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Dynamics of solitons in a weakly coupled discrete sine–Gordon system

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Abstract. We study the effects of discreteness on the motion of coupled solitons of two weakly coupled discrete sine–Gordon systems. A collective coordinate method associated with Dirac's formalism of constrained Hamiltonian dynamics is used to derive the equations of motion for the centres of the solitons and for the dressing or discreteness corrections of the continuum solitons. We show that the dynamics of the coupled solitons can be described by a set of two non-linear differential equations. It is also shown that the coupling reduces (increases) the trapping processes in the case where the two solitons have the same polarity (different polarities). A numerical analysis of the static dressing equations is performed. We find that the dressing lowers the potential energy of solitons and increases the Peierls–Nabarro barrier.

1. Introduction

The dynamics and statics of weakly coupled chains are now a subject of growing interest. These systems, each with a specific type of coupling, occur in various branches of physics; for instance, in electronics to describe the interaction between two parallel long-Josephson junctions (Mineev *et al* 1981, Holst *et al* 1990), in condensed matter physics to describe the frontier between two half-infinite arrays of atoms absorbed on a metal surface (Coutinho *et al* 1981, Braun *et al* 1988) and to describe the coupling between polaron or magnon waves, and acoustic waves in elastic ferroelectric or ferromagnetic systems (Pouget and Maugin 1984, Maugin and Miled 1986). In biophysics, it has recently been shown that the base–rotator dynamical model of a double helix of deoxyribonucleic acid can be described by a Hamiltonian in which the coupling is due to the H-bond energy and dipole–dipole interaction energy (Yomosa 1983, 1984, Takeno and Homma 1983, Homma and Takeno 1984, Zhang 1987, Gen-fa Zhou 1989).

Equations derived from the coupled systems are non-linear equations which, in the continuum limit, give rise to non-linear waves or solitons with complicated dynamics yet to be understood.

Because of the non-integrability of the coupled equations, the investigation of soliton excitations has taken two principal directions. The first approach is to solve the coupled equations for certain special cases as when the soliton of the second chain has the same amplitude and velocity as that of the first chain. The second approach is to solve the equation of motion in a general case by means of the perturbation method. Details are given in section 2.

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The weakly coupled sine–Gordon system is the most widely studied example. It admits fluxon soliton solutions. Experimental, numerical and theoretical investigations of this system perturbed by small damping and power input mechanisms have produced interesting results. For instance, it has been demonstrated that due to dissipation, fluxons belonging to different chains or junctions can fuse into a bound state (bifluxon). In addition radiative effects accompanying the collision of the two fluxons have been observed (Kivshar and Malomed 1988, Holst *et al* 1990, Grønbech-Jensen *et al* 1990).

These important results characterizing the propagation of the coupled solitons are obtained in the continuum medium where the soliton extensions are large compared with the lattice spacing. When this is not the case, the continuum approximation becomes inadequate to describe the motion of the solitons and the discreteness should be taken into account explicitly. Up until now, published works concerning the influence of the discreteness of the physical systems have focused on systems with single-soliton solutions. Interesting results have been obtained. In general, the solitons become trapped by the Peierls–Nabarro lattice potential (Nabarro 1967) and their motion occurs with dissipation (Aubry 1978, Peyrard and Remoissenet 1982, Combs and Yip 1983, Peyrard and Kruskal 1984, Willis *et al* 1986, Stancioff *et al* 1986, Boesch *et al* 1989, Woafo *et al* 1991).

Our aim in this paper is to model a solution of the motion of solitons of the coupled systems with the effects of discreteness taken into account. The particular model considered is the weakly coupled sine–Gordon system, the basic ideas of which we review in section 2. The continuum description is presented and the two approaches mentioned earlier are developed. In section 3, we present the theory of the effect of discreteness. The mathematical foundation of the theory is the collective coordinate method associated with Dirac's constrained Hamiltonian dynamics (Dirac 1964, Tomboulis 1975). New dynamical variables are introduced: the positions of the centres of the solitons and the corrections or dressings on the continuum soliton solutions due to discreteness. By means of a suitable canonical transformation, we derive an equation of motion in these new variables. We discuss the particular limit where the discreteness corrections can be neglected. It is found that the coupled solitons experience the periodic Peierls–Nabarro potential.

In section 4, a numerical analysis is performed to solve the discrete equations of dressings. It is found that the inclusion of the static dressing lowers the depth of the Peierls–Nabarro potential. Section 5 summarizes our conclusions and ideas for further work.

