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NONLINEAR WAVES

Wave motions along lattices with nonlinear on-site and inter-site potentials. Cooperation and/or competition leading to lattice solitons and/or discrete breathers

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Abstract. We consider the wave dynamics of a one-dimensional lattice where both on-site and inter-site vibrations, coupled together, are governed by Morse interactions. We focus attention on the onset of lattice solitons and discrete breathers (DBs, aka intrinsic localized modes, ILM). We show how varying the relative strength of the on-site potential to that of the inter-site potential permits transition from one mode of (travelling or otherwise) localized excitation to the other.

Key words: lattice soliton, discrete breather, intrinsic localized mode, Morse potential, on-site potential, inter-site potential.

1. INTRODUCTION

There is experimental evidence supporting the need of analysing the evolution of wave-like excitations in crystal lattices where non-linear on-site (Einstein, non-dispersive; diagonal depending on the coordinate of a single oscillator) and inter-site (Debye, dispersive; off-diagonal depending on the coordinates of two or more different units, hence relative interdistances) modes interact, thus cooperating or competing in the system's dynamical evolution. This is clearly shown with data on phase transitions and electron transport in conducting polymers and in bio-molecules such as DNA (natural and otherwise) [1–4].

Here we shall concentrate on a one-dimensional model where both on-site and inter-site vibrations are governed by empirical Morse interactions. Our aim is to uncover possibilities offered by varying their relative significance. We shall show that both lattice solitons and discrete breathers (DBs, aka intrinsic localized modes, ILM) are possible [5–14]. Furthermore, we shall show how one mode appears and eventually gives way to the other as we vary appropriate parameters. We have in mind that discreteness provides bounds and gaps to the spectrum of linear oscillations whereas nonlinearity makes the amplitude of oscillation frequency-dependent. We also have in mind that the inter-site Morse potential favours the excitation of soliton-like modes. It also permits the onset of (pinned) DBs albeit with some constraints, like being assisted by on-site oscillations, due to is 'soft' character (frequency of small amplitude oscillations

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around minimum decreases when amplitude increases; its well width goes outside the harmonic potential or, to put it differently, its spring stiffness decreases with the widening of the inter-site separation).

Discrete breathers could be mobile (subsonic or otherwise), pinned, or even impossible depending indeed on parameter values, whereas solitons would always be supersonically moving [15,16]. Coupling the inter-site Morse potential to the on-site Morse potential offers a variety of possibilities as the latter favours the onset of DB (for the case of on-site harmonic oscillations coupled to inter-site harmonic oscillations see [17] and references therein).

Note that, at variance with the Morse potential, DB are always possible with a 'hard' potential (frequency of small amplitude oscillations around minimum increases with increasing amplitude or spring stiffness increases with the widening of the separation; $x^2/2 \pm x^4/4$ is hard/soft with the positive/negative quartic term; otherwise in soft/hard the force is smaller/greater than the linear force alone). Note also that when two coupled harmonic oscillators are resonant, any amount of energy initially given to one of them alternates periodically between them with a frequency proportional to the strength of their coupling. Then in a lattice/chain with coupled identical harmonic oscillators there is energy propagation. In order for the energy to remain localized, resonance has to be broken and this is feasible when there are defects or disorder along the lattice. If, however, the oscillators are nonlinear as their frequencies depend on amplitude when two are coupled and energy is given to one of them in a way that its frequency is equal to the harmonic approximation of the other, resonance is generally broken after some energy transfer because the frequencies change and then the transfer stops. However, it was shown that resonance between two weakly coupled anharmonic oscillators may persist under particular conditions [12].

In Section 2 we pose the mathematical problem in the form of nonlinear evolution equations. Their solutions are discussed in Section 3 for two extreme opposite cases of relative parameter values, and in Section 4 with more generality. Section 5 is devoted to a summary of results.

2. LATTICE EVOLUTION EQUATIONS

Before addressing the dynamics with Morse potentials it seems worth recalling results from the linear case. The evolution of small amplitude vibrations is generally described by a system of linear differential equations

$$\mathrm{d}^2 q_n/\mathrm{d}t^2 = -\omega_0^2 q_n + \omega_b^2 \left(q_{n+1} - 2q_n + q_{n-1}\right), \tag{1}$$

