International Journal of Theoretical Physics, Vol. 42, No. 4, April 2003 (© 2003)

Nonlinear Excitations in Hydrogen-Bonded Chains with Anharmonic Interatomic Interactions

Yuan-Fa Cheng[1]

Received September 1, 2002

We discuss the nonlinear excitations and the motion of a kink soliton pair in hydrogen-bonded chains with anharmonic interatomic interactions, based on a two-component soliton model, using a direct perturbation method. The expression for the asymmetric solutions of the kink soliton pair is found because of anharmonicity, and the energy, the momentum and the effective mass of a kink pair for cubic and quartic anharmonicity are calculated, which are in good agreement with the experimental data.

KEY WORDS: nonlinear excitations; hydrogen-bonded chains.

1. INTRODUCTION

It is well known that hydrogen-bonded chains consisting of hydrogen bonds occur in many solid state systems and living systems, such as, for example, solid alcohol, carbon hydrates, proteins, and ice. In the case of studies of proton transfer processes in hydrogen-bonded systems, for example, in ice, water, or proteins, the one-component soliton model for proton transport in hydrogen-bonded molecular chains has been investigated by a number of authors (Kashimori *et al.*, 1982; Xu, 1990). In the normal state of a chain each proton is linked to a heavy ion (or oxygen atom in ice) by a covalent bond in one case, or a hydrogen bond in the other. Therefore, there are two kinds of arrangements of hydrogen-bonded states in these systems, namely the type $X{-}H \cdots X{-}H \cdots X{-}H \cdots X{-}H$ and the type $H{-}X \cdots H{-}X \cdots H{-}X \cdots H{-}X$, where — indicates a covalent bond, and $\cdots$ represents a hydrogen bond. Obviously the two states should have the same energy. In such a case it is accepted that the potential energy of the proton should have the form of a double well with two minima corresponding to the two equilibrium positions of a proton between two neighboring heavy ions (or oxygen atoms). In the usual case, the protons in the hydrogen bonds are subject to harmonic vibration about their equilibrium positions.

[1]Department of Physics, Hubei University, Wuhan 430062, Hubei, China.

0020-7748/03/0400-0747/0

Considering the influence of the motion of the heavy-ion sublattice on the proton sublattice, the two-component soliton model was suggested by Xu (1992) and Xu Huang (1995). This model considers that the nonlinear excitations in the proton and the heavy-ion sublattices are all kinks, kink pairs have symmetric solutions in the harmonic interatomic interactions approximation (Xu, 1992). However it does not explain the asymmetry observed experimentally between the structures of L and D defects (Pnevmatikos *et al.*, 1989) and the differences observed experimentally between the mobilities of OH^- and H_3O^+ defects (Nagle and Nogle, 1983), which correspond to kink and antikink solitons in this model.

Because the heavy ion sublattice is not an ideal simplex atomic lattice. The heavy ion has an internal vibration, as for example the amide-I vibration in the peptide group of α-helical protein (Xu, 2000; Xu and Zhou, 1996) and the vibration of the oxygen ion in ice. In the present paper, taking into account the anharmonic interatomic interactions of the two sublattices, on the basis of the two-component soliton model, we discuss the nonlinear excitations due to anharmonicity and can account for the asymmetry feature in hydrogen-bonded chains. The energy, the momentum, and the effective mass of a kink pair due to anharmontcity are found, which agree with the experimental data (Nagle and Nagle, 1983; Pnevmatikos *et al.*, 1989).

2. KINK SOLITON PAIR

In the continuum model for the two-component soliton of the hydrogen-bonded molecular chain, the Hamiltonian of the system is (Xu, 1992).

$$H = \frac{1}{l}\int\left[\frac{1}{2}m\left(u_t^2 + c_0^2u_x^2\right) + \frac{1}{2}M\left(w_t^2 + \upsilon_0^2w_x^2\right) + V(u) - kw_x\left(u^2 - u_0^2\right)\right]dx \tag{1}$$