2. Weakly coupled sine–Gordon systems

2.1. The model

Our discrete model consists of two coupled one-dimensional sine–Gordon chains of particles with equal masses $m = 1$. Each chain is characterized by a harmonic elastic constant J and a natural period constant b. These constants are set equal to unity. A particle of the chain is subjected to the sinusoidal potential

$$V(U) = (1/a^2)(1 - \cos U)$$

where a is a constant which measures the amplitude of the sinusoidal potential and U is the displacement of the particle from its equilibrium site. Denoting by Y_i the displacement of the particle on the first chain in cell i and by W_i the same quantity on the second chain, we can express the total energy or Hamiltonian of the system as (the dot stands for the time derivative)

$$H = H_0 + H_1 \tag{2.1}$$

with

$$H_0 = \tfrac{1}{2}\sum_{i=1}^{N}(\dot{Y}_i^2 + \dot{W}_i^2) + \tfrac{1}{2}\sum_{i=1}^{N}[(Y_{i+1} - Y_i)^2 + (W_{i+1} - W_i)^2] + \frac{1}{a^2}\sum_{i=1}^{N}(2 - \cos Y_i - \cos W_i) \tag{2.2}$$

and

$$H_1 = -\epsilon\sum_{i=1}^{N}(Y_{i+1} - Y_i)(W_{i+1} - W_i). \tag{2.3}$$

H_0 is the expression for the total energy of the two sine–Gordon systems with no coupling. H_I denotes the interaction energy. It takes into account the interaction between the relative displacements of particles in both chains. ϵ is the coupling constant between the chains. It is assumed to be small and positive throughout this paper.

The Hamiltonian (2.1), with an appropriate scaling, can be seen as the total energy of two discrete parallel long-Josephson junctions inductively coupled (Mineev *et al* 1981, Kivshar *et al* 1988, Holst *et al* 1990, Grønbech-Jensen *et al* 1990). In this sense, Y_i and W_i represent fluxons that propagate along the junctions and the time derivatives of Y_i and W_i are the voltages. H_I is then a discrete version of the energy of topological charges in the two coupled long-Josephson chains. In the case where H describes the Hamiltonian of two coupled chains of adatoms, H_I accounts for the interaction between the density of the excess adatoms in both parallel adatomic chains (Braun *et al* 1988).

The equations of motion derived from (2.1) are

$$Y_{i+1} + Y_{i-1} - 2Y_i - \ddot{Y}_i - \frac{1}{a^2}\sin Y_i = \epsilon(W_{i+1} + W_{i-1} - 2W_i) \tag{2.4a}$$

$$W_{i+1} + W_{i-1} - 2W_i - \ddot{W}_i - \frac{1}{a^2}\sin W_i = \epsilon(Y_{i+1} + Y_{i-1} - 2Y_i) \tag{2.4b}$$

where the dots are differentiations with respect to time t.

To solve equations (2.4), we shall assume the continuum approximation $U_i(t) \to U(x,t)$ and $U_{i+1} + U_{i-1} - 2U_i \simeq U_{2x}(U_i = Y_i, W_i)$. Then equations (2.4) reduce to (the subscript $2x$ is the spatial second derivative of the function U)

$$Y_{2x} - \ddot{Y} - \frac{1}{a^2}\sin Y = \epsilon W_{2x} \tag{2.5a}$$

$$W_{2x} - \ddot{W} - \frac{1}{a^2}\sin W = \epsilon Y_{2x}. \tag{2.5b}$$

When $\epsilon = 0$, the system turns into uncoupled, exactly integrable sine–Gordon equations. The solutions corresponding to fluxons or kinks (antifluxons or antikinks) are

$$Y^0(x,t) = 4\tan^{-1}\exp(\sigma_1\gamma(v_1)Z_1) \tag{2.6a}$$

$$W^0(x,t) = 4\tan^{-1}\exp(\sigma_2\gamma(v_2)Z_2) \tag{2.6b}$$

where

$$Z_j = (x - v_jt)/a \qquad (j = 1, 2)$$
$$\gamma(v_j) = 1/(1 - v_j^2)^{1/2}$$

and $\sigma_1, \sigma_2 = \pm 1$ are the polarities of the kinks. The plus (minus) sign corresponds to the kink (antikink). v_j are the kink's velocities. We assume for the rest of the paper that $v_j \ll 1$ and the Lorentz contraction factor $\gamma(v_j)$ reduces to unity.

When $\epsilon \neq 0$, the interaction between the junctions distorts the solitons' shape and the system (2.5) cannot be solved exactly. However, it is easy to see that $Y = W = 0$ is a solution of the system (2.5) and that the case $W = 0$, $Y \neq 0$ (or $W \neq 0$, $Y = 0$) reduces the system to the well known sine–Gordon equation which has recently been analysed theoretically and numerically in the discrete limit by many authors (Peyrard and Kruskal 1984, Willis *et al* 1986, Stancioff *et al* 1986, Boesch *et al* 1989). The case where there are non-linear excitations in both chains will be divided into two parts. The first part concerns some special assumptions for which the system of equations becomes uncoupled and yields special solutions. In the second part, the system is solved by expanding its solutions in power series of the coupling constant ϵ.

