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Kink dynamics in a lattice model with long-range interactions

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Abstract

This paper proposes a one-dimensional lattice model with long-range interactions which, in the continuum, keeps its nonlocal behaviour. In fact, the long-time evolution of the localized waves is governed by an asymptotic equation of the Benjamin–Ono type and allows the explicit construction of moving kinks on the lattice. The long-range particle interaction coefficients on the lattice are determined by the Benjamin–Ono equation.

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1. Introduction

This paper is concerned with the effects of long-range interactions in the behaviour of solitons (kinks) in a lattice system. In particular, we show that the introduced lattice model asymptotically leads to a nonlocal continuum equation. By nonlocal we mean the model where the localized solution is of the order of the scale parameter (i.e. the parameter which has the dimension of length), and thus it is physically acceptable to consider wavelengths comparable with the scale parameter. Its equation of motion contains integral, integro-differential or finite difference operators in the spatial variables, while the wave propagation velocity depends on the wavelength. In the present model there are two characteristic lengths: (a) the lattice spacing and (b) the radius of particle interaction range.

The nonlocal models can be divided into two classes: discrete and continuous. For specific cases, it is simpler and easier to use the quasicontinuum description of the discrete medium. Its essence is an interpolation of functions of discrete argument by a special class of analytic functions in such a way that a correspondence condition between the quasicontinuum and the discrete medium is fulfilled. The advantages of such an approach is the description of discrete and continuum media within a unified formalism and their correct generalization. In that case the quasicontinuum model is also applicable to macrosystems. Analytic solutions valid for

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wide nonlinear excitations have been obtained using the continuum approximation in [1, 2] and the quasicontinuum approximation in [3–5]. In particular, in [1, 6] it has been shown that very narrow soliton-like excitations can propagate without any energy loss due to discreteness effects.

The lattice model we study possesses an inherent nonlocal behaviour, i.e. the motion of a particle at node n depends on the motion of its neighbours. Such models for different kinds of particle interactions have been studied in a series of papers [7–9]. Thus far the classical procedure for studying them, at the continuum limit, is to assume slowly varying fields and expand them using Taylor's series. Then, approximate partial differential equations for the continuous fields were obtained.

In this paper, we show how to keep the nonlocal behaviour of the lattice model at the continuum level, or in other words, how to describe the nonlocality at the continuum level. This transition from the continuum to the discrete system with long-range interactions and vice versa is straightforward due to the quasicontinuum approximation. The idea of preserving the nonlocality at the continuum limit occurs in condensed-matter physics to describe phase transition in crystals, nonlinear waves in crystals and biological molecules. For example, modified versions of the discrete nonlinear Schrödinger equation which keep the nonlocality at the continuum and describe problems in biomolecules have been studied in the past [10, 11].

It is worthwhile mentioning some interesting studies of anharmonic atomic chains including long-range interactions due to large Coulomb coupling between particles [12–15]. The long-range potential is of the inverse power-type or Kac–Baker form. In the case of inverse power type of the fourth order, the continuum limit yields an integro-differential equation involving a Hilbert transform [15]. Using a perturbative technique the authors derive a mixed modified Korteweg–de-Vries with Benjamin–Ono equations [15], which is close to the result presented in what follows.

This paper is organized as follows: in section 2 we introduce the lattice model, while in section 3 we deal with its continuum approximation and show that it leads to the Benjamin–Ono equation for long-time evolution. In section 4, we derive the type of long-range particle interactions on the lattice using the fact that the lattice model asymptotically leads to the Benjamin–Ono equation. Finally, numerical simulations of the discrete model based on the Benjamin–Ono soliton are given and discussed in section 5.

2. The lattice model

We consider a one-dimensional lattice with mass M, lattice spacing b and long-range interactions. The Lagrangian of the system is

$$\mathcal{L} = \sum_n \tfrac{1}{2} M \dot{u}_n^2 - \sum_{nn'} \tfrac{1}{4} \Psi(n-n')\ (u_n - u_{n'})^2 - \sum_n \tfrac{1}{3} k_3 (u_{n+1} - u_n)^3. \quad (2.1)$$

Figure 1 presents a one-dimensional chain of masses and springs with second neighbour interactions.

