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Motion of a soliton pair in an inhomogeneous hydrogen-bonded chain

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Abstract. In a hydrogen-bonded chain with a symmetric double-well potential, there are slow-mode kink–antikink pairs and fast-mode kink–kink pairs. However, in a hydrogen-bonded chain with an asymmetric double-well potential, there are slow-mode bell-shaped soliton–antisoliton pairs corresponding to two parallel electric dipoles and fast-mode bell-shaped soliton–soliton pairs corresponding to two antiparallel electric dipoles. Propagating in a spatial inhomogeneous chain, soliton pairs may transform from slow-mode soliton–antisoliton pairs into fast-mode soliton–soliton pairs or the converse process. For bell-shaped soliton pairs, this transformation is accompanied by a reversion of the electric dipoles in one of the two sublattices. In the case of repulsion-type impurities, there is a critical velocity v_{cr} for the incident soliton pair. If the velocity v of the incident soliton pair equals v_{cr}, its trajectory of motion in phase space will branch while, for $v < v_{cr}$, forbidden regions and allowed regions for its motion will exist.

1. Introduction

The hydrogen bridge exists in many biological molecular chains and solid state systems. It has two types, namely symmetric type X–H···X and asymmetric type X–H···Y, where the —— indicates a covalent bond, and ······ indicates a hydrogen bond. For example, the hydrogen bridge in an ice lattice is symmetric, in which protons exist in a symmetric potential with double minima. However, for α-helical proteins, the hydrogen bridge is asymmetric, in which protons exist in an asymmetric potential with double minima [1]. The symmetric or asymmetric potential with double minima may be written in the following general form:

$$U(u) = \tfrac{1}{2}Au^2 \pm \tfrac{1}{3}Bu^3 + \tfrac{1}{4}Cu^4 \qquad (1)$$

where $u = u(x,t)$ is the displacement of a proton (mass m_1) from one of the minima of the double-well potential. A, B and C are constants relating to temperature. If $B^2 = \frac{9}{2}AC$, then $U(u)$ is a symmetric potential with a double well while if $B^2 \neq \frac{9}{2}AC$, $U(u)$ is an asymmetric potential with a double well. The signs + and − in equation (1) correspond to the cases $u < 0$ and $u > 0$, respectively.

In the transfer process, the proton moves from one well of the double-well potential to the other well; solitonic defects are excited in the proton sublattice of the hydrogen-bonded chain. 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

[2–6]. The results show that solitonic defects in the proton sublattice and in a heavy-ion sublattice may exist. Solitonic defects in two sublattices propagate in pairs along the chain with the same velocity, i.e. they form soliton pairs [2].

According to the two-component soliton model, coupling between the proton sublattice and the heavy-ion sublattice is either a linear type [3,4] or a non-linear type [5,6]. In this paper, we investigate the motion of the soliton in an inhomogeneous hydrogen-bonded chain with a double-well potential (1) on the basis of linear coupling. In section 2, we shall show that kink pairs will be excited in a hydrogen-bonded chain with a symmetric double-well potential and bell-shaped soliton pairs will be excited in a hydrogen-bonded chain with an asymmetric double-well potential. A bell-shaped soliton pair corresponds to two parallel (or antiparallel) electric dipoles lying on a chain. A slow-mode soliton–antisoliton pair is more stable than a fast-mode soliton–soliton pair. In section 3, we shall discuss the interaction between soliton pairs and impurities. When a soliton pair moves in an impurity region, transformation from a slow-mode soliton–antisoliton pair into a fast-mode soliton–soliton pair will occur. For a bell-shaped soliton pair, this transformation corresponds to the reversion of an electric dipole in one of the two sublattices. In the case of repulsion-type impurities, there is a critical velocity v_{cr} for soliton pairs. For incident soliton pairs with velocity $v < v_{cr}$, allowed regions and forbidden regions will exist for its motion. The motion of a soliton pair in the vicinity of an impurity is discussed in section 4. We shall show that the vibrational amplitude and the vibrational frequency of the soliton pair around the impurity depend on the change in the model parameters in the vicinity of this impurity and the distribution of neighbouring impurities.