2.2. Special solutions

In addition to the particular cases mentioned earlier, another interesting case is $W = \pm Y$. In this case, the system of equation (2.5) reduces to a sine–Gordon equation with a small correction to the disperson coefficient (coefficient of Y_{2x} or W_{2x}).

$$\ddot{Y} - (1 \mp \epsilon)Y_{2x} + (1/a^2)\sin Y = 0. \tag{2.7}$$

The single-soliton solution of equation (2.7) is

$$Y(x,t) = 4\tan^{-1}\left\{\exp\left(\sigma_1\frac{x - \sqrt{1 \mp \epsilon}v_1t}{\sqrt{1 \mp \epsilon}a}\right)\right\}. \tag{2.8}$$

2.3. Perturbation method

In the general case where $|Y| \neq |W|$, there is currently no exact solution for equation (2.5). Since the coupled chains are similar (e.g. they have the same physical parameters), we assume that the difference between $|Y|$ and $|W|$ appears in the positions of the centres of the two solitons. This assumption is fulfilled when the initial waves entering the chains (or transmission lines) have the same amplitude and velocity. Intrachain damping, inhomogeneities and external noises can cause one of the solitons to be slightly slowed down or accelerated. The difference will be characterized by a parameter d standing for the spatial distance between the two solitons.

$$d = X_1 - X_2 \tag{2.9}$$

where X_1 and X_2 are, respectively, the positions of the centres of the first (Y) and the second (W) solitons. In the continuum limit, $X_j = v_j t + X_{0j}$ where X_{0j} are the initial positions of the solitons. One should recall that d is a small parameter since we have assumed slight acceleration or deceleration.

Remembering that the coupling constant ϵ is small, it is reasonable to expand the solution of equations (2.5) into an ϵ power series (Zhang 1987, Braun *et al* 1988) which would have the form

$$Y = Y^0 + \epsilon Y^1 + \mathrm{O}(\epsilon^2) \qquad W = W^0 + \epsilon W^1 + \mathrm{O}(\epsilon^2) \tag{2.10}$$

and Y^0 and W^0 are soliton solutions (2.6) of the uncoupled equations ($\epsilon = 0$). Inserting (2.10) into (2.5) and assuming that Y^1 and W^1 are solitary waves with the same velocities as Y^0 and W^0 (the perturbations Y^1 and W^1 are distortions of the kink shapes) one obtains

$$Y^1_{Z_1Z_1} = (2\tanh^2\sigma_1 Z_1 - 1)Y^1 - 2\,\mathrm{sech}\,\sigma_2 Z_2 \tanh\sigma_2 Z_2 \tag{2.10a}$$

$$W^1_{Z_2Z_2} = (2\tanh^2\sigma_2 Z_2 - 1)W^1 - 2\,\mathrm{sech}\,\sigma_1 Z_1 \tanh\sigma_1 Z_1. \tag{2.10b}$$

Equations (2.10) are linear ordinary differential equations. They have been integrated numerically (for any d) and analytically (for $d = 0$) by using the associated Legendre polynomials of the first and second kind. While solving equations (2.10) one assumes that the solitons Y and W tend asymptotically to 2π for $Z_j = +\infty$ and to zero for $Z_j = -\infty$. It is also assumed that $|Y| = \pi$ and $|W| = \pi$ for $Z_j = 0$ ($j = 1, 2$). Under these constraints and after some algebraic manipulations (see Zhang (1987)), the perturbation solutions may be written as

$$Y^1 = \pm\Bigg\{\mathrm{sech}\,\sigma_1 Z_1(\sigma_1 Z_1 + \ln 2\tanh\sigma_1 Z_1 - \tan^{-1}\tanh\sigma_1 Z_1) - \sinh\sigma_1 Z_1 \ln\left(\frac{1+\tanh^2\sigma_1 Z_1}{2}\right)\Bigg\}$$

$$W^1 = \pm\Bigg\{\mathrm{sech}\,\sigma_2 Z_2(\sigma_2 Z_2 + \ln 2\tanh\sigma_2 Z_2 - \tan^{-1}\tanh\sigma_2 Z_2) - \sinh\sigma_2 Z_2 \ln\left(\frac{1+\tanh^2\sigma_2 Z_2}{2}\right)\Bigg\}.$$

The plus sign corresponds to the case where the two solitons have the same polarity and the minus sign for opposite polarities. Numerical calculation reveals that Y^1 and W^1 slightly change the shape of the uncoupled solutions Y^0 and W^0.

3. Discreteness effects theory

The study of the dynamics of topological solitons has been facilitated by the discovery of the collective coordinate method (Branco *et al* 1974, Gervais and Sakita 1975, Tomboulis 1975). This method, currently applied to non-linear field theories that possess exact space-dependent solutions, is based on the introduction of two new dynamical variables: a coordinate describing the position of the soliton's centre and another coordinate which is a small amplitude field accounting for the radiated phonons that occur during the propagation of the solitons.

Recently Flesch *et al* (1987) have used this theory to describe the motion of the Klein–Gordon kink in the presence of a weak, localized perturbation. Also, a complete Hamiltonian dynamics of discrete kinks has been developed (Willis *et al* 1986). We follow this approach to study the motion of discrete coupled solitons. Since the coupling parameter is assumed to be small and the coupling distortions negligible, we can assume for this complicated problem that the solution of equations (2.5) is given by (2.6). That is $Y(x,t) \simeq Y^0(x,t)$ and $W(x,t) \simeq W^0(x,t)$.

The discrete variables Y_i and W_i are separated in the following manner:

$$Y_i = f_{1,i}(X_1) + \psi_{1,i} \qquad W_i = f_{2,i}(X_2) + \psi_{2,i} \tag{3.1}$$

where

$$f_{j,i} = 4\tan^{-1}\exp\left(\sigma_j \frac{x_i - X_j(t)}{a}\right)$$

are the continuum soliton solutions at the cell i ($x_i = i$ since $b = 1$). The $\psi_{j,i}$ field will account for the discrete corrections or dressing of the continuum solitons and for the radiated phonons emitted by the solitons during their propagation. In addition, because of the coupling, part of $\psi_{j,i}$ might be due to the coupling corrections of the soliton's shape since (2.6) is not the exact continuum solutions of equations (2.5).