The equations of motion obtained from the variation of (2.1) are

$$M\ddot{u}_n = \sum_{m=1}^{\mathcal{M}} \Psi(m)\,(u_{n+m} + u_{n-m} - 2u_n) + k_3\big[(u_{n+1} - u_n)^2 - (u_n - u_{n-1})^2\big] \quad (2.2)$$

where k_3 is a positive constant ($k_3 < 1$). $\Psi(n)$ are the interaction coefficients of the particles, related to the force constants $\Phi(n)$ (see equation (2.4)) which determine the effective characteristics of the elastic bonds between the particles. The lattice parameters $\Psi(n)$ can be obtained from the interaction potential between particles or atomic bonds in crystals (the same

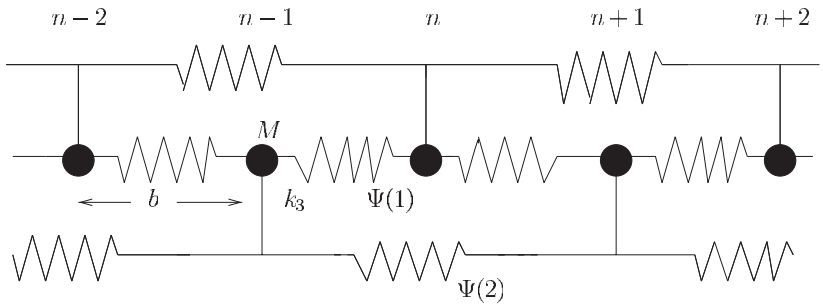

Figure 1. A one-dimensional atomic chain of masses and springs with first and second neighbour interactions.

as for $\Phi(n)$), e.g. the Born–Meyer potential, the Morse potential, the Lennard–Jones potential, the covalent potential, etc.

Here, we consider the chain to be homogeneous and so, the unique definition of $\Phi(n)$ leads to the identity $\Phi(n) = \Phi(-n)$. If $\Phi(n)$ differs from zero for $|n| \leqslant \mathcal{M}$, then every particle interacts with $\mathcal{M}$ neighbours to the right and to the left. The case $\mathcal{M} = 1$ corresponds to the simplest model of interaction between first nearest neighbours; while in real mechanical systems the action at a distance is always restricted, i.e. $\mathcal{M}$ is finite.

The distances between the particles do not change and therefore the forces acting on them are equal to zero [16]. This leads to the following condition for the force constants:

$$\Phi(0) = -\sum_{n}{}' \Phi(n) \tag{2.3}$$

where $\sum_n'$ means the summation over all $n \neq 0$. This equation is deduced from the lattice energy invariance, i.e. the invariance by translation of the chain as a whole.

Assume now that the particles interact nonlocally with measure $\Psi(n)$. Then it can be shown that [16]

$$\Phi(n) = -\Psi(n) \qquad n \neq 0 \qquad \Phi(0) = \sum_{n}{}' \Psi(n). \tag{2.4}$$

Note that for real mechanical systems all $\Psi(n) > 0$ and hence $\Phi(0) > 0$, $\Phi(n) < 0$ ($n \neq 0$). However, a system may be constructed for which some particles would have negative interaction coefficients, which is the case of our model described below.

3. The continuum approximation

The set of nonlinear differential equations for a discrete system is generally complex and, quite often, its continuum approximation is considered (which is the case here). By assuming that the displacements are slowly varying over the lattice spacing, the continuum approximation may be derived as follows.

3.1. The nonlocal model

The Lagrangian (2.1) in the form that is invariant with respect to n and x representations can be written as

$$\mathcal{L} = \tfrac{1}{2}\langle \rho\dot{u}, \dot{u}\rangle + \tfrac{1}{2}\langle u,\ \Phi u\rangle - \tfrac{1}{3}\langle \Delta u,\ k_3 \Delta u^2\rangle \tag{3.5}$$

where ρ is the mass density, while $u = u_n(t)$, $\Delta u = b^{-1}(u_{n+1} - u_n)$ and $u = u(x,t)$, $\Delta u = u_x$ in the discrete and continuum space.

The various terms in (3.5) for both the discrete and the continuum representations are given as follows:

$$\begin{aligned}\tfrac{1}{2}\langle u,\ \Phi u\rangle &= \tfrac{1}{4}\sum_{nn'}\Phi(n-n')(u_n - u_{n'})^2 \\ &= \tfrac{1}{2}\int_{R^2}\Phi(x-x')\,u(x)\,u(x')\,\mathrm{d}x\,\mathrm{d}x' \qquad (3.6)\end{aligned}$$

$$\begin{aligned}\tfrac{1}{3}\langle \Delta u,\ k_3\Delta u^2\rangle &= \tfrac{1}{3}\sum_{n} k_3(u_{n+1} - u_n)^3 \\ &= \tfrac{1}{3}\int_{R} k_3\,u_x^3\,\mathrm{d}x. \qquad (3.7)\end{aligned}$$

The above forms contain elastic (long-range) interactions for both the discrete model and its quasicontinuum counterparts.