2. Kink pairs and bell-shaped soliton pairs

We assume that coupling between the proton sublattice and the heavy-ion sublattice is a linear type [3,4], and the Hamiltonian of a hydrogen-bonded molecular chain, in the continuum model, is

$$H = \frac{1}{\ell}\int [\tfrac{1}{2}m_1(u_t^2 + c_0^2 u_x^2) + \tfrac{1}{2}m_2(\eta_t^2 + v_0^2\eta_x^2) + U(u) + K u_x \eta_x]\,\mathrm{d}x. \tag{2}$$

Here ℓ is the lattice spacing. $\eta = \eta(x,t)$ is the displacement of the heavy ion (mass m_2). c_0 and v_0 are characteristic sound velocities of the proton and the heavy-ion sublattices, respectively. K is the coupling constant between the two sublattices. The Euler–Lagrange equations of motion corresponding to equation (2) are as follows:

$$m_1(u_{tt} - c_0^2 u_{xx}) - K\eta_{xx} + Au \mp Bu^2 + Cu^3 = 0 \tag{3}$$

$$m_2(\eta_{tt} - v_0^2\eta_{xx}) - K u_{xx} = 0. \tag{4}$$

When $B^2 = \frac{9}{2}AC$, equations (3) and (4) have kink solutions:

$$u^{\mathrm{K}} = \sigma u_0\{1 + \tanh[\tfrac{1}{2}\sqrt{\alpha}(x - vt)]\} \tag{5}$$

$$\eta^{\mathrm{K}} = q u^{\mathrm{K}}. \tag{6}$$

When $B^2 > \frac{9}{2}AC$, equations (3) and (4) have bell-shaped soliton solutions:

$$u^{\mathrm{B}} = \sigma \frac{3A}{B\{1 + (1 - 9AC/2B^2)^{1/2}\cosh[\sqrt{\alpha}(x - vt)]\}} \tag{7}$$

$$\eta^{\mathrm{B}} = q u^{\mathrm{B}} \tag{8}$$

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

$$\alpha = \frac{A}{m_1(c_0^2 - v^2) - K^2/m_2(v_0^2 - v^2)} \tag{9}$$

$$q = -\frac{K}{m_2(v_0^2 - v^2)} \tag{10}$$

and v is the velocity of the soliton. Solitons may be classified, by their velocity, into two modes [3], namely a fast mode given by

$$c_0^2 - \frac{K}{\sqrt{m_1 m_2}} > v^2 \geqslant v_0^2 + \frac{K}{\sqrt{m_1 m_2}}$$

and a slow mode given by

$$v_0^2 - \frac{K}{\sqrt{m_1 m_2}} \geqslant v^2 > 0.$$

Kinks and antikinks correspond to local lattice expansion and contraction, respectively. For the proton sublattice, the local lattice expansion and contraction are accompanied by a local decrease and a local increase, respectively, in positive charge density. The change in the charge density depends directly on $\rho^{\mathrm{K}} = -\partial u^{\mathrm{K}}/\partial x$ [3]. However, equations (6) and (10) show that, if the proton sublattice produces a slow-mode kink (or antikink), then the heavy-ion sublattice produces a slow-mode antikink (or kink). They propagate along the chain *with the same velocity in pairs. In other words, they form a slow-mode kink–antikink pair.* Similarly the fast-mode kinks (or antikinks) in the proton and heavy-ion sublattices will form a fast-mode kink–kink (or antikink–antikink) pair.

There is a local lattice contraction on one side of the centre of the bell-shaped soliton, and there is a local lattice expansion on the other side. The excessive charge density depends directly on $\rho^{\mathrm{B}} = -\partial u^{\mathrm{B}}/\partial x$, in the proton sublattice. ρ^{B} has a maximum at a_0 and a minimum at $-a_0$, where

$$a_0 = \frac{1}{\sqrt{\alpha}} \operatorname{arc}\left[\cosh\left(\frac{1 + (3/B)(B^2 - 4AC)^{1/2}}{2(1 - 9AC/2B^2)^{1/2}}\right)\right]. \tag{11}$$