Transformation (3.1) yields

$$\dot{Y}_i = \dot{\psi}_{1,i} + \dot{X}_1 f_{1,i}^{(1)}(X_1) \qquad \dot{W}_i = \dot{\psi}_{2,i} + \dot{X}_2 f_{2,i}^{(1)}(X_2) \tag{3.2}$$

where the superscript (1) denotes the differentiation of $f_{j,i}$ with respect to X_j. In order to conserve the number of degrees of freedom which has been increased by the introduction of X_j and $\psi_{j,i}$, the system is subjected to the following conditions of constraint:

$$C_j = \sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)\psi_{j,i} = 0 \qquad C_j' = \sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)\dot{\psi}_{j,i} = 0. \tag{3.3}$$

The transformation (3.1) and (3.2) under constraints (3.3) is a canonical transformation (Tomboulis 1975). Introducing (3.1) and (3.2) into the discrete Hamiltonian (2.1), one obtains

$$H = \frac{P_1^2}{2M_1} + \frac{P_2^2}{2M_2} + \tfrac{1}{2}\sum_{i=1}^{N} p_{1,i}^2 + \tfrac{1}{2}\sum_{i=1}^{N} p_{2,i}^2 + \sum_{i=1}^{N} V_1(\psi_{1,i} + f_{1,i}) + \sum_{i=1}^{N} V_2(\psi_{2,i} + f_{2,i}) + \sum_{i=1}^{N} V_{12}(\psi_{1,i} + f_{1,i}, \psi_{2,i} + f_{2,i}) \tag{3.4}$$

with

$$V_j(\psi_{j,i}+f_{j,i}) = \tfrac{1}{2}(\psi_{j,i+1}+f_{j,i+1}-\psi_{j,i}-f_{j,i})^2 + \frac{1}{a^2}(1-\cos(\psi_{j,i}+f_{j,i}))$$

$$V_{12}(\psi_{1,i}+f_{1,i},\psi_{2,i}+f_{2,i}) = -\epsilon(\psi_{1,i+1}+f_{1,i+1}-\psi_{1,i}-f_{1,i})(\psi_{2,i+1}+f_{2,i+1}-\psi_{2,i}-f_{2,j})$$

$$M_j = \sum_{i=1}^{N}(f_{j,i}^{(1)}(X_j))^2 \qquad P_j = M_j\dot{X}_j \qquad p_{j,i} = \dot{\psi}_{j,i}.$$

P_j and $p_{j,i}$ are, respectively, the conjugate momenta of variables X_j and $\psi_{j,i}$ and the M_j are the dimensionless masses of the solitons.

Under constraints (3.3), we are in the presence of a constrained dynamical system. Thus, we can apply Dirac's formalism of constrained Hamiltonian dynamics (Dirac 1964). Following the formalism elaborated by Willis *et al* (1986) one obtains the equations of motion for the dynamical variables X_j

$$M_j\ddot{X}_j + \tfrac{1}{2}\dot{X}_j^2\frac{\mathrm{d}M_j}{\mathrm{d}X_j} = -\frac{\partial U_j}{\partial X_j} \tag{3.5}$$

with

$$\frac{\partial U_j}{\partial X_j} = -\sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)\{\psi_{j,i+1}+\psi_{j,i-1}-2\psi_{j,i}+f_{j,i+1}+f_{j,i-1}-2f_{j,i}$$
$$-\frac{1}{a^2}\sin(\psi_{j,i}+f_{j,i})\} + \epsilon\sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)$$
$$\times\{\psi_{j',i+1}+\psi_{j',i-1}-2\psi_{j',i}+f_{j',i+1}+f_{j',i-1}-2f_{j',i}\} \tag{3.6}$$

and for the dressing $\psi_{j,i}$

$$\ddot{\psi}_{j,i} = \psi_{j,i+1}-2\psi_{j,i}+f_{j,i+1}+f_{j,i-1}-2f_{j,i}-\frac{1}{a^2}\sin(\psi_{j,i}+f_{j,i})+\psi_{j,i-1}-f_{j,i}^{(1)}(X_j)$$
$$\times\left\{\ddot{X}_j+\tfrac{1}{2}\dot{X}_j^2\frac{\mathrm{d}\ln M_j}{\mathrm{d}X_j}\right\}$$
$$+\epsilon(\psi_{j',i+1}+\psi_{j',i-1}-2\psi_{j',i}+f_{j',i+1}+f_{j'i-1}-2f_{j',i}) \tag{3.7}$$

where $(j,j')=(1,2)$ or $(2,1)$.

Since the parameter d, due to the slight deceleration or acceleration of one of the two coupled solitons, is considered to be small, one can write

$$f_{j,i}(X_j) \simeq f_{j',i}(X_{j'}) \pm d f_{j',i}^{(1)}(X_{j'}). \tag{3.8}$$

The plus sign is for $j=1$ and the minus sign for $j=2$.