Here, l is the lattices spacing. $u(x,t)$ and $w(x,t)$ are the displacement fields of the proton (mass m) and the heavy ion (mass M); respectively. c_0 and υ_0 are the characteristic velocities of the proton and the heavy-ion sublattices, respectively. k is the coupling constant between the two sublattices.

$$V(u) = \in_0\left(1 - \frac{u^2}{u_0^2}\right)^2 \tag{2}$$

is the proton potential energy in each hydrogen bond $\in_0$ is the barrier height, u_0 is the distance between the central maximum and one of the minima of the double well. The Euler–Lagrange equations of motion corresponding to Eq. (1) are as follows.

$$u_{tt} - c_0^2u_{xx} - \frac{2k}{m}uw_x + V'(u) = 0 \tag{3}$$

$$w_{tt} - \upsilon_0^2 w_{xx} - \frac{2k}{M} u u_x = 0 \tag{4}$$

Considering anharmonic interatomic interactions in the two sublattices, generally, $U(u_x)$ and $P(w_x)$, which are the interaction potentials in the proton and the heavy-ion sublattices, respectively, may be written as (Davydov, 1991).

$$U(u_x) = \frac{1}{2} m c_0^2 u_x^2 - \lambda_1 g(u_x) \tag{5}$$

$$U(w_x) = \frac{1}{2} M \upsilon_0^2 w_x^2 + \lambda_2 \rho(w_x) \tag{6}$$

Where λ_1 and λ_2 represent a small constant parameter, and $U(u_x)$ and $P(w_x)$ account for anharmonic interatomic interactions in the proton and in the heavy-ion sublattices, respectively. Replacing the model parameters in Eq. (1) by the corresponding parameters in Eqs. (5) and (6), we get the Hamiltonian of the anharmonicity,

$$H = \frac{1}{l} \int \left[\frac{1}{2} m u_t^2 + U(u_x) + V(u) \frac{1}{2} M w_t^2 + P(w_x) - k w_x \left(u^2 - u_0^2\right) \right] dx \tag{7}$$

The equations of motion corresponding to the Hamiltonian (7) are

$$m u_{tt} - U^{tt}(u_x) u_{xx} - \frac{2k}{M \upsilon_0^2} u P'(w_x) + V'(u) = 0 \tag{8}$$

$$M w_{tt} - P''(w_x) w_{xx} - \frac{2k}{M c_0^2} u U'(u_x) = 0 \tag{9}$$

When $\lambda_1 = 0$ and $\lambda_2 = 0$, Eqs. (8) and (9) reduce to Eqs. (3) and (4), respectively, that is, in the harmonic interatomic interactions approximation, the symmetric solutions of kink pair in the following form (Xu, 1992).

$$u = \sigma u_0 \tanh \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] \tag{10}$$

$$w = D u \tag{11}$$

Here, $\sigma = \pm 1$ is the polarity of soliton, and

$$\alpha = \frac{1}{m\left(c_0^2 - \upsilon^2\right)} \left[\frac{4 \in_0}{u_0^2} - \frac{2k^2 u_0^2}{M\left(\upsilon_0^2 - \upsilon^2\right)} \right] \tag{12}$$

$$D = -\frac{\sqrt{2} k \alpha^{-1/2} u_0}{M\left(\upsilon_0^2 - \upsilon^2\right)} \tag{13}$$

Equation (10), (11), and (13) show that, in the case $\upsilon < \upsilon_0$ 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 alone the hydrogen-bonded chains in pairs with the same velocity.

3. THE ASYMMETRIC SOLUTIONS OF THE KINK PAIK

When the perturbation is included ($\lambda_1 \neq 0$, $\lambda_2 \neq 0$), it is usually impossible to obtain on exact analytical solutions of Eqs. (8) and (9), we use a direct perturbation method, and assume that the solutions of Eqs. (8) and (9) have the following form (Braun and Vazquez, 1991).