The equation of motion of the medium in the (x,t) representation is

$$\rho\ddot{u}(x,t) = -\int_R \Phi(x-x')u(x',t)\,\mathrm{d}x' + k_3(u_x^2)_x. \qquad (3.8)$$

The corresponding condition (2.3) in the x representation becomes $\int_R \Phi(x-x')\,\mathrm{d}x' = 0$, which implies that $\Phi(x-x')$ can be represented as

$$\Phi(x-x') = \psi(x)\,\delta(x-x') - \Psi(x-x') \qquad (3.9)$$

with $\Psi(x-x') = \Psi(x'-x)$ and $\psi(x) \doteq \int \Psi(x-x')\,\mathrm{d}x'$.

Its quasicontinuum counterparts are of the form

$$\Phi(n-n') = \psi(n)\,\delta(n-n') - \Psi(n-n') \qquad (3.10)$$

with $\Psi(n-n') = \Psi(n'-n)$ and $\psi(n) \doteq \sum_{n'}\Psi(n-n')$. Thus $\Psi(n-n')$ and $\Psi(x-x')$ are the interaction coefficients and the interaction coefficient density of the model connecting the points (n, n') and (x, x'), respectively.

In the x representation the force constant can be expressed as [16]

$$\Phi(x-x') = \frac{\partial^2}{\partial x\,\partial x'}c(x-x') \qquad (3.11)$$

where $c(x-x')$ is the so-called kernel operator of elastic moduli.

Then, after integration by parts, equation (3.8) becomes

$$\rho\ddot{u}(x,t) = \frac{\partial}{\partial x}\int_R c(x-x')\frac{\partial u(x')}{\partial x'}\,\mathrm{d}x' + k_3(u_x^2)_x \qquad (3.12)$$

which is quite similar to the equation obtained from the nonlocal elasticity of the one-dimensional linear case (i.e. with the k_3 term vanishing) [17, 18].

In this case, by using the kinematical definition for the strain $\epsilon(x',t) = \partial u(x',t)/\partial x'$ and the nonlocal constitutive equation for the stress $\sigma(x,t) = \int_{-l}^{l} c(x-x')\,\epsilon(x',t)\,\mathrm{d}x'$, where l is the interaction range length, equation (3.12) can be recast into

$$\rho\ddot{u}(x,t) = \sigma_x \qquad (3.13)$$

which is the equation of motion of a one-dimensional elastic medium. (Note that, the integral over a finite radius of interaction defines the finiteness of action at a distance determined by this radius (that is, $l = \mathcal{M}b$). Specifically, $\Phi(y)$ is not zero for $y \in [-l, l]$ and it is equal to zero otherwise; however, if the chain is bounded within an interval $2L$ then $l \ll L$.)

In this connection, equation (3.13) is the starting point in continuum mechanics and expresses the balance of linear momentum. It is endowed with appropriate constitutive equations for the stress leading to partial differential equations for the determination of the displacement field. For example, a simple linear elastic model of the form $\sigma = E\epsilon$ with E denoting the Young modulus (identified as c_0^2 below) leads to the classical wave equation $u_{tt} = c^2 u_{xx}$ ($c^2 \equiv E/\rho$). If a gradient-dependent nonlinear elasticity model is adopted [19] of the form $\sigma = f(\epsilon) - \tilde{c}\epsilon_{xx}$ the appropriate equation of motion reads $f(u_x)u_{xx} - \tilde{c}u_{xxxx} = \rho u_{tt}$, which contains the $k_3(u_x^2)_x$ term listed above, even though a more interesting case results when $f'(u_x)$ is nonmonotonic. Other types of such constitutive models and their corresponding equations of motion are discussed in [20]. A case of particular interest in terms of its discrete model counterpart arises when viscosity is considered.

For a simple Kelvin–Voigt model of the form $\sigma = E\epsilon + \mu\dot{\epsilon}$ where μ is the viscosity and $\dot{\epsilon}$ the strain rate, the resultant equation of motion with $\lambda \equiv \mu/\rho$ is $u_{tt} = c^2 u_{xx} + \lambda \dot{u}_{xx}$, i.e. the damped wave equation. It is an open question to examine a Lagrangian-like lattice version of this model.

On the other hand, by letting

$$c = c_0^2\,\delta(x - x') + c_1(x - x') \tag{3.14}$$

where c corresponds to the local response with c_0^2 denoting the local elastic modulus and c_1 describing the nonlocal behaviour of the model, equation (3.12) simplifies to

$$\rho\ddot{u}(x,t) = c_0^2\,u_{xx} + \frac{\partial}{\partial x}\int_R c_1(x - x')\frac{\partial u(x')}{\partial x'}\,\mathrm{d}x' + k_3(u_x^2)_x \tag{3.15}$$

which is examined further below.