In the case where the soliton width $a \gg b$, all $\psi_{j,i}$ approach zero. Then, after using the Taylor expansion of $f_{j,i\pm1}$ to the fourth-order derivative, that is

$$f_{j,i\pm1} \simeq f_{j,i} \pm f_{j,i}^{(i)} + \frac{1}{2!}f_{j,i}^{(2i)} \pm \frac{1}{3!}f_{j,i}^{(3i)} + \frac{1}{4!}f_{j,i}^{(4i)}$$

with the aid of (3.8) and the identity $f_{2,i}^{(2i)} = (1/a^2)\sin f_{j,i}$, (3.6) reduces to

$$\frac{\partial U_j}{\partial X_j} = F_j(X_j) + \epsilon G_j(X_j) \tag{3.9a}$$

where

$$F_j(X_j) = -\frac{2}{4!}\sum_{i=1}^{N} f_{j,i}^{(1)} f_{j,i}^{(4i)} \tag{3.9b}$$

and

$$G_j(X_j) = \sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)\left\{f_{j,i}^{(2i)} + \frac{2}{4!}f_{j,i}^{(4i)}\right\} \pm d\sum_{i=1}^{N} f_{j,i}^{(1)}(X_j)\left\{f_{j,i}^{(3i)} + \frac{2}{4!}f_{j,i}^{(5i)}\right\}. \tag{3.9c}$$

The notation $f_{j,i}^{(mi)}$ stands for the mth-order derivative of $f_{j,i}$ with respect to the integer i assumed for the circumstance to behave like a *continuous* real variable.

$F_j(X_j)$ and the first part of $G_j(X_j)$ are odd in X_j while the second part of $G_j(X_j)$ is even in X_j. Moreover, $F_j(X_j)$ and $G_j(X_j)$ are periodic functions in X_j with a period equal to the natural period b. Hence, we can expand these quantities in a Fourier series. After some algebraic calculations, we obtain the following results:

$$\frac{\partial U_j}{\partial X_j} = -\sum_{n=1}^{\infty}(F_{jn} + \sigma_1\sigma_2\epsilon G_{jn})\sin(2\pi n X_j) \pm \sigma_1\sigma_2\epsilon d\left(C_{j0} + \sum_{n=1}^{\infty} C_{jn}\cos(2\pi n X_j)\right) \tag{3.10a}$$

where

$$F_{jn} = \frac{1}{3a^2}\frac{4\pi^3 n^2}{\sinh(n\pi^2 a)}(2q_s + 1) \tag{3.10b}$$

$$G_{jn} = -F_{jn} - \frac{16\pi^2 n^2}{\sinh(n\pi^2 a)} \tag{3.10c}$$

$$C_{jn} = \frac{4\pi^2 n}{a^2\sinh(n\pi^2 a)}\left\{\frac{-16}{15a^2}(q_s+1)(q_s+4) + \frac{1}{3}\left(16 + \frac{40}{3a^2}\right)(q_s+1) - \left(4 + \frac{1}{3a^2}\right)\right\} \tag{3.10d}$$

and

$$C_{j0} = \frac{4}{a^3}\left(\frac{4}{3} - \frac{7}{45a^2}\right) \tag{3.10e}$$

with

$$q_s = \pi^2 n^2 a^2.$$

In formula (3.10a), we have the plus sign for $j = 1$ and the minus sign for $j = 2$. We have also found that the dimensionless mass $M_j(X_j)$ has a periodic structure like the potential energy U_j:

$$M_j(X_j) = M_{j0} + \sum_{n=1}^{\infty} M_{jn}\cos(2\pi n X_j) \tag{3.11a}$$

where

$$M_{j0} = 16/a \qquad \text{and} \qquad M_{jn} = \frac{16\pi^2 n}{\sinh(n\pi^2 a)}. \tag{3.11b}$$

It is clear that we have the same Fourier coefficients for $j = 1$ and for $j = 2$. Because of the presence of the hyperbolic sine functions in the denominators of the Fourier coefficients, the contribution of second-order harmonics or more can be neglected. Then, the equations of motion for the centres of the coupled solitons are coupled through a set of two non-linear differential equations in the form

$$M_1\ddot{X}_1 + \tfrac{1}{2}\dot{X}_1^2\frac{\mathrm{d}M_1}{\mathrm{d}X_1} = E_1\sin(2\pi X_1) - \sigma_1\sigma_2\epsilon(X_1 - X_2) \times (C_{10} + C_{11}\cos(2\pi X_1)) \tag{3.12a}$$

$$M_2\ddot{X}_2 + \tfrac{1}{2}\dot{X}_2^2\frac{\mathrm{d}M_2}{\mathrm{d}X_2} = E_1\sin(2\pi X_2) + \sigma_1\sigma_2\epsilon(X_1 - X_2) \times (C_{10} + C_{11}\cos(2\pi X_2)) \tag{3.12b}$$

where we have substituted d by $X_1 - X_2$ and

$$E_1 = (1 - \epsilon\sigma_1\sigma_2)F_{11} - \epsilon\sigma_1\sigma_2\frac{16\pi^3}{\sinh(\pi^2 a)}. \tag{3.13}$$

