Dynamics of solitary waves in diatomic chains with long-range Kac-Baker interactions

1993 J. Phys. A: Math. Gen. 26 6477

(http://iopscience.iop.org/0305-4470/26/22/041)

J. Phys. A: Math. Gen. 26 (1993) 6477–6491. Printed in the UK

Dynamics of solitary waves in diatomic chains with long-range Kac–Baker interactions

C Tchawoua, T C Kofane and A S Bokosah

Laboratoire de Mécanique, Faculté des Sciences, Université de Yaoundé, BP 812, Yaoundé, Cameroun

Received 19 November 1992, in final form 10 June 1993

Abstract. An analytical study of the influence of the long-range atomic interactions on the properties of soliton-like excitations in a one-dimensional (1D) anharmonic chain is presented. The model chosen is a nonlinear diatomic chain in which atoms are assumed to interact via a cubic and/or quartic nonlinear short-range potential and a linear long-range Kac–Baker type pair potential. In the continuum approximation, using scaling arguments, it is shown that the coupled nonlinear difference-differential equations for the motion of the two different masses can be decoupled and reduced to a generalized Boussinesq equation which admits supersonic and subsonic acoustic kink (pulse) solitons, long-wavelenth acoustic oscillating solutions of breather type and optical envelope type solitons of a nonlinear Schrödinger equation. A possible alternation of envelope and dark is found that can exist not only for acoustic mode but also for optical mode.

1. Introduction

The dynamics of nonlinear lattices and the related soliton-like excitations have been intensively studied since the introduction of solitons [1]. More recently, attempts have been made to study lattices, such as metals or ferroelectrics [2], in which long-range interatomic forces may be significant. Using a 1D lattice with long-range coupling of Lennard–Jones type, Ishimori [3] showed that the value of the force range parameter contributes not to the nonlinear term but to the dispersive terms in the equation of propagation in the continuum limit. In magnetic systems it is well known that in the presence of the phase transition in a 1D system, the model must consist of very long-range interaction forces [4]. A well studied example of long-range interaction potential is the so-called Kac–Baker [5, 6] potential in which the interactions between particles fall off exponentially as the distance between them increases. It is commonly encountered in systems undergoing phase transition and has been recently used to investigate thermodynamic properties, in connection with topological soliton excitations, of a 1D ϕ^4 system in continuum [7] as well as in discrete limits [8]. It has also been used to describe the dynamics of solitons in an anharmonic non-magnetic chain [9], a sine–Gordon system [10] and a magnetic Heisenberg-chain [11]. Most of the aforementioned studies have been limited to models with one atom per unit cell. These studies could also be applied to ferroelectric crystals like $SrTiO_3$, $BaTiO_3$ and $KTaO_3$ that have got a diatomic structure along their (100) direction and present structural phase transition, soft mode and central peak phenomena [12].

0305-4470/93/226477+15 $07.50

Since the pioneering work of Zubusky and Deem [13] on optical excitations in monoatomic chains, the study of nonlinear acoustic and optical excitations in diatomic chains has been of considerable interest [2, 14–23]. However, because of mathematical complexities, most of the models studied to date have been limited to one dimension and to nearest-neighbour interactions only.

This paper is devoted to a further study of the dynamics of nonlinear quasi-1D diatomic systems in which the long-range interaction of Kac–Baker type plays a significant role. In section 2, we present the model Hamiltonian and the derived equations of motion in the continuum approximation. In section 3 we apply a decoupling ansatz (section 3.1) to obtain the kink or pulse soliton solutions, the long-wavelength acoustic oscillatory excitations of breather type (section 3.2) and optical envelope type (section 3.3). The influence of long-range interactions on the conditions of existence of the soliton solutions of modulated-wave type are examined simultaneously. Section 4 gives concluding remarks and a brief summary.

2. The model Hamiltonian and equations of motion

We consider a 1D chain with two ions (atoms) of masses M_1 and M_2 per unit cell with a spacing of '$2a$' between cells (a is the lattice spacing). The Hamiltonian for the discrete lattice is taken to be

$$H=(1/2)\sum_n (M_1\dot{u}_n^2+M_2\dot{v}_n^2)+\sum_n (U_{1n}+U_{2n})$$

$$+(1/2)\sum_{n\neq j} (V_{1nj}(u_n-u_j)^2+V_{2nj}(v_n-v_j)^2) \tag{1}$$

where u_n, $\dot{u}_n(v_n, \dot{v}_n)$ are the displacement from the equilibrium position, respectively the velocity for odd (even) ions of masses M_1 (M_2) of the nth cell. These ions are assumed to interact through linear long-range pair potentials V_{1nj} and V_{2nj} and through nonlinear short-range potentials $U_{1n}(v_n-u_n)$ and $U_{2n}(u_{n+1}-v_n)$. V_{1nj} and V_{2nj} are taken to be the Kac–Baker form in which the interactions between ions fall off exponentially as $\exp(-\gamma|x|)$ as the distance x between them increases:

$$V_{1nj}=J_1\frac{(1-S)}{2S}S^{|n-j|} \tag{2a}$$

$$V_{2nj}=J_2\frac{(1-S)}{2S}S^{|n-j|}. \tag{2b}$$

The coefficients J_1 and J_2 are constants measuring the elastic energy of the lattice. The parameter $S=\exp(-\gamma)$ defines the range of interaction with $0\leqslant S<1$ and can be seen as a measure of the ratio $V_{1nj+1}/V_{1nj}(V_{2nj+1}/V_{2nj})$ of the elastic coupling coefficient between the nth and $(j+1)$th odd (even) ions on one hand, and the nth and jth odd (even) ions on the other. The absolute difference $|n-j|$ measures the distance between the odd (even) ions of cells n and j. The virtue of this interaction potential, commonly encountered in physical systems such as the Ising ferromagnetic lattice, is that the range of interaction can be varied continuously. Indeed, when S increases, the range of interaction (the coupling coefficient $V_{1nj}(V_{2nj})$ between the odd (even) ions on cells n and j) continuously increases. For a given S, $V_{1nj}(V_{2nj})$ decreases when $|n-j|$ increases. Experimentally, one can relate the parameter S to the number of neighbouring interactions. Due to the mathematical complexity and in order to model the physical situations where the weight of the long-range coupling is smaller than the short-range one, we have neglected long-range interactions between odd and even ions.