This means that there is a positive excessive charge density on one side of the centre and there is a negative excessive charge density on the other side. Therefore, a bell-*shaped soliton in a proton sublattice corresponds to an electric dipole lying on a chain.* Similarly, a bell-shaped soliton in a heavy-ion sublattice corresponds to an electric dipole lying on a chain too. Obviously, equations (8) and (10) show that if a proton sublattice produces a slow-mode bell-shaped soliton, then a heavy-ion sublattice produces a slow-mode bell-shaped antisoliton. Hence, they form a slow-mode bell-shaped soliton–antisoliton pair corresponding to two parallel electric dipoles. Fast-mode bell-shaped solitons in protons and heavy-ion sublattices will form a fast-mode bell-shaped soliton–soliton pair corresponding to two antiparallel electric dipoles. The soliton–antisoliton pair and soliton–soliton pair are referred to as a soliton pair sometimes for short. It is noteworthy that it differs from the usual soliton–antisoliton pair in the same sublattice.

The minimum energy needed to transform from a slow-mode kink–antikink pair into a fast-mode kink–kink pair, obtained from equations (2), (5) and (6), is

$$\Delta E_{\mathrm{K}} = \frac{4KA^{3/2}}{3\ell C[m_2(c_0^2 - v_0^2)]^{1/2}} \tag{12}$$

while the minimum energy needed to transform from a slow-mode bell-shaped soliton–antisoliton pair into a fast-mode bell-shaped soliton–soliton pair, obtained from equations (2), (7) and (8), is

$$\Delta E_{\mathrm{B}} = \frac{24KA^{5/2}}{5\ell B^2[m_2(c_0^2 - v_0^2)]^{1/2}} \left(1 - \frac{9AC}{2B^2}\right) F \tag{13}$$

where $F = F(\frac{5}{2}, 2; \frac{7}{2}; 9AC/2B^2)$ is a hypergeometric function. In the process of transformation, the reversion of an electric dipole in one of the two sublattices will happen. Thus, it is clear that a slow-mode soliton–antisoliton pair should be more stable than a fast-mode soliton–soliton pair. However, the supersonic soliton has been investigated by researchers in other cases, too [7].

3. Interaction between a soliton pair and an impurity

In this section, we shall consider the interaction between a soliton pair and an impurity. In the presence of impurities, we assume that model parameters in the vicinity of impurities are changed as follows [8]:

$$\begin{aligned} m_1'(x) &= m_1\left(1 + \sum_i^N \epsilon_1^i \delta(x - a_i)\right) \qquad & m_2'(x) &= m_2\left(1 + \sum_i^N \epsilon_2^i \delta(x - a_i)\right) \\ c_0'^2(x) &= c_0^2\left(1 + \sum_i^N \epsilon_c^i \delta(x - a_i)\right) \qquad & v_0'^2(x) &= v_0^2\left(1 + \sum_i^N \epsilon_v^i (x - a_i)\right) \\ K'(x) &= K\left(1 + \sum_i^N \epsilon_K^i \delta(x - a_i)\right) \qquad & U'(u) &= U(u)\left(1 + \sum_i^N \epsilon_0^i \delta(x - a_i)\right) \end{aligned} \tag{14}$$

where N is the number of impurities. ϵ^i indicates the strength of the ith inhomogeneity. a_i is the position of the ith impurity. Replacing the model parameters in equation (2) by the corresponding parameters in equation (14), we obtain the Hamiltonian of an inhomogeneous chain:

$$\begin{aligned} H' = {} & \frac{1}{\ell} \int [\tfrac{1}{2}m_1(u_t^2 + c_0^2 u_x^2) + \tfrac{1}{2}m_2(\eta_t^2 + v_0^2\eta_x^2) + Ku_x\eta_x + \tfrac{1}{2}Au^2 \mp \tfrac{1}{3}Bu^3 + \tfrac{1}{4}Cu^4]\,\mathrm{d}x \\ & + \frac{1}{\ell}\sum_i^N \int [\tfrac{1}{2}m_1(\epsilon_1^i u_t^2 + c_0^2 \bar{\epsilon}_1^i u_x^2) + \tfrac{1}{2}m_2(\epsilon_2^i \eta_t^2 + \bar{\epsilon}_2^i v_0^2 \eta_x^2) + K\epsilon_K^i u_x \eta_x \\ & + \epsilon_0^i(\tfrac{1}{2}Au^2 \mp \tfrac{1}{3}Bu^3 + \tfrac{1}{4}Cu^4)]\delta(x - a_i)\,\mathrm{d}x \end{aligned} \tag{15}$$