Setting $\epsilon = 0$ in (3.12), we obtain two uncoupled equations of motion for the solitons' centres. In the case where the distance between the two moving solitons is equal to zero ($d = 0$; $X_1 = X_2$), equations (3.12) reduce to a single equation, for example

$$M_1\ddot{X}_1 + \tfrac{1}{2}\dot{X}_1^2\frac{\mathrm{d}M_1}{\mathrm{d}X_1} = E_1\sin(2\pi X_1). \tag{3.14}$$

The quantity $E_{\mathrm{PN}} = E_1/\pi$ stands for the Peierls–Nabarro potential amplitude (Nabarro 1967). One can immediately see that the presence of the coupling between the chains induces a modification of the trapping potential. This modification is measured by the variation

$$E_{\mathrm{v}} = \frac{(E_1 - F_{11})}{\pi} = \frac{\epsilon\sigma_1\sigma_2 G_{11}}{\pi} \tag{3.15}$$

of the Peierls–Nabarro potential barrier.

The expression of E_{v} suggests that, when the two solitons have the same polarity (e.g. the kink–kink and antikink–antikink), the pinning potential barrier suffered by the kink is smaller than that experienced by a single soliton of a single sine–Gordon chain since $E_v < 0$. The opposite situation is observed when the polarities are different (e.g. the propagating solitons are a kink in the first chain and an antikink in the second chain). If it is assumed that $M_j \simeq M_{j0}$ since $M_{j1} \ll M_{j0}$, then from equation (3.14), one obtains the small-amplitude frequency W_p of the soliton in the potential well located at $X_j = \frac{1}{2}$ (the middle of a cell of the system)

$$W_p^2 = 2\pi E_1/M_{j0}. \tag{3.16}$$

The presence of the hyperbolic sine functions in the denominator of E_{PN} and W_p^2 make these quantities decrease exponentially when the soliton width a increases.

When $\psi_{j,i} \neq 0$, the full equation of dressing (3.7) has to be analysed. In the one-component field systems such as the sine–Gordon or ϕ^4 model, it has been shown that the dressing $\psi_{j,i}$ has important effects on dynamical properties such as the kink pinning frequency W_p, the depth of the Peierls–Nabarro potential and the spontaneous radiation of phonons by the moving kink (Combs and Yip 1983, Stancioff *et al* 1986, Boesch *et al* 1989). Section 4 which follows deals with the numerical investigation of the static form of the dressing equation (3.7) for certain special cases. The effect of the static solution for $\psi_{j,i}$ on dynamical properties of the soliton's motions is presented. The full dynamical equation will be analysed in a further paper.

4. Numerical analysis of static dressing: effects on the Peierls–Nabarro depth

When the soliton width is reduced to a few natural periods of the system, $\psi_{j,i}$ cannot be neglected in the calculation of the potential force $-\partial U_j/\partial X_j$. This section is devoted to the analysis of the effects of $\psi_{j,i}$, which accounts for the difference between the continuum and discrete shapes of the solitons, on the Peierls–Nabarro barrier. However, because of the complexity of the model, we have restricted our computations to some physically justifiable special cases.

The dressings in the static form verify the non-linear discrete equation:

$$\psi_{j,i+1} + \psi_{j,i-1} - 2\psi_{j,i} - \frac{1}{a^2}\sin(\psi_{j,i} + f_{j,i}) + f_{j,i+1} + f_{j,i-1} - 2f_{j,i}$$
$$+ \epsilon(\psi_{j',i+1} + \psi_{j',i-1} - 2\psi_{j',i} + f_{j',i+1} + f_{j',i-1} - 2f_{j',i}) = 0. \tag{4.1}$$

Since a similar equation can be written by changing the positions of j and j' it is easy to reduce (4.1) into the form

$$\psi_{j,i+1} + \psi_{j,i-1} - 2\psi_{j,i} - \frac{1}{a^2}\sin(\psi_{j,i} + f_{j,i}) + f_{j,i+1}$$
$$+ f_{j,i-1} - 2f_{j,i} + \frac{\epsilon}{a^2}\sin(\psi_{j',i} + f_{j',i}) = 0 \tag{4.2}$$

where we have used $\epsilon^2 \ll 1$.

Assuming that the $\psi_{j,i}$ are small enough to justify the expansion of the sine expression in the manner $\sin(\psi_{j,i} + f_{j,i}) \simeq \psi_{j,i}\cos f_{j,i} + \sin f_{j,i}$, equation (4.2) becomes

$$-\psi_{j,i+1} + \left(2 + \frac{1}{a^2}\cos f_{j,i}\right)\psi_{j,i} - \psi_{j,i-1} - \left(\frac{\epsilon}{a^2}\cos f_{j',i}\right)\psi_{j',i}$$
$$= f_{j,i+1} + f_{j,i-1} - 2f_{j,i} - \frac{1}{a^2}\sin f_{j,i} + \frac{\epsilon}{a^2}\sin f_{j',i}. \tag{4.3}$$

In matrix notation, equation (4.3) has the form

$$\mathbf{A}_j\psi_j + \mathbf{A}_{j'}\psi_{j'} = \mathbf{F} \tag{4.4}$$

where

$$\psi_j = (\ldots, \psi_{j,i}, \ldots) \qquad \psi_{j'} = (\ldots, \psi_{j',i}, \ldots)$$

$$\vdots$$

$$\mathbf{F} = \left(f_{j,i+1} + f_{j,i-1} - 2f_{j,i} - \frac{1}{a^2}\sin f_{j,i} + \frac{\epsilon}{a^2}\sin f_{j',i} \right)$$

$$\vdots$$

$$(A_j)_{ik} = -\delta_{i,k-1} + \left(2 + \frac{1}{a^2}\cos f_{j,i}\right)\delta_{i,k} - \delta_{i-1,k}$$

and

$$(A_{j'})_{ik} = \left(-\frac{\epsilon}{a^2}\cos f_{j',i}\right)\delta_{ik}$$

where δ_{ik} is the Kronecker delta.