3.2. The long-time evolution of the localized wave

In this section we investigate the asymptotic behaviour of equation (3.15) for large times. By assuming that the contribution of the nonlinear term is significant throughout we rescale the nonlinear and the dispersive terms by introducing a small parameter $\varepsilon < 1$ as follows:

$$2k_3 = \gamma\,\varepsilon \qquad c_1 = \varepsilon\,g. \tag{3.16}$$

Here, γ is the rescaled nonlinearity coefficient and g is the rescaled elastic kernel. Then, for large times, the asymptotic expansion for the displacement field can be expressed as

$$u(x,t) = u_0(\xi,\tau) + \varepsilon\,u_1(x,t) + \mathrm{O}(\varepsilon^2) \tag{3.17}$$

where $\xi = x - vt$ is a shifted coordinate and $\tau = \varepsilon t$ is the slow time variable.

Using equations (3.16) and (3.17) and keeping terms of order ε only, equation (3.15) becomes

$$2\,\rho\,v\,u_{0\xi\tau} + \frac{\partial}{\partial\xi}\int_R g(\xi - \xi')\,u_{0\xi'}\,\mathrm{d}\xi' + \gamma\,u_{0\xi}\,u_{0\xi\xi} = -c_0^2\,u_{1xx} + \rho\,u_{1tt} \tag{3.18}$$

where $c_0^2 = \rho v^2$.

Then, the secularity condition [21] implies that both the left- and right-hand sides of (3.18) are zero. Thus, the right-hand side leads to the standard linear wave equation for u_1, while the left-hand side gives the long-time behaviour of u_0, i.e.

$$2\,\rho\,v\,u_{0\xi\tau} + \frac{\partial}{\partial\xi}\int_R g(\xi - \xi')\,u_{0\xi'}\,\mathrm{d}\xi' + \gamma\,u_{0\xi}\,u_{0\xi\xi} = 0. \tag{3.19}$$

Finally, by letting

$$u_{0\xi} = \mathcal{F} \qquad g(z) = \frac{\partial}{\partial z}G(z) \tag{3.20}$$

where $z = \xi - \xi'$ and $y = \xi - z$, equation (3.19) becomes

$$2\,\rho\,v\,\mathcal{F}_\tau + \gamma\,\mathcal{F}\,\mathcal{F}_\xi + \int_R G(\xi - y)\frac{\partial^2}{\partial^2 y}\mathcal{F}(y,\tau)\,\mathrm{d}y = 0 \tag{3.21}$$

which transforms to the Benjamin–Ono equation for

$$\tau = \frac{1}{2\rho v}T \qquad \mathcal{F} = \frac{1}{\gamma}U \qquad G(\xi - y) = -\frac{\alpha}{\pi}\frac{1}{\xi - y}. \tag{3.22}$$

Note that, on interchanging the role played by x and t in (3.21), we arrive at an integro-differential equation usually met in nonlinear wave propagation in active media with a dissipative process [22]. The latter is due to viscoelasticity described by an integral law involving an exponential kernel in the integral part of the equation of motion. This kernel is then a function of time introduced by a relaxation process.

3.3. The Benjamin–Ono equation

The Benjamin–Ono evolution equation

$$U_T + U\,U_\xi + \alpha\,H(U_{\xi\xi}) = 0 \tag{3.23}$$

with α being a positive parameter, was originally derived in [23–25] for interval-wave propagation in a two-layer system: one shallow and the other infinitely deep. In this context, $U(\xi, T)$ represents the amplitude of the interfacial wave produced by an initial disturbance, say $U(\xi, 0)$. The operator H designates the one-dimensional Hilbert transform, i.e.

$$\alpha\,H(U_{\xi\xi}) = \frac{\alpha}{\pi}\int_R \frac{1}{y - \xi}\,U_{yy}\,\mathrm{d}y \tag{3.24}$$

which implies that (3.23) is an integro-differential weakly nonlinear evolution equation.

Equation (3.23) has a simple solitary wave solution in the form of a Lorentzian (algebraic) shape [21, 26], i.e.

$$U(\xi, T) = \frac{4\nu}{(\frac{\nu}{\alpha})^2(\xi - \nu T)^2 + 1} \tag{3.25}$$

where 4ν is the amplitude of the wave and $\frac{\alpha}{\nu}$ measures the wavelength. The velocity of the soliton is amplitude dependent and is equal to ν.

Remark. Regarding the long-wavelength limit of the lattice model, the classical continuum approximation (i.e. Taylor's expansion for the fields) of (3.15) leads to the local nonlinear partial derivative equation of Boussinesq type [1, 2]

$$u_{tt} - c^2 u_{xx} + a u_x u_{xx} + b u_{xxxx} = 0 \tag{3.26}$$

where the parameters c, a and b depend on the atomic interactions. Alternatively, equation (3.26) may be directly deduced as a special case from the continuum approximation of (2.2).