where q denotes a deviation from the equilibrium state and ω_0 and ω_b correspond, respectively, to the on-site and inter-site oscillations. Equation (1) accounts for both types of oscillations due to the symmetry of the parabolic potentials. Each temporal behaviour $q_n(t)$ is a harmonic component of a Fourier expansion, i.e., $q_n \sim \exp[i(\omega t - kna)]$. The corresponding dispersion relation, i.e., $D(\omega, k) = 0$ is $\omega^2 = \omega_0^2 + 4\omega_b^2 \sin^2(ka/2)$. The (half) Brillouin plot is depicted in Fig. 1. In general, there are two critical frequencies in a dispersion relation of a chain of interacting oscillators: $\omega_{cr1} = \omega_0$, $\omega_{cr2} = \sqrt{\omega_0^2 + 4\omega_b^2}$. The region $\omega_{cr1} < \omega < \omega_{cr2}$, with $\mathrm{Im}k(\omega) = 0$, and $\mathrm{Re}k(\omega) \neq 0$, is the so-called 'phonon' or 'transparency' band. Solutions corresponding to this band are waves travelling freely from $-\infty$ to $+\infty$ with a constant amplitude. This defines delocalization (Bloch theory) offering the possibility of phonon-assisted transport. For $\omega < \omega_{cr1}$ and $\omega > \omega_{cr2}$ we have $\mathrm{Im}k(\omega) \neq 0$, $\mathrm{Re}k(\omega) = 0$ and we are outside, below, or above, the phonon band, respectively. Then (say below unity in Fig. 1) there are no energy losses as the dynamics is conservative. We have left to right and converse motions with reflections expressing lack of 'transparency'. Looking again at Fig. 1, we can say that, provided adequate nonlinearity is added to the dynamics, lattice solitons are expected inside the phonon band when there is moderate wave dispersion (from around the centre to the upper right corner of the solid lines). (Pinned) DB can be searched for frequencies above ω_{cr2} (upper right corner) and below ω_{cr1} (lower left corner) as long as the harmonics are not resonant with the phonon band. With weak on-site potentials it is hard, eventually impossible to excite (pinned) DB in the gap as its harmonics may enter the phonon band. Thus it appears easier when such band is very narrow like in the right panel of Fig. 1, which shows the result of a strong enough on-site potential. Inside the phonon band

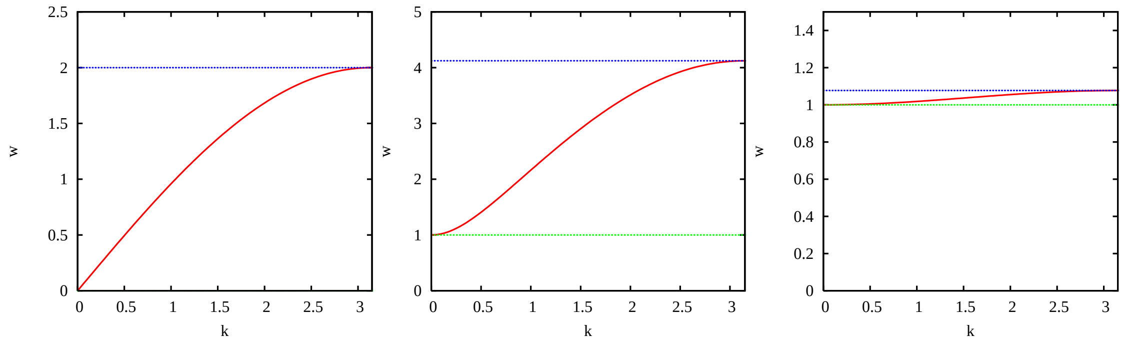


Fig. 1. Brillouin dispersion relation (half) plots (with appropriate dimensionless units) for a lattice of identical oscillators. In each case the region between the solid line and the upper dotted line is the so-called phonon or transparency band. Left panel: $\omega_0 = 0$ (no on-site potential; gapless due to conservation of linear total momentum); central panel: general case, $\omega_0 \sim \omega_b$ (here, in particular, $\omega_b = 2\omega_0$; gap); right panel: very weak inter-site bond, $\omega_b << \omega_0$ (here $\omega_b = 0.2\omega_0$). Clearly, for DB to appear the existence of a (lower) gap may be sufficient (as with strong enough on-site and soft inter-site potentials) but certainly is not necessary (as with hard potentials).

DB are not possible since any resonance of the DB or harmonics with the extended phonons will radiate the DB away.

In view of the above, our problem corresponds to the following evolution equations $(n = 1, \ldots, N)$:

$$\frac{\mathrm{d}^2 q_n}{\mathrm{d}t^2} + \left[\left(\frac{\partial U_M^{\text{inter-site}}}{\partial r} \right) |_{r=|q_{n+1}-q_n|} - \left(\frac{\partial U_M^{\text{inter-site}}}{\partial r} \right) |_{r=|q_n-q_{n-1}|} \right] + \frac{\partial}{\partial r} U_M^{\text{on-site}} |_{r=q_n} = 0, \tag{2}$$

with $q_n = b(x_n - x_{n0}) = b_{\text{inter-site}}(x_n - n\sigma)$ and $U_M = D\left(e^{-2br} - 2e^{-br}\right)$, where D and b characterize, respectively, the potential well depth (or dissociation energy level) and its stiffness; for a first approach and simplification we take $\sigma_{\text{on-site}} = \sigma_{\text{inter-site}}$; σ is the equilibrium inter-site distance. For universality in the argument and convenience in our discussion of cooperation and/or competition between the on-site and inter-site Morse potentials we rescale the problem using the following relationships: $\tau = \omega_M^{\text{inter-site}} t$, $\eta_b = b_{\text{on-site}}/b_{\text{inter-site}}$ (ratio of widths of potential wells/stiffnesses), and $\eta_D = D_{\text{on-site}}/D_{\text{inter-site}}$ (ratio of depths of potential wells). Thus, for one-sided motions, in dimensionless variables

$$\frac{\mathrm{d}^2 q_n}{\mathrm{d}t^2} = \left[1 - e^{(q_n - q_{n+1})}\right] e^{(q_n - q_{n+1})} - \left[1 - e^{(q_{n-1} - q_n)}\right] e^{(q_{n-1} - q_n)} + \eta_b \eta_D \left[1 - e^{\eta_b q_n}\right] e^{\eta_b q_n}. \tag{3}$$