Recalling that the coupled chains have the same physical parameters, we can correctly set $\psi_{j',i} = \psi_{j,i}(d = 0)$ when the two solitons have the same polarity and $\psi_{j',i} = -\psi_{j,i}$, when the polarities are different. Then equations (4.4) reduce to the tridiagonal matrix problem

$$\mathbf{A}\psi_j = \mathbf{F} \tag{4.5}$$

submitted to constraints (3.3) with the matrix elements $(A)_{ik}$ given by

$$(A)_{ik} = -\delta_{i,k-1} + \left(2 + \frac{1}{a^2}\cos f_{j,i} \mp \frac{\epsilon}{a^2}\cos f_{j',i}\right)\delta_{i,k} - \delta_{i-1,k}.$$

The negative (positive) sign corresponds to kink–kink (kink–antikink) propagation.

We have considered a system of N unit cells with $N = 200$. The solitons' centres are situated far from the extreme points of the system in order to avoid end effects. Since the dressings are localized around the solitons, we have truncated the matrix $\mathbf{A}$ by attributing the value zero to $\psi_{j,i}$ for all i which are not contained in the integer domain (int $(5a)$, N-int $(5a)$) where int $(5a)$ is the integer obtained from the conversion of real $5a$ to the integer type. The parameter a is the soliton width and therefore plays the role of the discreteness parameter. During the numerical calculation, we have observed that the magnitude of the constraint C_j increases with the coupling parameter. For instance, it does not exceed 2×10^{-8} for $\epsilon = 0$. For $\epsilon = 0.0001$, $C_j = 2 \times 10^{-5}$ and for $\epsilon = 0.01$, it reaches 7×10^{-4}. The ϵ-dependence of the constraint can be explained by this fact. When the coupling parameter increases, the distortion of the soliton's shape also increases so that for some range of the coupling parameter, the zero-order perturbation solution $f_{j,i}$ taken as the solitons' shape is invalid. Taking the first-order perturbation solution $f_{j,i} + \epsilon Y_i^1(\epsilon W_i^1)$, we have obtained a reduction in C_j by 5%. It is clear that the constraints C_j' are always satisfied since $\dot{\psi}_{j,i} = 0$.

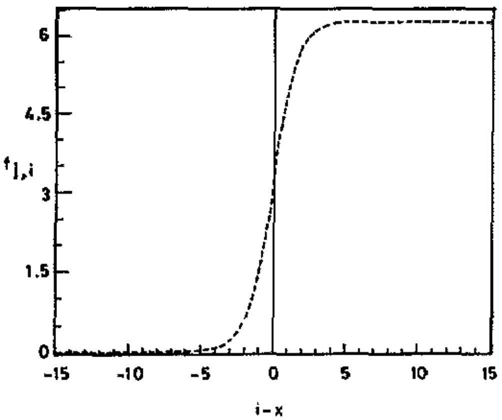

Figure 1. Shape of the continuum soliton $f_{j,i}$ plotted against $i - X$ for $a = 2$.

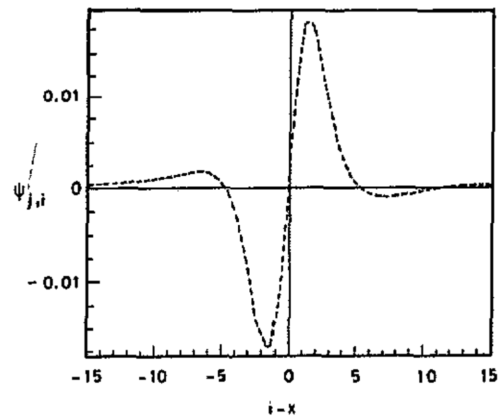

Figure 2. Static dressing $\psi_{j,i}$ as a function of the distance from the centre of the soliton for $a = 2$ and $\epsilon = 0.0005$.

When $\psi_{j,i}$ is added to the soliton shape, we observe that the deviation from the continuum shape given in the cell i by $f_{j,i}$ (figure 1) increases when a decreases. But the deviation still remains small even if a is reduced to one natural period of the system. Figure 2 shows the plot of the static dressing $\psi_{j,i}$ (which is a measure of the deviation from the continuum model) for $a = 2$ and $\epsilon = 0.0005$.