The long-time evolution of (3.26) is given by the Korteweg–de-Vries equation,

$$V_t + V\,V_x + V_{xxx} = 0 \tag{3.27}$$

when multi-scale techniques (or perturbation methods) as described in section 3.2 are used. In addition, the Benjamin–Ono equation (3.23) can be transformed into the Korteweg–de-Vries equation by replacing $\alpha\,H(U_{\xi\xi})$ with $U_{\xi\xi\xi}$; however, this transition is not an obvious one.

4. Evaluation of the interaction coefficients

In this section we derive the lattice interaction coefficients $\Psi(n)$ of the model (2.1) using the fact that its asymptotic expansion, for large times, leads to the Benjamin–Ono equation; and therefore, the kernel of the operator of elastic moduli $c(x)$ is known.

Since there is a correspondence between functions of discrete argument and a certain class of analytic functions, the interaction coefficients can be evaluated either in the space of functions of discrete argument or in the space of analytic functions. However, since all these spaces are isomorphic to each other the interaction coefficients are obtained using the x representation (due to simplicity).

By setting $x - x' \to x$, equation (3.11) becomes

$$\begin{aligned}\Phi(x) &= -\frac{\partial^2}{\partial x^2}c(x)\\ &= -c_0^2\delta''(x) - \varepsilon\, g''(x)\end{aligned} \tag{4.28}$$

where (3.14) and (3.16) were used. However, from the long-time evolution analysis of the localized wave the explicit form of the function g is known. Thus, using (3.20) and (3.22) we obtain

$$\begin{aligned}\Phi(x) &= -c_0^2\delta''(x) - \varepsilon\, G'''(x)\\ &= -c_0^2\delta''(x) - \frac{6\varepsilon\alpha}{\pi}\frac{1}{x^4}.\end{aligned} \tag{4.29}$$

Due to Fourier transform, the force constants in the space of discrete arguments are related with the ones in the space of analytic functions as [16]

$$\begin{aligned}\Phi(n) = \Phi(nb) &= \int_R \Phi(x)\,\delta_b(x - nb)\,\mathrm{d}x\\ &= -c_0^2\,\mathcal{I}_1(n) - \frac{6\alpha\varepsilon}{\pi}\,\mathcal{I}_2(n)\end{aligned} \tag{4.30}$$

where $\delta_B(x) \doteq (2\pi)^{-1}\int_B \mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x = \sin(\pi x)(\pi x)^{-1}$ and

$$\begin{aligned}\mathcal{I}_1(n) &= \int_R \delta''(x)\frac{\sin[\frac{\pi}{b}(x - nb)]}{\pi(x - nb)}\,\mathrm{d}x\\ \mathcal{I}_2(n) &= \int_R \frac{1}{x^4}\frac{\sin[\frac{\pi}{b}(x - nb)]}{\pi(x - nb)}\,\mathrm{d}x.\end{aligned} \tag{4.31}$$

Thus, it is a matter of algebra to evaluate the two integrals and obtain

$$\begin{aligned}\mathcal{I}_1(0) &= -\frac{\pi^2}{3\,b^3}\\ \mathcal{I}_2(0) &= \frac{\pi^4}{24\,b^4}\end{aligned} \tag{4.32}$$

while for $n \neq 0$

$$\begin{aligned}\mathcal{I}_1(n) &= -\frac{2}{b^3}\frac{(-1)^n}{n^2}\\ \mathcal{I}_2(n) &= \frac{\pi^2}{b^4}\frac{(-1)^n}{n^2}\left[\frac{1}{2} + \frac{(-1)^n - 1}{n^2\,\pi^2}\right].\end{aligned} \tag{4.33}$$

Therefore, the lattice force constants are given by

$$\begin{aligned}\Phi(0) &= \frac{c_0^2\pi^2}{3b^3} - \frac{\alpha\varepsilon\pi^3}{4b^4}\\ \Phi(n) &= \frac{2c_0^2}{b^3}\frac{(-1)^n}{n^2} - \frac{6\alpha\varepsilon\pi}{b^4}\frac{(-1)^n}{n^2}\left[\frac{1}{2} + \frac{(-1)^n - 1}{n^2\,\pi^2}\right] \qquad n \neq 0.\end{aligned} \tag{4.34}$$

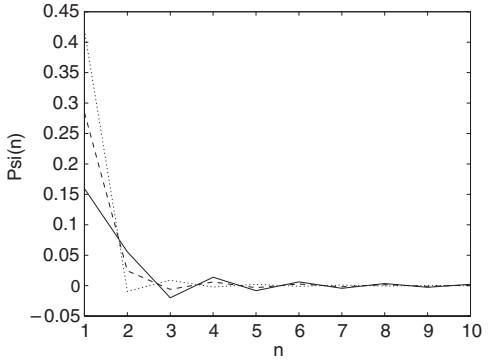

Figure 2. The function $\Psi(n)$ given by (4.34), (4.35) for $\alpha = 1$, $\nu = 1/4$, $\varepsilon = 0.1$, $n_0 = 125$ and phase velocity: (a) $c_0 = 0.6$ solid curve; (b) $c_0 = 0.65$ dashed curve; (c) $c_0 = 0.7$ dotted curve.