$$u(\xi) = u_0(\xi) + \lambda\varphi(\xi) \tag{14}$$

$$w(\xi) = D\,u(\xi) \tag{15}$$

where $\xi = x - \upsilon t$, $u_0(\xi)$ is the kink of the unperturbed system ($\lambda = 0$) in the proton sublattice. Using $u_{tt} = \upsilon^2 u_{\xi\xi}$, $u_{xx} = u_{\xi\xi}$, $U(u_\xi) = \frac{1}{2} m c_0^2 u_\xi^2 + \lambda_1 g(u_\xi)$, $P(w_\xi) = \frac{1}{2} M \upsilon_\xi^2 c_\xi^2 + \lambda_2 \rho(w_\xi)$, and substituting Eqs. (14) and (15) into Eq. (8), we obtain

$$-mc_0^2\gamma^{-2}u_{\xi\xi} - \lambda_1 g''(u_\xi)u_{\xi\xi} - \frac{2k}{M\upsilon_0^2}uP'(w_\xi) + V'(u) = 0 \tag{16}$$

Multiplying Eq. (16) by u_ξ and integrating over $(-\infty, \xi)$, we have

$$\int_{-\infty}^{\xi} -mc_0^2\gamma^{-2}u_{\xi\xi}\cdot u_\xi\,d\xi - \int_{-\infty}^{\xi} \lambda_1 g''(u_\xi)u_{\xi\xi}\cdot u_\xi\,d\xi$$
$$-\int_{-\infty}^{\xi} \frac{2k}{M\upsilon_0^2}uP'(w_\xi)\cdot u_\xi\,d\xi + \int_{-\infty}^{\xi}\frac{dV(u)}{du}u_\xi\,d\xi = 0 \tag{17}$$

we let

$$s = \int_{-\infty}^{\xi} g''(u_\xi)u_{\xi\xi}\cdot u_\xi\,d\xi = u_\xi g'(u_\xi) - g(u_\xi) \tag{18}$$

$$\delta = \int_{-\infty}^{\xi} \frac{2k}{M\upsilon_0^2}uP'(w_\xi)u_\xi\,d\xi = \frac{k}{M\upsilon_0^2}u^2P'(w_\xi) \tag{19}$$

and we have

$$\int_{-\infty}^{\xi} -mc_0^2\gamma^{-2}u_{\xi\xi}\cdot u_\xi\,d\xi = -\frac{1}{2}mc_0^2\gamma^{-2}u_\xi^2 \tag{20}$$

$$\int_{-\infty}^{\xi}\frac{dV(u)}{du}u_\xi\,d\xi = V(u) \tag{21}$$

Inserting Eqs. (18)—(21) into (17), we obtain

$$-\frac{1}{2}mc_0^2\gamma^{-2}u_\xi^2 - mc_0^2\lambda(s+\delta^*) + V(u) = 0 \tag{22}$$

here

$$\delta^* = \delta/\left(mc_0^2\lambda\right), \quad \lambda = \lambda_1/\left(mc_0^2\right), \quad \gamma = \left(1 - \frac{\upsilon^2}{c_0^2}\right)^{-1/2},$$

Substituting Eq. (14) into Eq. (22), and using the expansion

$$V(u_0 + \lambda\varphi) \approx V(u_0) + \lambda V'(u_0)\varphi \tag{23}$$

and

$$V(u_0) = \frac{1}{2}mc_0^2\gamma^{-2}u_0'^2 \tag{24}$$

we come to the following first-order equation

$$\gamma^{-2}u_0'\varphi' - \gamma^{-2}u_0''\varphi = -(s + \delta') \tag{25}$$

From Eq. (25) we get

$$\varphi(\xi) = u_0' \int \frac{-(s + \delta')\gamma^2}{u_0'^2}\, d\xi \tag{26}$$