When $S=0$, the model reduces to a second nearest-neighbour problem. On the other hand, the limit $S\to 1$ defines the infinite-range problem. $V_{1nj}(V_{2nj})$ is constructed such that the total potential experienced by one ion due to all others is finite for all S so that a thermodynamic limit exists. Then we have

$$\sum_{j\neq n} V_{inj}=J_i \qquad (i=1,2). \tag{3}$$

The nonlinear short-range potentials between ions are a polynomial approximation to a realistic potential such as Lennard–Jones and Morse potentials and have the form

$$U_{1n}=\tfrac{1}{2}k_2(v_n-u_n)^2+\tfrac{1}{3}k_3(v_n-u_n)^3+\tfrac{1}{4}k_4(v_n-u_n)^4 \tag{4a}$$

$$U_{2n}=\tfrac{1}{2}k_2(u_{n+1}-v_n)^2+\tfrac{1}{3}k_3(u_{n+1}-v_n)^3+\tfrac{1}{4}k_4(u_{n+1}-v_n)^4 \tag{4b}$$

where k_2, k_3, k_4 are force constants. From Hamiltonian (1), the equations of motion for u_n and v_n are

$$M_1\ddot{u}_n=k_2(v_n-2u_n+v_{n-1})+k_3((v_n-u_n)^2-(u_n-v_{n-1})^2)+k_4((v_n-u_n)^3-(u_n-v_{n-1})^3)$$
$$-J_1\frac{(1-S)}{S}\sum_{j\neq n}S^{|j-n|}(u_n-u_j) \tag{5a}$$

$$M_2\ddot{v}_n=k_2(u_{n+1}-2v_n+u_n)+k_3((u_{n+1}-v_n)^2-(v_n-u_n)^2)+k_4((u_{n+1}-v_n)^3-(v_n-u_n)^3)$$
$$-J_2\frac{(1-S)}{S}\sum_{j\neq n}S^{|j-n|}(v_n-v_j). \tag{5b}$$

The overdots ($\cdot\cdot$) denote time differentiation.

Let

$$J_i\frac{(1-S)}{S}\sum_{j\neq n}S^{|j-n|}=2J_i \qquad (i=1,2)$$

and define the auxiliary quantities

$$L_{1n}=\ddot{u}_n+2\frac{J_1}{M_1}u_n-F_{1n} \tag{6a}$$

$$L_{2n}=\ddot{v}_n+2\frac{J_2}{M_2}v_n-F_{2n} \tag{6b}$$

where

$$F_{1n}=\frac{k_2}{M_1}(v_n-2u_n+v_{n-1})+\frac{k_3}{M_1}((v_n-u_n)^2-(u_n-v_{n-1})^2)+\frac{k_4}{M_1}((v_n-u_n)^3-(u_n-v_{n-1})^3) \tag{7a}$$

$$F_{2n}=\frac{k_2}{M_2}(u_{n+1}-2v_n+u_n)+\frac{k_3}{M_2}((u_{n+1}-v_n)^2-(v_n-u_n)^2)+\frac{k_4}{M_2}((u_{n+1}-v_n)^3-(v_n-u_n)^3). \tag{7b}$$

Equations (5) can be rewritten as

$$L_{1n}=\frac{J_1}{M_1}\frac{(1-S)}{S}\sum_{j\neq n}S^{|j-n|}u_j \tag{8a}$$

$$L_{2n}=\frac{J_2}{M_2}\frac{(1-S)}{S}\sum_{j\neq n}S^{|j-n|}v_j \tag{8b}$$

with L_{1n} and L_{2n} satisfying the recursive relations

$$(S+1/S)L_{1n}=L_{1n+1}+L_{1n-1}+\frac{J_1}{M_1}\frac{(1-S)}{S}(u_{n+1}+u_{n-1}-2Su_n) \tag{9a}$$

$$(S+1/S)L_{2n}=L_{2n+1}+L_{2n-1}+\frac{J_2}{M_2}\frac{(1-S)}{S}(v_{n+1}+v_{n-1}-2Sv_n). \tag{9b}$$

We can apply the continuum approximation to the displacement of each mass separately and write

$$\begin{aligned}
&u_n(t)\to u(x,t)\\
&v_n(t)\to v(x,t)\\
&L_{in}(t)\to L_i(x,t)\\
&F_{in}(u_n(t),v_n(t))\to F_i(u(x,t),v(x,t))\\
&u_{n+1}+u_{n-1}=2u+4a^2u_{xx}+(4/3)a^4u_{xxxx}+O(\varepsilon^{4+\alpha})\\
&v_{n+1}+v_{n-1}=2v+4a^2v_{xx}+(4/3)a^4v_{xxxx}+O(\varepsilon^{4+\alpha})\\
&L_{in+1}+L_{in-1}=2L_i+4a^2L_{ixx}+(4/3)a^4L_{ixxxx}+O(\varepsilon^{4+\alpha}).
\end{aligned} \tag{10}$$