where

$$\bar{\epsilon}_1^i = \epsilon_1^i + \epsilon_c^i + 2\epsilon_1^i\epsilon_c^i \qquad \bar{\epsilon}_2^i = \epsilon_2^i + \epsilon_v^i + 2\epsilon_2^i\epsilon_v^i.$$

The Euler–Lagrange equations of motion corresponding to equation (15) are

$$\begin{aligned} m_1(u_{tt} - c_0^2 u_{xx}) - K\eta_{xx} + Au \mp Bu^2 + Cu^3 = {} & \sum_i^N \{-m_1\epsilon_1^i u_{tt}\delta(x - a_i) + m_1 c_0^2 \bar{\epsilon}_1^i [u_x\delta(x - a_i)]_x \\ & - \epsilon_0^i(Au \mp Bu^2 + Cu^3)\delta(x - a_i) + K\epsilon_K^i[\eta_x\delta(x - a_i)]_x\} \end{aligned} \tag{16}$$

$$\begin{aligned} m_2(\eta_{tt} - v_0^2\eta_{xx}) - Ku_{xx} = {} & \sum_i^N \{-m_2\epsilon_2^i \eta_{tt}\delta(x - a_i) + m_2 v_0^2 \bar{\epsilon}_2^i [\eta_x\delta(x - a_i)]_x \\ & + K\epsilon_K^i[u_x\delta(x - a_i)]_x\}. \end{aligned} \tag{17}$$

The right-hand sides of equations (16) and (17) are the terms perturbed by impurities. A collective coordinate $y(t)$ is introduced to describe this perturbation, i.e. we assume that the solutions of equations (16) and (17) have the following forms:

$$u^{\mathrm{K}} = \sigma u_0[\![1 + \tanh\{\tfrac{1}{2}\sqrt{\alpha}[x - y(t)]\}]\!] \tag{18}$$

$$\eta^{\mathrm{K}} = q u^{\mathrm{K}} \tag{19}$$

for a kink and

$$u^{\mathrm{B}} = \sigma \frac{3A}{B[\![1 + (1 - 9AC/2B^2)^{1/2}\cosh\{\sqrt{\alpha}[x - y(t)]\}]\!]} \tag{20}$$

$$\eta^{\mathrm{B}} = q u^{\mathrm{B}} \tag{21}$$

for a bell-shaped soliton. From equations (16) and (17), and considering the boundary conditions of equations (18)–(21), we obtain the equation of motion for a soliton pair:

$$\begin{aligned}\frac{\mathrm{d}P}{\mathrm{d}t} = {} & \frac{1}{\ell}\sum_i^N\{m_1\epsilon_1^i u_x u_{tt} + m_1 c_0^2 \bar{\epsilon}_1^i u_x u_{xx} + \epsilon_0^i[U(u)]_x + K\epsilon_K^i u_{xx}\eta_x\}_{x=a_i} \\ & + \frac{1}{\ell}\sum_i^n (m_2\epsilon_2^i \eta_x \eta_{tt} + m_2 \bar{\epsilon}_2^i v_0^2 \eta_x \eta_{xx} + K\epsilon_K^i u_x \eta_{xx})_{x=a_i}\end{aligned} \tag{22}$$

where

$$P = -\frac{m_1}{\ell}\int u_x u_t \,\mathrm{d}x - \frac{m_2}{\ell}\int \eta_x \eta_t \,\mathrm{d}x = M^* \dot{y} \tag{23}$$