Finally, the lattice interaction coefficients $\Psi(n)$ in (2.2) (due to (3.10)) are given by

$$\Psi(n) = \Phi(0)\delta(n) - \Phi(n). \tag{4.35}$$

As one can observe from figure 2, by keeping the nonlocality of the discrete model to the continuum one, and specifically, the choice of an integrable nonlocal equation as its asymptotic limit for large times, leads to the construction of a lattice model with negative interaction coefficients between its particles. In fact, figure 2 illustrates the change of sign of $\Psi(n)$ and its variation with n for an atomic chain where each particle interacts with its ten neighbour particles. (The values of the other parameters, i.e. (a, b, ε, c_0) are listed in the figure caption.)

5. Numerical simulations

The behaviour of genuinely discrete systems is quite different than the one of their continuum counterparts and these differences have been studied in numerous papers both from the mathematical and the physical point of view. Many of the methods used and their physical implementation in models with nearest neighbour interactions can be found in [27–29]. In addition, in [30, 31] the effects of discreteness in solitary waves in nearest neighbour lattices have been mathematically investigated.

In our case, the lattice model keeps its nonlocal behaviour at the continuum when its asymptotical limit for large times is the Benjamin–Ono equation. However, it is not obvious if the solution of the Benjamin–Ono equation will also be the solution of the lattice model. Thus, in this section we investigate the dynamical behaviour of the lattice model (2.2) numerically, using as an initial condition the soliton solution given in section 3.3.

We use a numerical scheme by directly considering the lattice equations (2.2), employing a Runge–Kutta method of fourth order and imposing pseudo-periodic boundary conditions, i.e.

$$u(N + i) = u(i) + u_0 \qquad i \in [-\mathcal{M}, \mathcal{M}] \tag{5.36}$$

where N is the number of particles in the lattice, $\mathcal{M}$ the range of particle interactions considered and u_0 the amplitude of the initial kink.

The initial conditions for the displacements and the velocities of each lattice particle are given by the analytic expression

$$u(x, t) = \frac{2\varepsilon\alpha}{k_3} \arctan\left[\frac{\nu}{\alpha}\left(x - x_0 - c_0\left(1 + \frac{\varepsilon\nu}{2c_0^2}\right)t\right)\right] \tag{5.37}$$

and its time derivative, respectively. Here, x_0 denotes the soliton position and we have set the mass density equal to one ($\rho = 1$). This solution represents a kink with thickness $\Delta = \alpha\pi/\nu$,

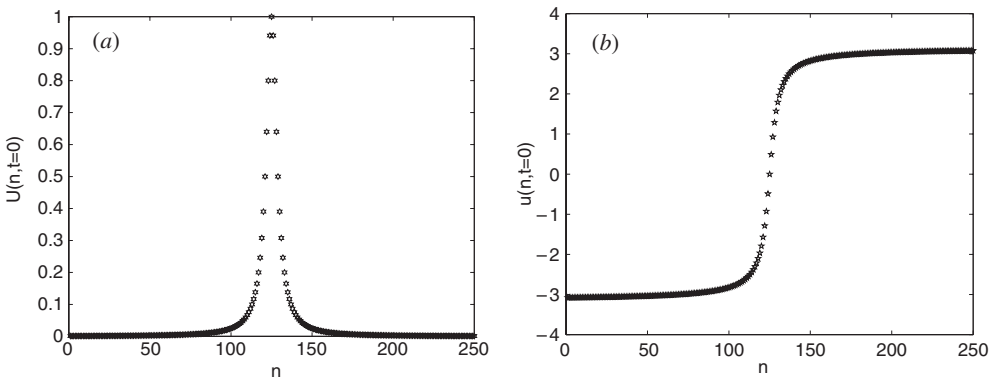

Figure 3. (*a*) Initial soliton solution (3.25) and (*b*) initial kink solution (5.37) for $\alpha = 1$, $\nu = 1/4$ and $n_0 = 125$.

i.e. the number of particles participating in the kink solution is proportional to the kernel factor α and decreases as the wave parameter ν increases. (The solution (5.37) has been obtained from the solitary wave solution of the Benjamin–Ono equation (3.25) after using the change of variables and fields given in section 3.2.) Figure 3 illustrates (*a*) the soliton solution $U(\zeta)$ with $\zeta = \xi - \nu T$ given by (3.25) and (*b*) the kink solution $u(x)$ given by (5.37) for the choice $b = 1$.