In equation (10) ε is a small scaling parameter (ε is $O(a/10)$) such that $\partial/\partial x$ is $O(\varepsilon)$ and $\partial/\partial t$ is $O(\varepsilon)$ and we have neglected terms of higher order than $\varepsilon^{4+\alpha}$ ($\alpha=1,2$). The parameter α is determined by the balance of the highest-order dispersive and nonlinear terms. For the quartic potential ($k_3=0$) the fourth-order dispersive term and nonlinear term are balanced if u is $O(1)$, i.e. with $\alpha=1$, but for the cubic potential ($k_4=0$) if u is $O(\varepsilon)$, so that $\alpha=2$. Using these approximations where we keep terms up to fourth derivatives, equations (9a) and (9b) yield

$$\left(u-4a^2\frac{S}{(1-S)^2}u_{xx}\right)_{tt}=F_1+\frac{4a^2}{(1-S)^2}\left((1+S)\frac{J_1}{M_1}u_{xx}-SF_{1xx}\right)$$
$$+(4/3)\frac{a^4}{(1-S)^2}\left((1+S)\frac{J_1}{M_1}u_{xxxx}-SF_{1xxxx}\right) \tag{11a}$$

$$\left(v-4a^2\frac{S}{(1-S)^2}v_{xx}\right)_{tt}=F_2+\frac{4a^2}{(1-S)^2}\left((1+S)\frac{J_2}{M_2}v_{xx}-SF_{2xx}\right)$$
$$+(4/3)\frac{a^2}{(1-S)^2}\left((1+S)\frac{J_2}{M_2}v_{xxxx}-SF_{2xxxx}\right) \tag{11b}$$

where $F_1=F_1(u,v)$ and $F_2=F_2(u,v)$ are given in the appendix.

3. Soliton solutions in the continuum approximation

3.1. *The decoupling ansatz*

The two equations (11*a*) and (11*b*) are decoupled by using the following ansatz [1, 17, 22]

$$v=\sigma(u+b_1au_x+(b_2/2)a^2u_{xx}+(b_3/6)a^3u_{xxx}+(b_4/24)a^4u_{xxxx}+b_0a^4u_x^2u_{xx}). \qquad (12)$$

To determine the constants σ, b_1b_2, b_3, b_4 and b_0, the procedure is to substitute $v(x,t)$ and its derivatives in equations (11) and impose the condition that the two equations for $u(x,t)$ resulting from (11) are equivalent. In the continuum approximation there are two values for σ: $\sigma=1$ and $\sigma=-M_1/M_2$. By analogy with the linear chain $\sigma=1$ corresponds to an acoustic mode where the ions move in phase with slowly varying amplitudes. The value $\sigma=-M_1/M_2$ gives an optical mode where the ions move out of phase with amplitude ratios equal to σ. In the following, we shall examine each mode separately.

3.2. *Acoustic mode* ($\sigma=1$)

3.2.1. Kink and pulse soliton solutions. Following the procedure described earlier we can calculate the coefficients in (12) for the acoustic mode and obtain

$$\begin{aligned}
b_1&=1\\
b_2&=2M_0\left(1/M_1+J_0\frac{1+S}{(1-S)^2}\right)\\
b_3&=6M_0\left(\frac{2M_1-M_2}{3M_1M_2}+J_0\frac{1+S}{(1-S)^2}\right)\\
b_4&=24M_0\left((1/3)M_2-(b_2^2/4)M_1+J_0\frac{1+S}{(1-S)^2}\left(b_2/2+1/3+\frac{4S}{(1-S)^2}\right)\right)
\end{aligned} \qquad (13a)$$

with

$$M_0=M_1M_2/(M_1+M_2) \qquad (13b)$$

and

$$J_0=2(J_2/M_2-J_1/M_1)/k_2. \qquad (13c)$$

The nonlinear coefficient b_0 of (12) depends on the symmetry of nonlinear short-range potentials and has been determined for the case of the quartic potential ($k_3=0$ in (4)) and for the case of the cubic-quartic ($k_3\neq0$).

In the first case (quartic potential), the two equations arising from (11) are equivalent if b_0 is given by

$$b_0=-3M_0J_0\frac{(1+S)}{(1-S)^2}\,\frac{k_4}{k_2}. \qquad (14)$$

Then, one of the identical equations obtained is given by

$$u_{tt}-c^2(S)u_{xx}=3q(u_x)^2u_{xx}+h(S)u_{xxxx}+f(S)u_{ttxx}. \qquad (15)$$

For the case of the cubic-quartic potential, the two equations obtained from (11) are identical if the compatibility conditions

$$J_2/M_2 = J_1/M_1 \qquad \text{and} \qquad b_0 = 0 \tag{16}$$

are satisfied. With these conditions, the single equation obtained is of the form

$$u_{tt} - c^2(S)u_{xx} = 2pu_xu_{xx} + 3q(u_x)^2u_{xx} + h(S)u_{xxxx} + f(S)u_{ttxx} \tag{17}$$

which reduces to the form of a generalised Boussinesq (G-Bq) equation for $Z = u_x$ [9]

$$Z_{tt} - c^2(S)Z_{xx} = p(Z^2)_{xx} + q(Z^3)_{xx} + h(S)Z_{xxxx} + f(S)Z_{ttxx} \tag{18}$$

where

$$c^2(S) = (2k_2a^2/M_1)(b_2/2 + 2J_1(1+S)/k_2(1-S)^2) \tag{19a}$$

is the sound velocity

$$p = 2a^3k_3M_0/M_1^2 \tag{19b}$$

and

$$q = 2a^4k_4M_0/M_1^2 \tag{19c}$$

are the nonlinear coefficient while

$$h(S) = (2k_2a^4/M_1)(b_4/24 + 2J_1(1+S)/3k_2(1-S)^2 - 2Sb_2/(1-S)^2) \tag{19d}$$

and

$$f(S) = 4Sa^2/(1-S)^2 \tag{19e}$$

are the dispersion coefficients.

As expected, for $S = 0$ equation (18) reduces to the G-Bq equation, the well known limit of diatomic chain with nonlinear cubic and quartic interaction potential between first neighbours in the continuum approximation [22]. Moreover, the results of the monatomic chain are obtained if $M_1 = M_2$ [24]. An equation similar to (17) was derived recently by Roseneau [25] for a weakly nonlinear 1D lattice with N neighbouring interactions by using a method which correctly preserves the essential features of the discrete system. But no special link was assumed between the coupling coefficients of different neighbouring interactions. Consequently, the coefficient of the u_{xxtt} term, as well as that of the nonlinear interaction potential term, were given as sums over the N interacting particles. But in our equation (17), the coefficient of u_{xxtt} depends on the parameter S which measures the range of interaction. This is due to the exponential form (link) of the elastic coupling coefficients between the particles of the lattice.