is the momentum of a soliton pair. The dot denotes a derivative with respect to time. $M^* = m_1^* + m_2^*$ represents the effective mass of the soliton pair. $m_1^* = m_1 I$ and $m_2^* = m_2 I q^2$ are the effective masses of a solitonic defect in the proton and in the heavy-ion sublattices, respectively, in which

$$I = \frac{2\sqrt{\alpha}u_0^2}{3\ell} \tag{24}$$

for a kink and

$$I = \frac{6\sqrt{\alpha}A^2}{5\ell B^2}\left(1 - \frac{9AC}{2B^2}\right)F \tag{25}$$

for a bell-shaped soliton. Substituting equation (23) into equation (22) and multiplying both sides of the equation by $\dot{y}$, and then integrating, we obtain an expression for the velocity of a soliton pair:

$$\dot{y} = \pm\left[\left(D - \sum_i^N U_\epsilon^i f_i(y)\right)\Big/\left(M^* + \sum_i^N M_\epsilon^i f_i(y)\right)\right]^{1/2} \tag{26}$$

where D is an integral constant, and

$$M_\epsilon^i = L\alpha(m_1\epsilon_1^i + m_2\epsilon_2^i q^2) \tag{27}$$

$$U_\epsilon^i = L[\epsilon_0^i A + \alpha(m_1 c_0^2 \bar{\epsilon}_1^i + m_2 v_0^2 \bar{\epsilon}_2^i q^2 + 2K\epsilon_K^i q)] \tag{28}$$

in which

$$L = L_{\mathrm{K}} = \frac{u_0^2}{4\ell} \tag{29}$$

$$f_i(y) = f_i^{\mathrm{K}}(y) = \operatorname{sech}^4[\tfrac{1}{2}\sqrt{\alpha}(a_i - y)] \tag{30}$$

for a kink pair and

$$L = L_{\mathrm{B}} = \frac{81CA^3}{2\ell B^4}\left(\frac{2B^2}{9AC} - 1\right) \tag{31}$$

$$f_i(y) = f_i^{\mathrm{B}}(y) = \frac{\sinh^2[\sqrt{\alpha}(a_i - y)]}{\{1 + (1 - 9AC/2B^2)^{1/2}\cosh[\sqrt{\alpha}(a_i - y)]\}^4} \tag{32}$$

for a bell-shaped soliton pair. If the initial position of the soliton pair is in the homogeneous region of the chain, then $M_\epsilon^i = U_\epsilon^i = 0$. Hence, we get, from equation (26), $D = M^* v^2$.

For two identical impurities, we have $M_\epsilon^1 = M_\epsilon^2 = M_\epsilon$, $U_\epsilon^1 = U_\epsilon^2 = U_\epsilon$, $a_1 = \frac{1}{2}a$ and $a_2 = -\frac{1}{2}a$; here a is the distance between two impurities. So equation (26) can be written as follows:

$$\frac{\dot{y}}{v_0} = \pm\left(\frac{v^2/v_0^2 - (U_\epsilon/M^* v_0^2) f(y)}{1 + (M_\epsilon/M^*) f(y)}\right)^{1/2} \tag{33}$$

in which

$$f(y) = \operatorname{sech}^4[\tfrac{1}{2}\sqrt{\alpha}(\tfrac{1}{2}a + y)] + \operatorname{sech}^4[\tfrac{1}{2}\sqrt{\alpha}(\tfrac{1}{2}a - y)] \tag{34}$$

for the kink pair, and

$$f(y) = \frac{\sinh^2[\sqrt{\alpha}(\frac{1}{2}a + y)]}{\{1 + (1 - 9AC/2B^2)^{1/2}\cosh[\sqrt{\alpha}(\frac{1}{2}a + y)]\}^4} + \frac{\sinh^2[\sqrt{\alpha}(\frac{1}{2}a - y)]}{\{1 + (1 - 9AC/2B^2)^{1/2}\cosh[\sqrt{\alpha}(\frac{1}{2}a - y)]\}^4} \tag{35}$$