The result (26) describes a correction to the kink shape due to the anharmonic interatomic interactions, considering the cubic and quartic anharmonicity in the proton and in the heavy-ion sublattices, respectively,

$$\lambda_1 g(u_x) = \frac{1}{6}k_1u_x^3 + \frac{1}{12}k_2u_x^4 = \frac{1}{6}k_1u_\xi^3 + \frac{1}{6}k_1u_\xi^4 \tag{27}$$

$$\lambda_2 \rho(w_x) = \frac{1}{6}k_3w_x^3 + \frac{1}{12}k_4w_x^4 = \frac{1}{6}k_3w_\xi^3 + \frac{1}{6}k_4w_\xi^4 \tag{28}$$

where $k_1 - k_4$ are the anharmony parameters, we have

$$\lambda s = \frac{\lambda_1 s}{mc_0^2} = \frac{\lambda_1}{mc_0^2}[u_\xi g'(u_\xi) - g(u_\xi)] = \frac{1}{mc_0^2}\left(\frac{1}{3}k_1u_\xi^3 + \frac{1}{4}k_2u_\xi^4\right)$$

$$\lambda\varphi(\xi) = \lambda u_0' \int \frac{-(s + \delta^*)\gamma^2}{u_0'^2}\, d\xi = u_0' \int \frac{-\lambda s\gamma^2}{u_0'^2}\, d\xi + u_0' \int \frac{-\lambda\delta^*\gamma^2}{u_0'^2}\, d\xi$$

where

$$\begin{aligned} u_0' \int \frac{-\lambda s\gamma^2}{u_0'^2} d\xi &= \frac{-\gamma^2 u_0'}{mc_0^2} \int \frac{1}{u_0'^2}\left(\frac{1}{3}k_1u_\xi^3 + \frac{1}{4}k_2u_\xi'^4\right) d\xi \\ &\approx \frac{-\gamma^2 u_0'}{mc_0^2} \int \frac{1}{u_0'^2}\left(\frac{1}{3}k_1u_0'^3 + \frac{1}{4}k_2u_2'^4\right) d\xi \\ &= \frac{-\gamma^2 u_0'}{mc_0^2} \int \left(\frac{1}{3}k_1u_0' + \frac{1}{4}k_2u_0'\right) d\xi \end{aligned}$$

$$\int u_0' \, d\xi = \int \sqrt{\frac{\alpha}{2}} \sigma u_0 \, \mathrm{sech}^2 \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] d\xi = 2\sigma u_0$$

$$\int u_0'^2 \, d\xi = \int \frac{\alpha}{2} \sigma^2 u_0^2 \, \mathrm{sech}^4 \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] d\xi = \frac{2\sqrt{2}}{3} \alpha^{1/2} u_0^2$$

we further get

$$u_0' \int \frac{-\lambda s \gamma^2}{u_0'^2} \, d\xi = \frac{-\gamma^2 u_0'}{m c_0^2} \left(\frac{2}{3} k_1 \sigma u_0 + \frac{\sqrt{2}}{6} k_2 \, \alpha^{1/2} u_0^2 \right)$$

$$= -\gamma^2 u_0' \left(\frac{2}{3} k_1' \sigma u_0 + \frac{\sqrt{2}}{6} k_2' \, \alpha^{1/2} u_0^2 \right)$$

where $k_1' = \frac{k_1}{m c_0^2}$ and $k_2' = \frac{k_2}{m c_0^2}$, and using the same way

we have

$$u_0' \int \frac{-\lambda \delta^* \gamma^2}{u_0'^2} \, d\xi = -\gamma^2 u_0' \left(-4\sqrt{2} k_3' \alpha^{-1/2} D^3 u_0^2 + \frac{2}{9} k_4' \sigma D^4 u_0^3 \right)$$

hence

$$\lambda \varphi(\xi) = -\gamma^2 u_0' \left(\frac{2}{3} k_1' \sigma u_0 + \frac{\sqrt{2}}{6} k_2' \alpha^{1/2} u_0^2 - 4\sqrt{2} k_3' \alpha^{1/2} D^3 u_0^2 + \frac{2}{9} k_4' \sigma D^4 u_0^3 \right)$$

$$= - \left(\frac{\sqrt{2}}{3} k_1' \alpha^{1/2} \gamma^2 u_0^2 + \frac{1}{6} k_2' \alpha^{3/2} \sigma \gamma^2 u_0^3 - 4 k_3' \sigma \gamma^2 D^3 u_0^3 \right.$$