Neglecting the Z^2 and Z^3 terms in (18) and looking for small amplitude solutions of the form $Z(x,t) = Z_0 \sin(kx - \omega t)$, we obtain the dispersion relation for the phonons

$$\omega^2 = (c^2k^2 - hk^4)/(1 + fk^2) \tag{20}$$

where ω and k denote respectively the frequency and the wavevector. Equation (20) shows that the value of the range parameter S mainly contributes to the form of the dispersion relation. The frequency ω^2 remains positive if k satisfies, for each value of S, the following condition

$$c^2 - hk^2 > 0.$$

Looking for soliton solutions of the form

$$Z = Z(x - vt) = Z(\xi) \tag{21}$$

the full nonlinear equation equation (18) yields

$$(v^2 - c^2(S))Z_{\xi\xi} = p(Z^2)_{\xi\xi} + q(Z^3)_{\xi\xi} + h'(S)Z_{\xi\xi\xi\xi} \tag{22}$$

where

$$h'(S) = h(S) + f(S)v^2. \tag{23}$$

The kink-type solutions for (22) are presented in [24]. The analytical expression for the general case ($p \neq 0$, $q \neq 0$) is given as

$$u(x, t) = \pm \operatorname{sgn}(h')(8h'/q)^{1/2} \tan^{-1}\left(\frac{1}{P_1} \tanh\left(\frac{x - vt}{L} + x_1\right)\right) \tag{24}$$

with

$$P_1 = \left(\frac{[4p^2 + 18q(v^2 - c^2)]^{1/2} \pm 2p}{[4p^2 + 18q(v^2 - c^2)]^{1/2} \mp 2p}\right)^{1/2} \tag{25}$$

and

$$L = 2(h'/(v^2 - c^2))^{1/2}. \tag{26}$$

In (24) x_1 defines the initial position of the soliton while v is the velocity. The width of the soliton depends on both P_1 and L. The $+(-)$ sign (in (24)) means that the soliton can produce rarefaction (compression) in the lattice. The parameter $\operatorname{sgn}(h') = \pm 1$ depending on the sign of h'. The two special cases $q = 0$ or $p = 0$ reduce to the Boussinesq (Bq) or Modified Boussinesq (M-Bq) solitons:

(i) Bq ($p \neq 0, q = 0$)

$$u(x, t) = \operatorname{sgn}(h')3((h'(v^2 - c^2))^{1/2}/p) \tanh\left(\frac{x - vt}{L} + x_1\right) \tag{27}$$

(ii) M-Bq ($p = 0, q \neq 0$)

$$u(x, t) = \pm 2(2h'/q)^{1/2} \tan^{-1}\left\{\exp\left(\frac{2}{L}(x - vt) + x_1\right)\right\}. \tag{28}$$

The width and the amplitude of these solutions depend on the range parameter S and may, respectively, increase and decrease as S increases [9, 10]. For $S = 0$, equation (24) reduces to the well-known soliton solution of the G-Bq equation for $M_1 \neq M_2$ [22] and for $M_1 = M_2$ [24]. As in the case of monoatomic chains [9], the analysis of the possible types of solutions for equation (27) allows us to find subsonic and supersonic kink (pulse) solitons of dilatational or compressive type, and the condition of existence of subsonic solitons for both cooperative and competitive short- and long-range interactions.

3.2.2. Soliton solutions in the weakly nonlinear case. In order to obtain the low amplitude breather solutions of equation (17) we use a simplified version of the expansion method [26]. We assume

$$u \to \varepsilon u_1 \tag{29}$$

where $\varepsilon \ll 1$, and introduce the slow space and time independent variables:

$$x_n = \varepsilon^n x \qquad t_n = \varepsilon^n t. \tag{30}$$

Accordingly, the displacement field $u(x, t)$ in (17) is regarded as $u(x_0, x_1, \ldots, t_0, t_1, \ldots)$ and the derivative operators $(\partial/\partial x)$ and $(\partial/\partial t)$ are expanded as

$$\begin{aligned} \partial/\partial x &= \partial/\partial x_0 + \varepsilon \partial/\partial x_1 + \cdots \\ \partial/\partial t &= \partial/\partial t_0 + \varepsilon \partial/\partial t_1 + \cdots . \end{aligned} \tag{31}$$

To simplify the terminology thereafter we write x for x_0, X for x_1, t for t_0, T for t_1 and u for u_1. Then we assume for u a modulated wave solution of the form [9, 27]

$$u = F_0(X, T) + (F(X, T)\,\mathrm{e}^{i\theta} + \mathrm{c.c}) + \varepsilon(F_1(X, T)\,\mathrm{e}^{2i\theta} + \mathrm{c.c}) \tag{32}$$

which contains a DC term, a first- and a second-harmonic. Here $\theta = kx - \omega t$, the frequency ω and the wavevector k are related by the dispersion relation given by (20). Substituting (29) and (32) into (17) and equating DC, first and second harmonic terms we obtain

$$\varepsilon^2(F_{OTT} + c^2 F_{OXX} - 2pk^2 |F|^2_X) + O(\varepsilon^3) = 0 \tag{33a}$$

$$\begin{aligned} \{\varepsilon((-2ikc^2 + 4ihk^3 + 2ifk\omega^2)F_X - 2i\omega(1 + fk^2)F_T) \\ + \varepsilon^2((1 + fk^2)F_{TT} + (f\omega^2 + 6hk^2 - c^2)F_{XX} - 4fK\omega F_{XT} \\ - 4ipk^3 F^* F_1 + 2pk^2 F F_{OX} + 6k^4 q |F|^2 F)\}\mathrm{e}^{i\theta} + O(\varepsilon^3) = 0 \end{aligned} \tag{33b}$$

$$\{\varepsilon((-4\omega^2 + 4k^2c^2 - 16hk^4 - 16fk^2\omega^2)F_1 + 2ipk^3(F)^2)\}\mathrm{e}^{2i\theta} + O(\varepsilon^2) = 0. \tag{33c}$$