In the dynamical regime, it has been shown that the modification of the soliton's shape due to the discreteness is always accompanied by a strong emission of phonons. Consequently, this produces a decrease in the soliton velocity and the trapping processes (Currie *et al* 1977, Combs and Yip 1983, Peyrard and Kruskal 1984). In recent studies analysing the trapping potential in the ϕ^4 chain (Combs and Yip 1983) and in the sine–Gordon chain (Stancioff *et al* 1986), it was observed that the inclusion of the static dressing $\psi_{j,i}$ in the soliton solution lowers the potential and increases dramatically the depth of the potential. This yields incidentally the increase of the pinning frequency defined by (3.16). Similar results are obtained in the present paper.

In figure 3(a), we compared the Peierls–Nabarro barrier obtained numerically without dressing to that obtained with dressing for $1 \leqslant a \leqslant 2.5$. The figure shows an exponential decrease of the *barrier* as the soliton width increases. This decrease is also observed for large values of the kink width ($a \geqslant 2.5$). The square of the pinning frequency is plotted as function of kink width in figure 3(b). It appears from figure 3 that due to the inclusion of dressing, the Peierls–Nabarro barrier and the square of the pinning frequency are multiplied by a factor whose value is contained in the real interval (1.1, 1.3). The shapes of E_{PN} and W_{p} are in agreement with the theoretical predictions of section 3 where we obtained an exponential decay of E_{PN} (3.13). The modification of the potential amplitude given by the formula (3.16) has also been obtained in our numerical work. This suggests that in the case where both solitons have the same polarity, the trapping process is slightly reduced in a coupled system compared with what obtains in a single sine–Gordon lattice. When the polarities are different, the opposite holds, i.e. the trapping process is somewhat reduced in the single sine–Gordon lattice compared with the coupled system.

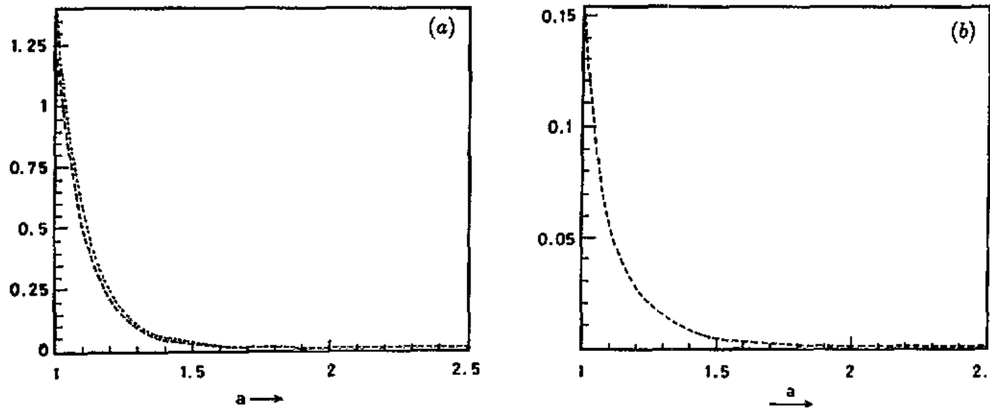

Figure 3. (*a*) Peierls–Nabarro barrier E_{PN} in hundreds as a function of kink width for $\epsilon = 0.0005$. The dotted curve is the dressed barrier and the broken curve is the barrier without dressing. (*b*) The pinning frequency W_p in hundreds obtained after inclusion of dressing as a function of kink width a for the same coupling constant as (*a*).

5. Conclusion

In the present paper, we have studied the effects of the discreteness of two weakly coupled sine–Gordon systems on the motion of the coupled solitons. After reviewing some analytical solutions of the systems in the continuum limit, we have carried out the collective coordinate method in which the coordinates X_j of the solitons' centres appear as dynamical variables. In addition, due to the discreteness, the continuum solitons' shapes were dressed by $\psi_{j,i}$. The variables X_j and $\psi_{j,i}$ have been expressed as functionals of the contiuum shape $f_{j,i}$ of the soliton by the requirement of constraining conditions. By using Dirac's formalism for constrained Hamiltonian systems, we have shown that the motion of the coupled solitons can be modelled by a set of two coupled non-linear differential equations.

An equation for the dressing $\psi_{j,i}$ has been obtained. We have analysed its static form. It has been shown that the inclusion of dressing effects considerably improves the accuracy in estimates of dynamical quantities such as the pinning frequency and the depth of the pinning potential.

At present, the full dynamical equation of dressing has not been analysed. It is hoped that the Green function method applied to the inhomogeneous partial differential equation resulting from a bound Taylor expansion of the dressing, will lead to an explicit time dependence for the energy potential. In an approximate calculation such as ours, it would be interesting to analyse the full non-linear dressing equation in a general way since, because of the coupling, the contribution of the non-linear terms might not be negligible. When this has been done, the application of the theory developed in this paper to some more complicated coupled models such as protein molecular chains, should lead to new important developments in the field of the propagation of coupled non-linear waves.

Due to the mathematical complexity of the coupled system, our model calculations have only covered a limited class of solitons (kink–kink and kink–antikink) solutions separated by a small distance parameterized by d. An analytical investigation for a possible generalization of our calculations to large values of parameter d is under consideration and will be published in a future work. Another interesting problem in connection with the discrete coupled chains is the analysis of the interaction between a topological soliton (kink or antikink) moving in one chain and the breather-like solution in the other chain.

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