$$\left. + \frac{\sqrt{2}}{9} k_4' \alpha^{1/2} \gamma^2 D^4 u_0^4 \right) \cdot \mathrm{sech}^2 \left[\sqrt{\frac{\alpha}{2}} (x - v t) \right] \quad (29)$$

we obtain from Eqs. (14), (15) and (29) the asymmetric solutions of the kink pair for cubic and quartic anharmonicity,

$$u(\xi) = \sigma u_0 \tanh \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] - \left(\frac{\sqrt{2}}{3} k_1' \alpha^{1/2} \gamma^2 u_0^2 + \frac{1}{6} k_2' \alpha^{3/2} \sigma \gamma^2 u_0^3 \right.$$

$$\left. -4 k_3' \sigma \gamma^2 D^3 u_0^3 + \frac{\sqrt{2}}{9} k_4' \alpha^{1/2} \gamma^2 D^4 u_0^4 \right) \cdot \ \mathrm{sech}^2 \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] \quad (30)$$

$$w(\xi) = D u(\xi) \quad (31)$$

Obviously, when $k_1' - k_4'$ are equal to zero, Eqs. (30) and (31) reduce to the symmetric solution of a kink pair of the unperturbed system. Because Eqs. (30) and

(31) include σ factor, the symmetric shape of the kink pair are broken because of the anharmonicity, the asymmetric solutions of the kink pair are obtained.

4. ELEMENTARY PROPERTIES OF THE KINK PAIK

In this section we investigate the elementary properties of the above kink soliton pair, but here we consider only some important physical quantities of the kink pair due to anharmonic interatomic interactions of the two sublattices.

4.1. Energy of the Kink Pair

Considering the cubic and quartic anharmonicity in the proton and in the heary-ion sublattices, respectively, the Hamiltonian (7) is rewritten as

$$H = \frac{1}{l}\int\Big[\frac{1}{2}m\big(u_t^2 + c_0^2 u_x^2\big) + \lambda_1 g(u_x) + \frac{1}{2}M\big(w_t^2 + \upsilon_0^2 w_x^2\big) + \lambda_2\rho(w_x) + V(u) - kw_x\big(u^2 - u_0^2\big)\Big]\,dx \tag{32}$$

Inserting $u_x = u_\xi,\ u_t = u_\xi(-\upsilon),\ w_x = w_\xi = Du_\xi,\ w_t = w_\xi(-\upsilon) = Du_\xi(-\upsilon)$ into (32), expression of the energy corresponding to (32) becomes

$$\begin{aligned} E &= \frac{1}{l}\int\Bigg[\frac{1}{2}m\big(\upsilon^2 + c_0^2\big)u_\xi^2 + \lambda_1 g(u_\xi) + \frac{1}{2}MD^2\big(\upsilon^2 + \upsilon_0^2\big)u_\xi^2 + \lambda_2\rho(w_\xi) \\ &\quad + V(u) - kD\big(u^2 - u_0^2\big)u_\xi\Bigg]d\xi \\ &\approx \frac{1}{l}\int\Bigg[\frac{1}{2}m\big(\upsilon^2 + c_0^2\big)u_0'^2 + \frac{1}{6}k_1 u_0'^3 + \frac{1}{12}k_2 u_0'^4 + \frac{1}{2}MD^2\big(\upsilon^2 + \upsilon_0^2\big)u_0'^2 \\ &\quad + \frac{1}{6}k_3 D^3 u_0'^3 + \frac{1}{12}k_4 D^4 u_0'^4 + V(u) - kD\big(u^2 - u_0^2\big)u_0'\Bigg]d\xi \end{aligned} \tag{33}$$

where

$$\int u_0'^3\,d\xi = \int\left(\frac{\alpha}{2}\right)^{3/2}\sigma u_0^3\,\mathrm{sech}^6\left[\sqrt{\frac{\alpha}{2}}(x - \upsilon t)\right]d\xi = \frac{8}{15}\sigma\alpha u_0^3 \tag{34}$$

$$\int u_0'^4\,d\xi = \int\left(\frac{\alpha}{2}\right)^{2}\sigma^4 u_0^4\,\mathrm{sech}^8\left[\sqrt{\frac{\alpha}{2}}(x - \upsilon t)\right]d\xi = \frac{8\sqrt{2}}{35}\alpha^{3/2}u_0^4 \tag{35}$$