for the bell-shaped soliton pair. According to equations (33) and (34), taking $\sqrt{\alpha} = 0.4$ Å^{-1}, $a = 60$ Å, $M_\epsilon/M^* = 0.1$ and $|U_\epsilon/M^* v_0^2| = 0.2$, the trajectories of motion in phase space for kink pair are drawn in figures 1 and 2, which describe two repulsion-type impurities ($U_\epsilon > 0$) and two attraction-type impurities ($U_\epsilon < 0$), respectively. The phase trajectories of motion for the bell-shaped soliton pair with two repulsion-type impurities ($U_\epsilon > 0$) is shown in figure 3, but the parameters of equation (33) and (35) are taken as follows: $\sqrt{\alpha} = 0.2$ Å^{-1}, $a = 60$ Å, $(1 - 9AC/2B^2)^{1/2} = 0.1$, $M_\epsilon/M^* = 0.1$ and $U_\epsilon/M^* v_0^2 = 0.2$.

For repulsion-type impurities ($U_\epsilon^i > 0$), the incident soliton pair has a critical velocity

$$v_{\mathrm{cr}} = \left[\frac{1}{M^*}\left(\sum_i^N U_\epsilon^i f_i(y)\right)_{\max}\right]^{1/2}. \tag{36}$$

When the incident soliton pair travels with the critical velocity v_{cr}, one of the following circumstances may occur: it may pass through the impurity region, it may be reflected by an

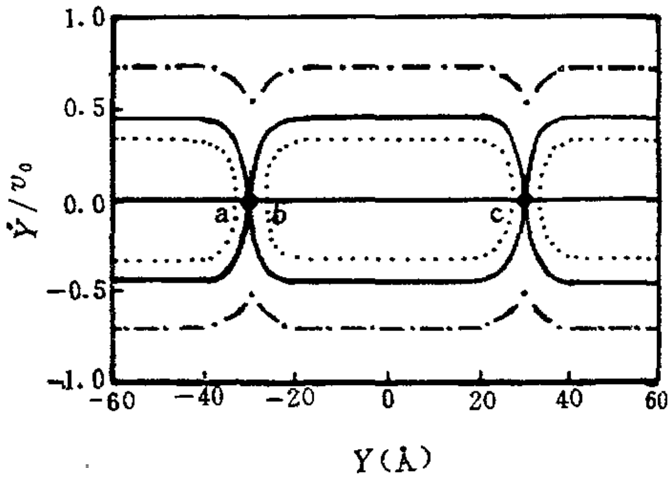

Figure 1. The phase trajectory of motion for a kink pair with two repulsion-type impurities: — · —, $D = 0.5M^*v_0^2$; ——, $D = 0.2M^*v_0^2$; ······, $D = 0.1M^*v_0^2$; ●, locations of impurities.

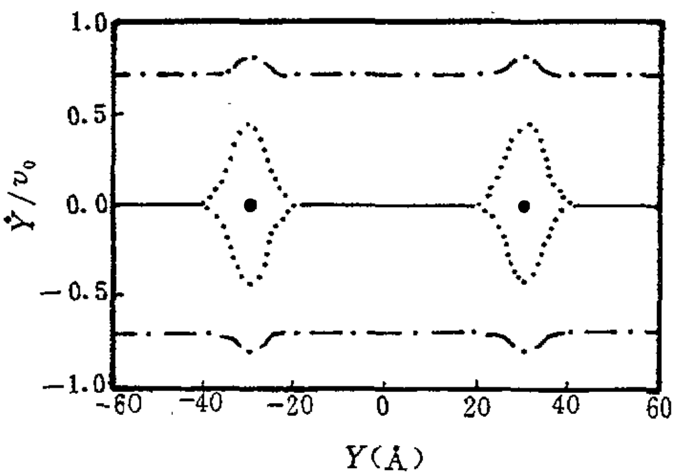

Figure 2. The phase trajectory of motion for a kink pair with two attraction-type impurities: — · —, $D = 0.5M^*v_0^2$; ······, $D = 0$; ●, locations of impurities.

impurity, or it may vibrate between two neighbouring impurities. In addition, a bell-shaped soliton pair may also vibrate around an impurity, but a kink soliton pair cannot, just as the cases shown by the full curves in figures 1 and 3, where the phase trajectory of motion for the soliton pair branches. The velocity of the soliton pair becomes zero at branch points. For a kink soliton pair, the branch point of the phase trajectory is just the location of the impurity. However, for a bell-shaped soliton pair, the branch points of the phase trajectory are located at both sides of impurity.