In all our simulations we have chosen the following fixed values: $k_3 = 0.1$, $\varepsilon = 0.1$, $b = 1$, $\alpha = 1$, $M = 1$. However, different values for the above parameters give qualitatively the same results. The initial position of the kink is chosen to be equal to $n_0 = 125$, while the value of the kink velocity c_0 is chosen such that the first interaction coefficient is positive (i.e. $\Psi(1) > 0$) and the total number of particles in the lattice is equal to 250.

Figure 4 summarizes the main results of our numerical simulations when models with different numbers of non-nearest neighbour interactions are considered and different values for the velocity and wavelength of the initial kink have been chosen. In particular, figures 4(*a*), (*e*) and (*f*) present a solution corresponding to a lattice model with first, tenth and twentieth neighbour particle interactions when the initial kink wavelength and phase velocity are: $\nu = 1/8$, $c_0 = 0.7$; $\nu = 1/4$, $c_0 = 0.6$; and $\nu = 1/8$, $c_0 = 0.6$, respectively. In each model, the kink contains from 12 up to 24 particles, which means that the continuum approximation is valid. (Recall that the kink thickness depends on the parameter ν, due to (5.37).) On the other hand, figures 4(*b*)–(*d*) present the kink dynamics for lattice models with second, fourth and seventh neighbour particle interactions. However, we choose the kink width in all three cases to be small, i.e. the kink contains six particles with $\nu = 1/2$, $c_0 = 0.54$ in the first case, and three particles with $\nu = 1$; $c_0 = 0.6$, $c_0 = 0.7$ in the last two.

From figure 4, one can observe that the initial soliton solution of the Benjamin–Ono equation is also a solution of the lattice model with long-range interactions given by (2.2). In fact, the initial lattice kink relaxes and propagates in the lattice space with small oscillations. It can be observed from figures 4(*a*), (*e*) and (*f*) that as the kink thickness increases (i.e. ν decreases) the lattice radiation is eliminated. Numerical simulations of the discrete nonlocal model for kink widths equal to three or six lattice spacings are presented in figures 4(*b*)–(*d*): at this level the kink changes slightly and loses energy by radiation of small amplitude waves. In all cases where the kink contains at least 20 particles, it is remarkable stable and emits (almost) no radiation.