$$\int V(u)\,d\xi = \int \epsilon_0\left(1 - \frac{u^2}{u_0^2}\right)^2 d\xi = \frac{4\sqrt{2}}{3}\,\epsilon_0\,\alpha^{-1/2} \tag{36}$$

$$\int u^2 u_0' \, d\xi = \int \sigma^2 u_0^2 \tanh^2 \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] \times \sqrt{\frac{\alpha}{2}} \sigma u_0 \, \mathrm{sech}^2 \left[\sqrt{\frac{\alpha}{2}} (x - \upsilon t) \right] d\xi = \frac{2}{3} \sigma u_0^3 \tag{37}$$

Substituting Eqs. (34)–(37) into Eq. (33), thus the energy of the kink soliton pair due to anharmonicity is

$$E = \frac{1}{l} \left[\frac{\sqrt{2}}{3} m \left(\upsilon^2 + c_0^2 \right) \alpha^{1/2} u_0^2 + \frac{\sqrt{2}}{3} M D^2 \left(v^2 + \upsilon_0^2 \right) \alpha^{1/2} u_0^2 + \frac{4}{45} (k_1 + k_3 D^3) \sigma \alpha u_0^3 + \frac{2\sqrt{2}}{105} (k_2 + k_4 D^4) \alpha^{3/2} u_2^4 + \frac{4\sqrt{2}}{3} \in \alpha^{-1/2} + \frac{4}{3} k D \sigma u_0^4 \right] \tag{38}$$

Because Eq. (38) contains the polarity factor σ of the soliton, we can see that the anharmonic interatomic interactions will increase the energy in the kink soliton and decrease the energy in the antikink soliton.

4.2. The Momentum and the Effective Mass of the Kink Pair

One can obtain the momentum P of the soliton pair due to anharmonicity (Cheng, 2000, 2001)

$$P = -\frac{1}{l} \int (m u_t u_x + M w_t w_x) \, dx = P_{\mathrm{k}} + P_{\mathrm{ak}} = (m^* + M^*) \upsilon = M_{\mathrm{sol}}^* \upsilon \tag{39}$$

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

$$P_k = -\frac{m}{l} \int u_t u_x \, dx = m^* \upsilon \tag{40}$$

$$m^* = \frac{m}{l} \int u_3^2 \, d\xi |_{\gamma=1} = \frac{m}{l} \left[\int u_0'^2 \, d\xi - \lambda \int (s + \delta^*) \, d\xi \right] = \frac{2\sqrt{2} m}{3l} u_0^2 \alpha^{1/2} - \frac{8m}{45l} \sigma k_1 u_0^3 \alpha - \frac{2\sqrt{2} m}{35l} k_2 u_0^4 \alpha^{3/2} - \frac{\sqrt{2} m}{15l} k_3' D^3 u_0^4 \alpha^{1/2} - \frac{8m}{315l} \sigma k_4' D^4 u_0^5 \alpha \tag{41}$$

m^* is the effective mass of the kink in the proton sublattice due to anharmonicity. $P_{\alpha\mathrm{k}}$ is the momentum of the antikink in the heary-ion sublattice,

$$P_{\alpha\mathrm{k}} = -\frac{M}{l}\int w_t w_x\, dx = M^* \upsilon \tag{42}$$

$$\begin{aligned} M^* &= \frac{D^2 M}{l}\int u_3^2\, d\xi\,|_{\gamma=1} \\ &= \frac{D^2 M}{l}\left[\int u_0'^2\, d\xi - \lambda\int (s+\delta^*)\, d\xi\right] \\ &= \frac{2\sqrt{2}D^2 M}{3l}u_0^2\alpha^{1/2} - \frac{8D^2 M}{45l}\sigma k_1 u_0^3\alpha - \frac{2\sqrt{2}D^2 M}{35l}k_2 u_0^4\alpha^{3/2} \\ &\quad -\frac{\sqrt{2}D^2 M}{15l}k_3' D^3 u_0^4\alpha^{1/2} - \frac{8D^2 M}{315l}\sigma k_4' D^4 u_0^5\alpha \end{aligned} \tag{43}$$