From (33) and introducing new scales

$$\xi = x - v_g T \qquad \tau = \varepsilon T \tag{34}$$

with

$$v_g = (\mathrm{d}\omega/\mathrm{d}k) = \frac{k}{\omega}\,\frac{(c^2 - 2hk^2 - hfk^4)}{(1 + fk^2)^2}. \tag{35}$$

we obtain

$$F_1 = 2ipk^3(F)^2/(4\omega^2 - 4k^2c^2 + 16hk^4) \tag{36}$$

and

$$F_{O\xi} = \frac{2k^2 p}{v_g^2 - c^2}(|F|^2 + \eta) \tag{37}$$

where η is the integration constant, subject to the following nonlinear equation:

$$-iF_\tau + PF_{\xi\xi} + Q|F|^2 F + B'F = 0 \tag{38}$$

with

$$P = \frac{k^2}{2\omega}\,\frac{(fc^2 + h)(c^2 - 2hk^2 + hfk^4)}{(c^2 - hk^2)(1 + fk^2)^3} \tag{39a}$$

$$Q = \frac{pk^2}{\omega}\left(\frac{p}{3(fc^2 + h)} + \frac{2pk^2}{(v_g^2 - c^2)(1 + fk^2)}\right) + 3\frac{k^4}{\omega} q \tag{39b}$$

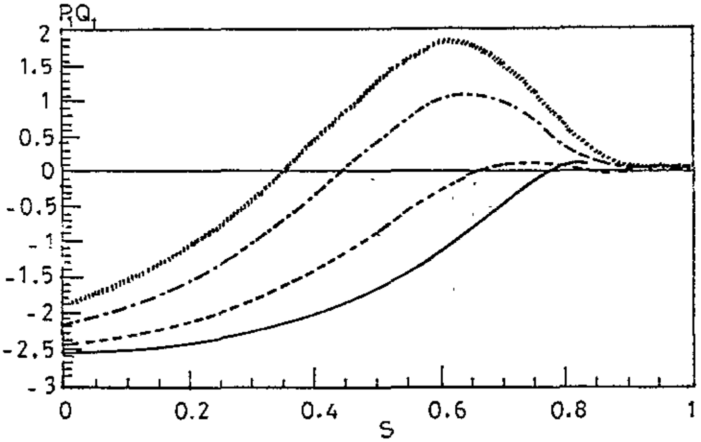

Figure 1. (Acoustic mode.) Plot of the quantity $P_1Q_1 = PQ\omega^2(1-fk^2)$ as a function of the range parameter S and for different values of $J_i\,(i=1,2)$ with $M_1=2M_2=1$, $k=0.2$, $k_2=k_3=k_4=1$ and $a=1$. Solid line: $J_1=2J_2=-0.005$; dashed line: $J_1=2J_2=0.01$; dotted-dashed line: $J_1=2J_2=0.05$; dotted line: $J_1=2J_2=0.1$.

and

$$B' = \frac{p^2k^4}{\omega(v_g^2-c^2)(1+fk^2)}\eta. \tag{40}$$

Putting

$$F = G\exp(-iB'\tau) \tag{41}$$

equation (38) yields the cubic nonlinear Schrödinger (NLS) equation

$$-iG_\tau + PG_{\xi\xi} + Q|G|^2G = 0. \tag{42}$$

The signs of the dispersive coefficient P and nonlinear coefficient Q determine the character of the solutions of (42). If $PQ<0$, equation (42) has an envelope soliton solution which has a vanishing amplitude at $|\xi|\to\infty$. If $PQ<0$, a typical solution of (42) is a dark (or envelope hole) soliton where the depression of an envelope propagates as a soliton with a finite amplitude at $|\xi|\to\infty$.

In figure 1, we plot the variations of the quantity PQ (multiplied by $4\omega^2(1+fk^2)$ which is always positive) as a function of the range parameter S, for different values of $J_i\ (i=1,2)$, and for $k_2=k_3=k_4=1$, $M_1=2M_2=1$, $a=1$, and $k=0.2$.

For $J_1=2J_2=1$ $(1=0.1, 0.05, 0.01)$, PQ can be alternately negative and positive as S increases. When $J_1=2J_2=-0.005$ (negative) we have $PQ<0$ for $0\leqslant S\leqslant 0.77$ and $PQ>0$ for $0.77<S\leqslant 0.83$ (the case $S>0.83$ is not physical because it gives $c^2<0$). When $J_1=2J_2=-0.1$ we have $PQ<0$ for $0\leqslant S\leqslant 0.38$ and $c^2<0$ for $S>0.38$. These results, although strictly valid only in the continuum approximation (small-k limit), show a new possible alternation of envelope and dark-soliton solutions which depends strongly on the long-range interactions (values of J_i and S). This alternation of solution can be obtained not only for competitive interactions ($J_i<$, $k_2>0$) as in the case when first and second-neighbour interactions are present, but also for cooperative interactions ($J_i>0$. $k_2>0$) [22].

Let us now give an explicit solution for the case $PQ>0$.