In comparison with the above situations, the incident soliton pair with a velocity $v > v_{cr}$ will directly pass through the impurity region, which is shown by the dot-dashed curves in figures 1 and 3.

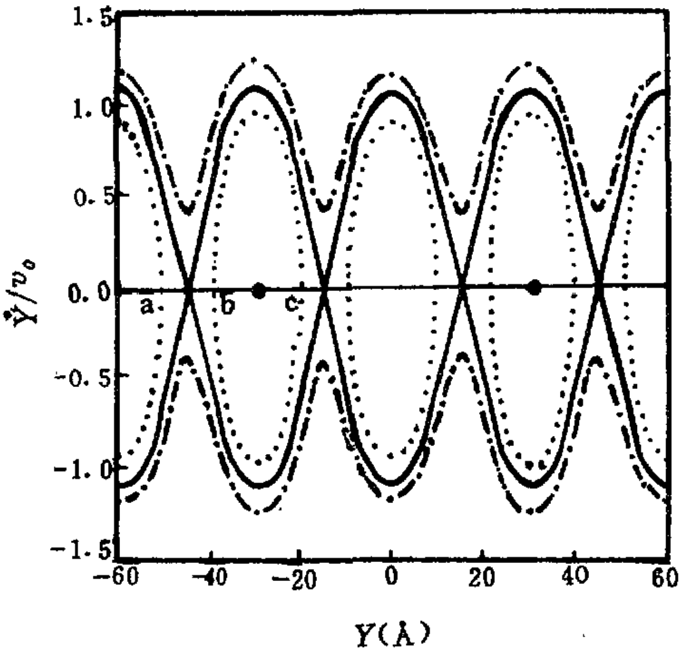

Figure 3. The phase trajectory of motion for a bell-shaped soliton pair with two repulsion-type impurities: — · —, $D = 1.5M^*v_0^2$; ——, $D = 1.237M^*v_0^2$; ······, $D = M^*v_0^2$; ●, locations of impurities.

While the incident soliton pair has velocity $v < v_{cr}$, it cannot pass directly through the impurity region but may be directly reflected by the impurity, which is shown by the dotted curves in figures 1 and 3, where there are allowed regions with $\dot{y}^2 > 0$ (e.g. region bc) and forbidden regions with $\dot{y}^2 < 0$ (e.g. region ab) for motion of a soliton pair. The velocity of the soliton pair becomes zero at the common boundary of the allowed region and the forbidden region. It is shown in figure 1 that a repulsion-type impurity is located in the forbidden region for motion of the kink pairs. This means that the repulsion-type impurity cannot capture a kink pair. However, in figure 3, a repulsion-type impurity is located in an allowed region of motion of a bell-shaped soliton pair. Therefore, this means that the bell-shaped soliton pair may vibrate around a repulsion-type impurity. In other words, a repulsion-type impurity can capture its neighbouring bell-shaped soliton pair.

For an attraction-type impurity ($U_\varepsilon^i < 0$), a soliton pair may pass through an impurity region or vibrate around an impurity, which are shown by the dot-dashed curves and dotted curves respectively, in figure 2. When the soliton pair propagates in an impurity region, its velocity will be changed. For this reason, transformation between a slow-mode soliton–antisoliton pair and a fast-mode soliton–soliton pair may occur.