M^* is the effective mass of the antikink soliton in the heavy-ion sublattice due to anharmonicity.

$$\begin{aligned} M_{\mathrm{sol}}^* &= m^* + M^* \\ &= \frac{2\sqrt{2}}{3l}(m + D^2 M)u_0^2\alpha^{1/2} - \frac{8}{45l}(m + D^2 M)\sigma k_1 u_0^3\alpha \\ &\quad -\frac{2\sqrt{2}}{35l}(m + D^2 M)k_2 u_2^4\alpha^{3/2} - \frac{\sqrt{2}}{15l}(m + D^2 M)k_3' D^3 u_0^4\alpha^{1/2} \\ &\quad -\frac{8}{315l}(m + D^2 M)\sigma k_4' D^4 u_0^5\alpha \end{aligned} \tag{44}$$

M_{sol}^* is the effective mass of the kink soliton pair due to anharmonicity.

When k_1, k_2, k_3, and k_4 are equal to zero, Eqs. (41), (43), and (44) become.

$$m^* = \frac{2\sqrt{2}m}{3l}u_0^2\alpha^{1/2} \tag{45}$$

$$M^* = \frac{2\sqrt{2}D^2 M}{3l}u_0^2\alpha^{1/2} \tag{46}$$

$$M_{\mathrm{sol}}^* = \frac{2\sqrt{2}}{3l}(m + D^2 M)u_0^2\alpha^{1/2} \tag{47}$$

Equation (45), (46), and (47) are the effective masses of the kink soliton in the proton, and the antikink soliton in the heavy-ion sublattices and the kink soliton pair of the unperturbed system, respectively, this result agrees with that of the harmonic interaction approximation (Xu, 1992).

From the above Eqs. (39)–(44), we can see that the anharmonic interatomic interactions 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, it can also be shown that anharmonicity will increase the momentum and the effective mass of the antikink soliton in the proton and the kink soliton in the heavy-ion sublattices, respectively.

5. CONCLUSIONS

In summary, we have studied the nonlinear excitations and the motion of a kink soliton pair in hydrogen-bonded chains with anharmonic interatomic interactions based on the two-component soliton model, using a direct perturbation method. The asymmetric solutions of the kink soliton pair are obtained because of anharmonicity, and the energy, the momentum and the effective mass of a kink pair for cubic and quartic anharmonicity are calculated. Because the influence of the anharmonic interatomic interactions in the different sublattices, the symmetries of the shape, the energy, the momentum, and the effective masses of the kink–antikink soliton are broken, which are in agreement with the experimental observations.

ACKNOWLEDGMENT

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

REFERENCES

Kashimori, Y., Kikuchi, T., and Nihimoto, K. (1982). *Journal of Chemical Physics* **77**, 1904.
Xu, J. Z. (1990). *Solid State Communications* **76**, 557.
Xu, J. Z. (1992). *Physics Letters A* **172**, 148.
Xu, J. Z. and Huang, J. N. (1995). *Physics Letters A* **197**, 127.
Pnevmatikos St. Tsironis, G. P. and Zolotaryuk, A. V. (1989). *J Mol. Liq.* **41**, 85.
Naqle, J. F. and Naqle, S. T. (1983). *Journal of Membrane Biology* **74**, 1.
Xu, J. Z. and Zhou, B. (1996). *Physics Letters A* **210**, 307.
Xu, J. Z. (2000). Chaos. *Solitons and Fractals*. **11**, 779.
Davydov, A. S. (1991). *Soliton in Molecular Systems, Vol. 95,* 2nd ed., Kluwer Academic, Dordrecht.
Braun, O. M. and Vazquez, L. (1991). *Physics Letters A* **157**, 241.
Cheng, Y. F. (2000). *Acta Physica Sinica.* **49**, 1.
Cheng, Y. F. (2001). *International Journal of Theoretical Physics* **40**, 1173.