For $PQ>0$ the envelope soliton solution of (42) is given by [28, 29]

$$G(\xi,\tau) = A\,\mathrm{sech}((Q/2P)^{1/2}A(\xi-u_e\tau))\exp(-i(u_e/2P)(\xi-u_c\tau)) \tag{43}$$

where A is the amplitude

$$A=((u_e^2-2u_e u_c)/(2PQ)) \tag{44}$$

where $u_e^2-2u_e u_c>0$, and u_e and u_c are the velocities of the envelope and the carrier waves. In the present case we obtain $B'=0$ from (40) because we have localized the solution such that $F_{0\xi}$, F and its derivatives tend to zero for $|\xi|\to\infty$. From equations (41), (34), (30) and (29) one can calculate

$$F\,e^{i(kx-\omega t)}=A\,\mathrm{sech}((x-V_e t)/L_e)\,e^{i(Kx-\Omega t)} \tag{45}$$

with

$$V_e=v_g+\varepsilon(u_e/P) \tag{46a}$$

$$K=k-\varepsilon(u_c/2P) \tag{46b}$$

$$\Omega=-(\varepsilon u_e/2P)(v_g+\varepsilon u_c/P)+\omega \tag{46c}$$

and where the quantity

$$L_e=\frac{2P}{\varepsilon(u_e^2-2u_e u_c)^{1/2}} \tag{46d}$$

is the width of the envelope.

Substituting expression (43) in (37) and integrating one obtains

$$F_0=\chi A(2P/Q)^{1/2}\tanh((AQ/2P)(\xi-u_e\tau/P))+D \tag{47}$$

where D is the integration constant. Thus from (31) we obtain

$$u=\varepsilon A_m\tanh((x-V_e t)/L_e)+\varepsilon A\,\mathrm{sech}((x-V_e t)/L_e)\cos(Kx-\Omega t) \\ +\varepsilon^2 A_m\,\mathrm{sech}^2((x-V_e t)/L_e)\sin(2(Kx-\Omega t)) \tag{48}$$

where

$$A_m=A\frac{2k^2p}{v_g^2-c^2}(2P/Q)^{1/2}. \tag{49}$$

Equation (48) has the form of an asymmetric envelope, i.e. the amplitude at infinity is finite and of opposite sign at $x=\pm\infty$. It is a superposition of a kink (DC term) and envelope solitons coupled and both moving at velocity V_e.

3.3. Optical mode ($\sigma=-M_1/M_2$)

Following the paper by Pnevmatikos *et al* [22], the compatibility condition is only possible if the cubic term of the interaction potential is set to zero ($k_3=0$). In this case we keep only terms to $O(\varepsilon^3)$ so that the terms uu_x^2 and u^2u_{xx} are of (ε^5) and can be omitted if their coefficients are of $O(1)$.

From the compatibility condition we obtain

$$b_1=1$$

$$b_2=2M_0\left(1/M_2-J_0\frac{1+S}{(1-S)^2}\right) \tag{50}$$

$$b_3=b_4=b_0$$

where M_0 and J_0 are given, respectively, by (13b) and (13c).

The equation for $u(x, t)$ is

$$u_{tt} + c_1(S)u_{xx} + c_2 u + c_3 u^3 = 0 \tag{51}$$

where

$$c_1(S) = 2\frac{k_2 a^2}{M_1 + M_2}\left(1 - \frac{2}{k_2}\left(J_1\frac{M_2}{M_1} + J_2\frac{M_1}{M_2}\right)\frac{(1+S)}{(1-S)^2} - \frac{4S}{(1-S)^2}\frac{(M_1+M_2)^2}{M_1 M_2}\right) \tag{52a}$$

$$c_2 = 2k_2\frac{(M_1 + M_2)}{M_1 M_2} \tag{52b}$$

$$c_3 = 2k_4\frac{(M_1 + M_2)^3}{M_1 M_2}. \tag{52c}$$

As expected, for $S = 0$

$$c_1 = 2\frac{k_2 a^2}{M_1 + M_2}\left(1 - \frac{2}{k_2}\left(J_1\frac{M_2}{M_1} + J_2\frac{M_1}{M_2}\right)\right) \tag{53}$$

and the equation (51) reduces to the Pnevmatikos *et al.* form [22]. We shall discuss the various solutions of equation (51).

If $c_2 < 0 (k_2 < 0)$, $c_3 > 0$ and $c_1 < 0$ there are kink solutions for u [30]

$$u(x, t) = u_0 \tanh\left(\frac{x - vt}{L} + x_0\right) \tag{54}$$

with

$$u_0 = \pm(-c_2/c_3)^{1/2} \tag{55}$$

and

$$L = (2(|c_1| - v^2)/|c_2|)^{1/2}. \tag{56}$$

As in the previous mode (acoustic mode), the width of the topological kink obtained here depends on the range parameter and may increase as S increases [10].

If $c_2 > 0$, we can find oscillating solutions by transforming (51) into a nonlinear Shrödinger (NLS) equation for the slowly varying complex envelope function $\phi(x, t)$ if we look for solutions of the form

$$u(x, t) = \phi(x, t)\exp(i(kx - \omega t)) + cc \tag{57}$$

where k and ω are chosen to satisfy the linear dispersion relation

$$\omega^2(k) = c_2^2 - c_1 k^2 \tag{58}$$

at the centre of the Brillouin zone ($k \neq 0$) for the optical branch. Working in a reference frame moving with the group velocity $v_g = d\omega/dk$, we obtain from (51) and (57) a NLS equation for the first harmonic $\phi(\xi, \tau)$, with

$$\xi = x - v_g t \qquad \text{and} \qquad \tau = \varepsilon t \tag{59a}$$

$$i\phi_\tau + \tfrac{1}{2}\mu\phi_{\xi\xi} + \phi|\phi|^2 = 0 \tag{59b}$$

where we neglect terms like $\phi_{\tau\tau}$, and $\mu = (d^2\omega/dk^2)$ is related to the dispersion while

$$Q_0 = -3c_3/2\omega. \tag{60}$$

We note that, for $S=0$, equation (59) reduces to the Pnevmatikos *et al.* form [22]. For $\mu Q_0>0$ ($c_1c_3>0$) it admits envelope solutions which, for the discrete diatomic chain, define spatially localized envelope solitons in the form of a wavepacket with an envelope function that modulates an essentially harmonic carrier wave. For $\mu Q_0<0$ ($c_1c_3>0$) we have dark solitons where the envelope has a finite amplitude as $|\xi|\to\infty$ and a compression near the soliton position.