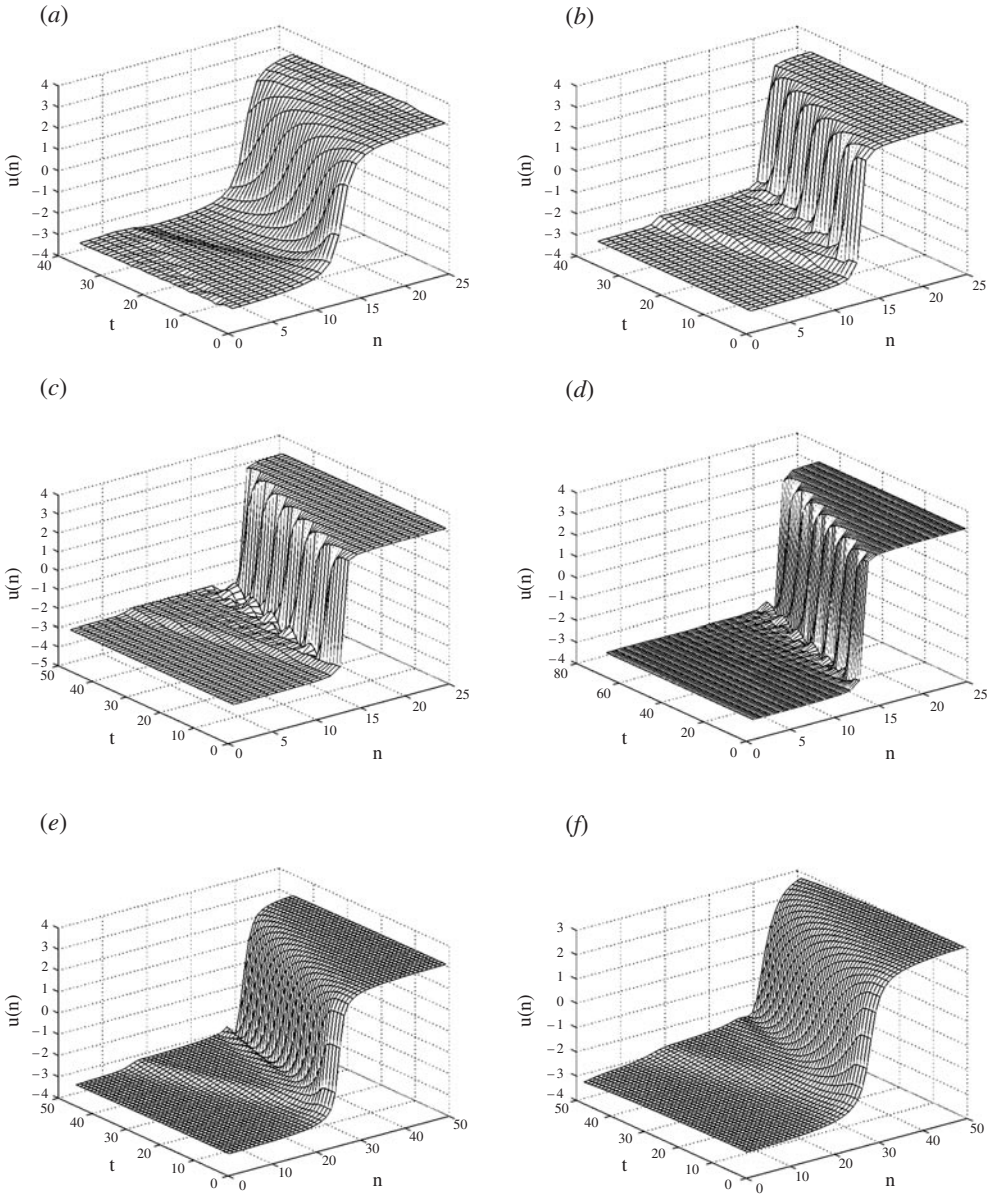

Figure 4. Kink plane for: (*a*) one-range interaction, $\nu = 1/8$, $c_0 = 0.7$; (*b*) two-range interaction, $\nu = 1/2$, $c_0 = 0.54$; (*c*) four-range interaction, $\nu = 1$, $c_0 = 0.6$; (*d*) seven-range interaction, $\nu = 1$, $c_0 = 0.7$; (*e*) ten-range interaction, $\nu = 1/4$, $c_0 = 0.6$; (*f*) 20-range interaction, $\nu = 1/8$, $c_0 = 0.6$.

Let us conclude by saying that, in the long-wavelength approximation (i.e. when the average kink wavelength is larger than the lattice spacing) the initial (continuum) kink, which has been derived using the quasicontinuum approximation of the discrete model, relaxes to a stable discrete kink without any oscillations and our method is accurate.

6. Concluding remarks

This paper is concerned with the dynamics of lattice models with long-range and nonlinear interactions. The main objective is the description of the dynamics of the lattice model, at the continuum level, by keeping the nonlocal nature of the discrete system. Our model is the simplest one consisting of a one-dimensional chain of point masses connected by springs. We have developed a theory for such a discrete system and introduced the notion of quasicontinuum which allows us to treat the discrete and continuum models in the framework of the same formalism. Attention has been focused on the analysis of an approximate model and its transition to nonlocal elasticity in the limit of long waves. In this formalism, we have set up a one-to-one correspondence between functions of discrete arguments and a class of analytic functions. The procedure is also applicable for integral operations on these functions. The method bears a resemblance to the problem of interpolation of a discrete function by a smooth function satisfying some smoothness conditions. The technique allows us (section 3) to use the same representation of the Lagrangian for all cases: discrete and analytic.

The equation of motion of the model in the continuum representation is similar to that of a nonlocal model of elasticity including a local nonlinear term. Nevertheless, such an equation of motion is not easy to deal with and a perturbation method has been employed. More precisely, we have considered the long-time evolution of nonlinear waves travelling in the lattice. The asymptotic method has been used to transform the equation of motion into an equation of Benjamin–Ono type, which governs the long-time evolution of the initial signal. For a particular choice of the nonlocal elastic kernel or interaction force function, the dispersive operator of the equation is a Hilbert transform corresponding to the Benjamin–Ono equation. In this particular situation, a localized wave solution of soliton type has been obtained. In order to test the analytical conjectures thus developed, some numerical simulations have been performed directly on the lattice model for different ranges of nonlocal action. It has been observed from numerics that the initial soliton (kink) solution propagates almost without perturbation and it is very stable. Moreover, wide kinks propagate in the lattice without any loss due to discreteness radiations.

Such a study can be extended to other kinds of nonlinear terms (double-well or sine-potential, higher-order interactions) or to arbitrary particle interactions. Extension to two-dimensional lattices can also be envisaged. The problems of kink collision or the influence of perturbations (forces, damping, lattice defects) on the kink motion is of interest. Some of these problems will be addressed in the future.

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