact that respond of the heavy ions to the force and damping are very much less than for the protons, the force and damping terms are only introduced in the equation of motion for the protons (Peyrard *et al.*, 1987). The equations of motion (7) and (8) are replaced by the following equations

$$m\left(u_{tt} - \upsilon_1^2 u_{xx}\right) - m\chi l^2 \rho_{xx} + m\Gamma u_t + \frac{dV'(u)}{du} = 0 \tag{10}$$

$$M\left(\rho_{tt} - c_0^2 \rho_{xx}\right) - m\chi l^2 u_{xx} = 0 \tag{11}$$

where Γ is the damping coefficient for the proton. In the external electric field E each proton has an additional potential energy $-eEu$:

$$V'(u) = \frac{1}{2}\alpha u^2 - \frac{1}{3} B u^3 + \frac{1}{4} C u^4 - eEu \tag{12}$$

here e is the protonic charge.

Using the variable transformation $\xi = x - \upsilon t, \; u = u(\xi), \; \rho = bu(\xi)$, Eqs. (10) and (11) become

$$\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right] u_{\xi\xi} + m\Gamma \upsilon u_\xi - \frac{dV'(u)}{du} = 0 \tag{13}$$

$$b = -\frac{m\chi l^2}{M\left(c_0^2 - \upsilon^2\right)} \tag{14}$$

Using the phase-plane method (Gordon, 1987), we shall obtain soliton solution. For this reason, we introduce the following notation

$$\frac{du}{d\xi} = y \tag{15}$$

Equation (13) can be written as

$$\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right] y_\xi + m\Gamma\upsilon y - C(u - u_1)(u - u_2)(u - u_3) = 0 \tag{16}$$

where

$$u_1 = \frac{B}{3C}\left(1 - 2\sqrt{1 - \frac{3\alpha C}{B^2}}\cos\frac{\theta}{3}\right) \tag{17}$$

$$u_2 = \frac{B}{3C}\left(1 + 2\sqrt{1 - \frac{3\alpha C}{B^2}}\cos\frac{\pi - \theta}{3}\right) \tag{18}$$

$$u_3 = \frac{B}{3C}\left(1 + 2\sqrt{1 - \frac{3\alpha C}{B^2}}\cos\frac{\pi + \theta}{3}\right) \tag{19}$$

$$\theta = \arccos\left[\frac{(1 - 9\alpha C/2B^2 + 27C^2 eE/2B^3)}{(1 - 3\alpha C/B^2)^{3/2}}\right] \tag{20}$$

here u_1, u_2 and u_3 are the roots of the equation $dV'(u)/du = 0 u_1$, u_2 correspond to minima of the potential $V'(u)$, u_3 corresponds to the top of potential barrier of the double-minimum potential.

Therefore, soliton solution which we seek corresponds to a trajectory in the (u, y) phase plane of the system of Eqs. (15) and (16). From (15) and (16) we obtain a differential equation for solution trajectory as

$$\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right] y\frac{dy}{du} + m\Gamma\upsilon y - C(u - u_1)(u - u_2)(u - u_3) = 0 \tag{21}$$

Equation (21) can be satisfied by a trajectory of the form

$$y = D(u - u_1)(u - u_2) \tag{22}$$

The substituting Eq. (22) into (21), we have

$$D = \frac{\sqrt{C}}{\sqrt{2\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right]}} \tag{23}$$

Inserting Eq. (22) into (15) and integrating (15), we obtain kink soliton solution

$$u = \frac{u_1 + u_2}{2} - \frac{u_1 - u_2}{2}\tanh\frac{\xi}{2W_k} \tag{24}$$

where W_k is the width of the soliton

$$W_k = \frac{\sqrt{2\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right]}}{\sqrt{C}(u_1 - u_2)} \tag{25}$$

Solution (24) is a topological excitation being a kink soliton. Because the charge density depends directly on $\delta_e = -\partial u/\partial x$ (Xu and Huang, 1995). Equation (24) show that the motion of this kink describes the propagation of the charge along the hydrogen-bonded chain and realize the mobility of the kink soliton.

4. VELOCITY AND MOBILITY

The substitution of (22) into (21) gives kink soliton velocity along hydrogen-bonded chain

$$\upsilon = \frac{B\sqrt{2\left[m\left(\upsilon_1^2 - \upsilon^2\right) + m\chi l^2 b\right]}}{m\Gamma\sqrt{C}}\sqrt{1 - \frac{3\alpha C}{B^2}}\cos\frac{\pi + \theta}{3} \tag{26}$$

From (26) we obtain soliton velocity

$$\upsilon = \frac{\left[1 + m\chi l^2 b/m\upsilon_1^2\right]^{1/2}\upsilon_1}{\left[1 + m\Gamma^2 C/2B^2(1 - 3\alpha C/B^2)\cos^2\frac{\pi+\theta}{3}\right]^{1/2}} \tag{27}$$

In case the weak coupling and $\upsilon \ll c_0$, we have coupling factor $m\chi l^2 b/m\upsilon_1^2 \ll 1$, Eq. (27) is written as

$$\upsilon = \upsilon_1\left[1 + \frac{m\Gamma^2 C}{2B^2(1 - 3\alpha C/B^2)\cos^2\frac{\pi+\theta}{3}}\right]^{-1/2} \tag{28}$$

Using the expansion

$$\upsilon = \upsilon|_{E=0} + \left.\frac{d\upsilon}{dE}\right|_{E=0} E = \upsilon|_{E=0} + \mu E \tag{29}$$

and when $E = 0$, we get

$$u_1 = \frac{B}{2C}\left(1 + \sqrt{1 - \frac{4\alpha C}{B^2}}\right) \tag{30}$$

$$u_2 = \frac{B}{2C}\left(1 - \sqrt{1 - \frac{4\alpha C}{B^2}}\right) \tag{31}$$

$$u_3 = 0 \tag{32}$$

$$\cos\left.\frac{\pi + \theta}{3}\right|_{E=0} = -\frac{1}{2\sqrt{1 - \frac{3\alpha C}{B^2}}} \tag{33}$$

From Eqs. (20), (28), (29) and (33) we get

$$v|_{E=0} = v_1 \left[1 + \frac{2m\Gamma^2 C}{B^2}\right]^{-1/2} \tag{34}$$

and the mobility of the kink soliton

$$\mu = \frac{-6mC^2 V_1 e\Gamma^2}{\alpha(B^2 + 2C\Gamma^2 m)^{3/2}} \tag{35}$$

Considering a symmetric double-well potential (Gordon, 1987)

$$V(u) = -\frac{1}{2}Au^2 + \frac{1}{4}Bu^4 \tag{36}$$

comparing Eqs. (36) and (12) and using $\alpha \to -A,\ B = 0,\ E = 0,\ C \to B$, Eq. (35) becomes

$$\mu = \frac{3V_1 e}{A\Gamma}\left(\frac{B}{2m}\right)^{1/2} \tag{37}$$

Equation (36) is the mobility of kink soliton with symmetric double-well potential in hydrogen-bonded chain. This result agrees with that given by Gordon (1987).

5. CONCLUSIONS

In conclusion, we have studied the nonlinear excitations and the motion of a kink soliton in hydrogen-bonded chains with an asymmetric double-well potential, in presence of an external force and damping using a new two-component soliton model. Solution (24) is a topological excitation being a kink soliton. It describes the propagation of the charge along the hydrogen-bonded chains. We also investigate soliton velocity and obtain the expression for the mobility of the kink soliton.

ACKNOWLEDGMENT

The author is grateful to professor J.Z. Xu for helpful discussions.

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