In figure 2, we plot the variations of the quantity μQ_0 as a function of the range parameter S, for different values of J_i ($i=1,2$), and for $k_2=k_4=1$, $M_1=M_2=1$, $a=1$ and $k=0,2$.

For $J_1=2J_2=l$ ($l=0.1$, 0.05, -0.1), the quantity μQ_0 decreases and changes sign as S increases. For small values of S ($S\leqslant 0.1$), μQ_0 is positive, when $S>0.1$, μQ_0 is negative. As in the previous case (acoustic mode), the above results show a new possible alternation of envelope and dark soliton solutions which can be obtained for both competitive ($J_i<0$, $k_2>0$) and cooperative ($J_i>0$, $k_2>0$) short- and long-range interactions. Let us now give explicit solutions for the case $\mu Q_0>0$.

For $\mu Q_0>0$ the envelope soliton solution of (59) is given by [28, 29]

$$\phi(\xi,\tau)=A\,\mathrm{sech}((Q/2P)^{1/2}A(\xi-u_e\tau)\exp(-\mathrm{i}(u_e/2P)(\xi-u_c\tau)) \qquad (61)$$

where A is the amplitude

$$A=((u_c^2-2u_eu_c)/(2PQ))^{1/2} \qquad (62)$$

where $u_e^2-2u_eu_c>0$, and u_e and u_c are the velocities of the envelope and the carrier waves. From equations (57), (59*a*), (61) and (62) we then obtain the symmetric envelope solution

$$u=\varepsilon A\,\mathrm{sech}((x-V_et)/L_e)\cos(Kx-\Omega t) \qquad (61)$$

with

$$V_e=v_g+\varepsilon(u_e/P) \qquad (62a)$$

$$K=k-\varepsilon(u_e/2P) \qquad (62b)$$

$$\Omega=-(\varepsilon u_e/2P)(v_g+\varepsilon u_c/P)+\omega \qquad (62)$$

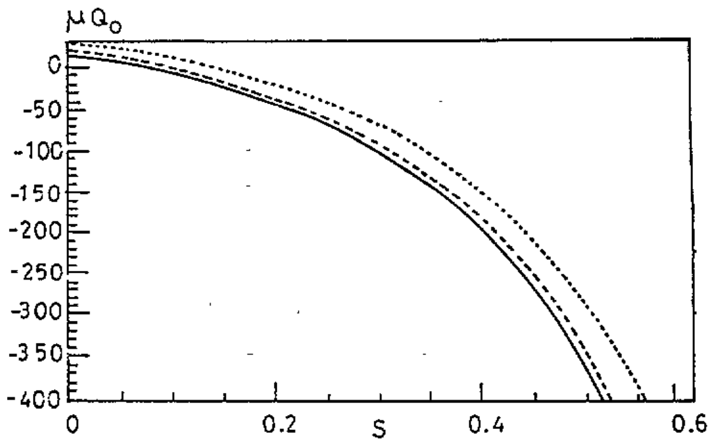

Figure 2. (Optical mode.) Plot of the quantity μQ_0 as a function of the range parameter S and for different values of J_i ($i=1,2$) with $M_1=2M_2=1$, $k=0.2$, $k_2=k_3=k_4=1$ and $a=1$. Solid line: $J_1=2J_2=-0.1$; dashed line: $J_1=2J_2=0.05$; dotted line: $J_1=2J_2=-0.1$.

and where the quantity

$$L_e = \frac{2P}{\varepsilon(u_e^2 - 2u_c u_e)^{1/2}} \tag{62c}$$

is the width of the envelope.

In contrast to the previous case (acoustic envelope), equation (61) has the form of a symmetric envelope. For $S=0$, it reduces to the result obtained for a diatomic chain with first and second nearest interactions [22].

4. Concluding remarks and brief summary

In this paper we have studied the effect of long-range interactions on acoustic and optical soliton-like excitations in a nonlinear (1D) diatomic lattice model in which the atoms were assumed to interact via a cubic and/or quartic nonlinear short-range pair potential and linear long-range pair potential. This long-range coupling falls off exponentially as the interparticle distance increases and has the virtue that the range of interactions can be varied continuously in a controlled manner.

We first used the continuum approximation which leads to nonlinear coupled equations for the displacement fields of the two different masses. We applied a decoupling ansatz to reduce, in the small-amplitude limit, these equations of motion to the well known generalized Boussinesq equation (GBq) which admits acoustic and optical soliton solutions.

In acoustic mode, both supersonic and subsonic kink (pulse) solitons of dilatational or compressive type are found. The subsonic soliton can exist for both cooperative and competitive short- and long-range interactions. Considering the small-amplitude nonlinear oscillations and using the multiple-scale expansion technique, we have derived a cubic NLS equation of motion for the first-harmonic term of the displacement. The analysis of the sign of the dispersive and nonlinear coefficients of this equation shows a possible alternation of envelope and dark soliton solutions which depends on the long-range interactions. It can be observed for both competitive and cooperative short- and long-range coupling. The modulated wave solution of the asymmetric envelope were calculated. Similar results have been obtained for the (1D) monoatomic lattice model [9].

In optical mode, considering the small-amplitude nonlinear wave, we have derived a ϕ^4 equation or, after using the multiple-scale expansion technique, a NLS equation which allow us to calculate, respectively, optical kink or symmetric envelope solutions. As in the acoustic mode, the analysis of the sign of the dispersive and nonlinear coefficients of the NLS equation shows a possible alternation of envelope and dark soliton solutions which can be observed for both competitive and cooperative short- and long-range coupling. An interesting problem related to these results is that a nonlinear system which supports envelope solitons is known to exhibit modulation instability. Consequently, the results obtained above reveal clearly that the long-range interactions will also control the modulation instability regimes. Another important point to outline is that, by setting $S=0$, our results reduce to those obtained from the model with first and second neighbour interactions.