4. Motion of a soliton pair in the vicinity of an impurity

We study the circumstances in the vicinity of the jth impurity. On the assumption that $y = a_j + \xi$, $\xi = \xi(t)$, is a small perturbation, equation (26) can be written approximately as

$$\dot{\xi}^2 = \Omega^2 \xi^2 + R. \tag{37}$$

This equation has a solution satisfying the condition $\xi(0) = 0$:

$$\xi = G \sinh(\Omega t) \tag{38}$$

where $G = \sqrt{R}/\Omega$ and

$$R = \gamma \frac{D_j}{M_j} \tag{39}$$

$$\Omega^2 = \frac{\alpha(M_j U_\epsilon^j + M_\epsilon^j D_j)}{\beta M_j^2} \tag{40}$$

$$D_j = D - \sum_{i \neq j}^{N} U_\epsilon^i f_i(a_j) \tag{41}$$

$$M_j = M^* + \sum_{i \neq j}^{N} M_\epsilon^i f_i(a_j) \tag{42}$$

in which

$$\gamma = \left(1 - \frac{U_\epsilon^j}{D_j}\right)\left(1 + \frac{M_\epsilon^j}{M_j}\right)^{-1} \qquad \beta = 2\left(1 + \frac{M_\epsilon^j}{M_j}\right)^2 \tag{43}$$

for a kink soliton pair and

$$\gamma = 1 \qquad \beta = -\left[1 + \left(1 - \frac{9AC}{2B^2}\right)^{1/2}\right]^4 \tag{44}$$

for a bell-shaped soliton pair. Equation (38) shows that the soliton pair may escape from the impurity if $\Omega^2 > 0$ or may vibrate around the impurity if $\Omega^2 < 0$. The amplitude and frequency of vibration depend not only on the change in model parameter in the vicinity of the impurity but also on the distribution of neighbouring impurities.

For $N = 1$, $\epsilon_1^j = \epsilon$ and $\epsilon_2^i = \epsilon_c^i = \epsilon_v^i = \epsilon_K^i = \epsilon_0^i = 0$, then we obtain

$$\Omega^2 = \Omega_{\mathrm{K}}^2 = \frac{m_1 \alpha^2 u_0^2 (D + M^* c_0^2)}{2[M^* + (\alpha m_1 u_0^2/4\ell)\epsilon]^2}\epsilon \tag{45}$$

for a kink pair and

$$\Omega^2 = \Omega_{\mathrm{B}}^2 = -\frac{81 m_1 C \alpha^2 A^3 (D + M^* c_0^2)}{2\ell M^{*2} B^4 [1 + (1 - 9AC/2B^2)^{1/2}]^4}\left(\frac{2B^2}{9AC} - 1\right)\epsilon \tag{46}$$

for a bell-shaped soliton pair. Because $\epsilon = 1$ for an isotopic impurity, we obtain $\Omega_{\mathrm{K}}^2 > 0$ and $\Omega_{\mathrm{B}}^2 < 0$ from equations (45) and (46), respectively. Therefore, a kink pair may escape from an isotopic impurity, but a bell-shaped soliton pair can be trapped by an isotopic impurity and vibrate around it. In other words, an isotopic impurity will attract a nearby bell-shaped soliton pair but repulse a neighbouring kink pair.

5. Conclusion

There are kink soliton pairs in a hydrogen-bonded chain with a symmetric double-well potential and bell-shaped soliton pairs in a hydrogen-bonded chain with an asymmetric double-well potential. A bell-shaped soliton pair corresponds to two parallel (or antiparallel) electric dipoles. Reversion of the electric dipole in one of the two sublattices, when the bell-shaped soliton pair propagates along an inhomogeneous chain, may occur. A bell-shaped soliton pair can be captured by a repulsion-type impurity and vibrate around it, but a kink soliton pair is certainly reflected by the repulsion-type impurity.

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References

[1] Ichinose S and Minato T 1992 *Chaos, Solitons & Fractals* **2** 147
[2] Xu J-Z 1992 *Phys. Lett.* **172A** 148
[3] Yomosa S 1983 *J. Phys. Soc. Japan* **52** 1866
[4] Dey B and Daniel M 1990 *J. Phys.: Condens. Matter* **2** 2331
[5] Zolotariuk A V, Spatschek K H and Laedke E W 1984 *Phys. Lett.* **101A** 517
[6] Halding J and Lomdahl P S 1988 *Phys. Rev.* A **37** 2608
[7] Christiansen P L, Eilbeck J C, Enol'skii V Z and Gaididei Ju B 1992 *Phys. Lett.* **166A** 129
[8] Kivshar Yu S 1991 *Phys. Rev.* A **43** 3117