In order to partially take into account the lattice effects that will occur in a real condensed matter system, it should be interesting to extend the study using the semi-discrete limit in which the envelope of a soliton is determined in the continuum limit while the fast oscillations of the quasi-harmonic carrier inside the envelope are treated exactly.

Appendix

The quantities F_1 and F_2 used in equations (11) are given as

$$
\begin{aligned}
F_1=\frac{2k_2}{M_1}\{ & v-u-av_x+a^2v_{xx}-\tfrac{2}{3}a^3v_{xx}-\tfrac{2}{3}a^3v_{xxx}+\tfrac{1}{3}a^4v_{xxxx}\} \\
& +\frac{4k_3}{M_1}\{(v-u)(av_x-a^2v_{xx}+\tfrac{2}{3}a^3v_{xxx}-\tfrac{1}{3}a^4v_{xxxx}) \\
& -a^2v_x^2-a^4v_{xx}^2+2a^3v_xv_{xx}-\tfrac{4}{3}a^4v_xv_{xxx}\} \\
& +\frac{2k_4}{M_1}\left\{(v-u)^3-3(v-u)^2\left(av_x-a^2v_{xx}+\tfrac{2}{3}a^3v_{xxx}-\frac{a^4}{3}v_{xxxx}\right)\right. \\
& \left.+6(v-u)(a^2v_x^2+a^4v_{xx}^2-2a^3v_xv_{xx}+\tfrac{4}{3}a^4v_xv_{xxx})-4a^3v_x^3+12a^4v_x^2v_{xx})\right\}
\end{aligned}
$$

$$
\begin{aligned}
F_2=\frac{2k_2}{M_2} & \left\{u-v+au_x+a^2u_{xx}+\tfrac{2}{3}a^3u_{xxx}+\frac{a^4}{3}u_{xxxx}\right\} \\
& +\frac{4k_3}{M_2}\left\{(u-v)\left(au_x+a^2u_{xx}+\tfrac{2}{3}a^3u_{xxx}+\frac{a^4}{3}u_{xxxx}\right)\right. \\
& \left.+a^2u_x^2+a^4u_{xx}^2+\tfrac{4}{3}a^4u_xu_{xxx}+2a^3u_xu_{xx}\right\} \\
& +\frac{2k_4}{M_2}\left\{(u-v)^3+3(u-v)^2\left(au_x+a^2u_{xx}+\tfrac{2}{3}a^3u_{xxx}+\frac{a^4}{3}u_{xxxx}\right)\right. \\
& \left.+6(u-v)(a^2u_x^2+a^4u_{xx}^2+2a^3u_xu_{xx}+\tfrac{4}{3}a^4u_xu_{xxx})+4a^3u_x^3+12a^4u_x^2u_{xx}\right\}.
\end{aligned}
$$

References

[1] Zabusky N J and Kruskal M D 1965 *Phys. Rev. Lett.* **15** 240
[2] Büttner H and Bilz H 1978 *Solitons and Condensed Matter Physics* eds A R Bishop and T Schneider (Berlin: Springer)
[3] Ishimori Y 1982 *Prog. Theor. Phys.* **68** 402
[4] Van Hove L 1949 *Physica* **15** 951
[5] Baker G A Jr 1961 *Phys. Rev.* **122** 1477
[6] Kac A M and Helfand B C 1973 *J. Math. Phys.* **4** 1078
[7] Sarker S K and Krumhansl J A 1981 *Phys. Rev.* B **23** 2374
[8] Woafo P, Kofane T C and Bokosah A S 1991 *J. Phys: Condens. Matter* **4** 3389
[9] Remoissenet M and Flytzanis N 1985 *J. Phys. C.: Solid State Phys.* **18** 1573
[10] Woafo P, Kenne J R and Kofane T C 1993 *J. Phys: Condens. Matter* **5** L123
[11] Ferrer R 1989 *Phys. Rev.* B **40** 1107

[12] Büttner H and Bilz H 1981 *Recent Developments in Condensed Matter Physics* vol 1 ed J T Devreese (New York: Plenum) p 49
[13] Zabusky N J and Deem G S 1967 *J. Comput. Phys.* **2** 126
[14] J. Tasi and M. J. P. Musgrave 1976 *J. Mech. Phys. Solid* **24** 43
[15] Yajima N and Satsuma J 1979 *Prog. Theor. Phys.* **62** 370
[16] Flytzanis N 1981 *Phys. Lett.* **85** A 353
[17] Dash P C and Patnaik K 1981 *Phys. Rev.* A **23** 959
[18] Dash P C and Patnaik K 1981 *Prog. Theor. Phys.* **65** 1526
[19] Henry B I, Oitmaa J and Revzen M 1982 *Solid State Commun.* **44** 511
[20] Pnevmatikos St, Remoissenet M and Flytzanis N 1983 *J. Phys. C: Solid State Phys.* **16** L305
[21] Henry B I and Oitmaa J 1985 *Solid State Commun.* **55** 587
[22] Pnevmatikos St, Flytzanis N and Remoissenet M 1986 *Phys. Rev.* B **4** 2308
[23] Dikande A M and Kofane T C 1991 *Phys. Lett.* **155A** 403
[24] Flytzanis N, Pnevmatikos St and Remoissenet M 1985 *J. Phys. C: Solid State Phys.* **18** 4603
[25] Roseneau Ph. 1987 *Phys. Rev.* B **36** 5868
[26] Kawahara T 1973 *J. Phys. Soc. Japan* **35** 1537
[27] Varma C M 1976 *Phys. Rev.* B **14** 244
[28] Hasegawa A 1975 *Plasma Instabilities and Nonlinear Effects* (Berlin: Springer)
[29] Scott A S, Chu F Y F and Mclaughlin D W 1973 *Proc. IEEE* **61** 1443
[30] Krumhansl A and Schrieffer J R 1975 *Phys. Rev.* B **11** 3535