3. WAVE EXCITATIONS IN THE ANHARMONIC LATTICE. SOLITON AND DB AS EXTREME OPPOSITE CASES

There are two extreme opposite 'ideal' cases.

1. Soliton in a Morse chain without on-site potential ($\eta_b = \eta_D = 0$). At a low to moderate level of excitation the Morse potential can be approximated by the Toda model and hence we shall make use of the known analytical solutions of the latter [15]. Thus we set as initial condition

$$q_n = q_{n+1} + \frac{1}{3} 1n \left[1 + sh^2\kappa/ch^2\left[\kappa(n - n_{\text{centr}}) - shk^* t\right]\right]_{t=0}, \; v_n = \mathrm{d}q_n/dt, \tag{4}$$

with κ denoting the inverse width of the localized excitation centred around n_{centr}. Its space–time evolution, exhibiting supersonic velocity, is depicted in Fig. 2. We have a lattice soliton growing in the phonon band when there is a bending of the $\omega(k)$ as k grows, hence allowing for dispersion. The balance of the latter

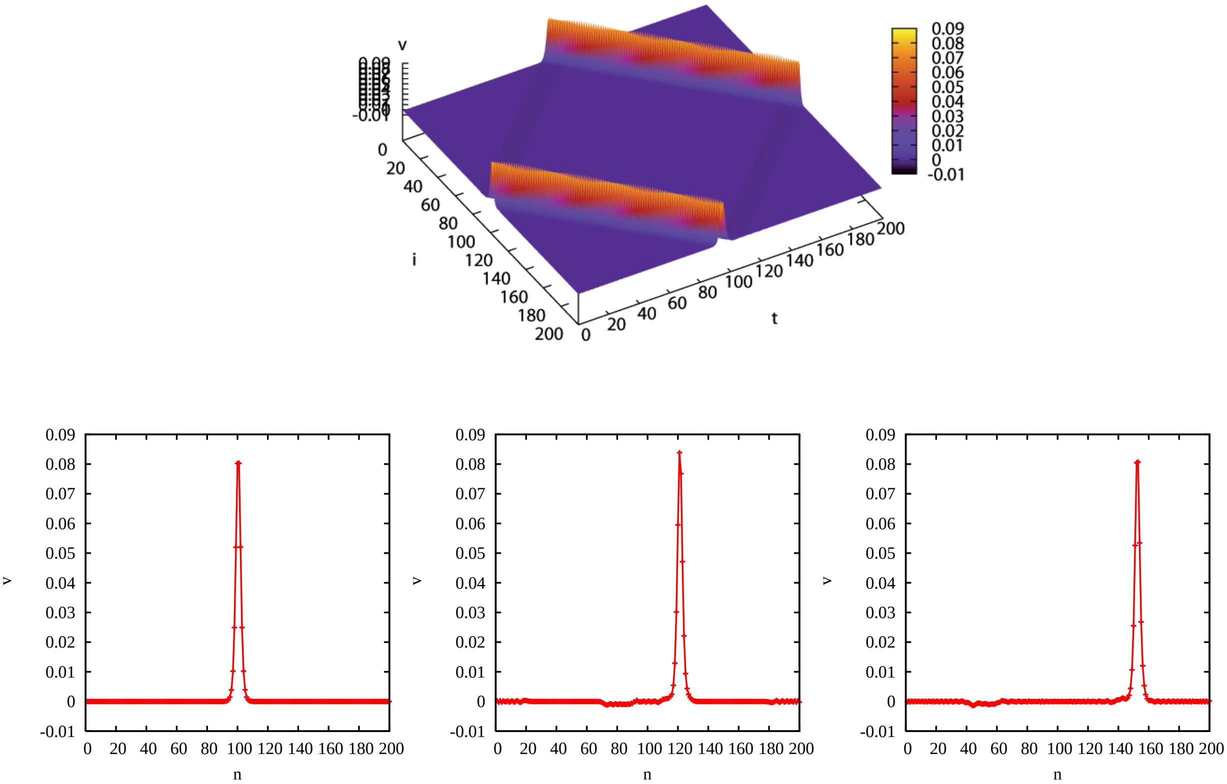


Fig. 2. 'Low' energetic lattice soliton, embracing ten lattice units, in a Morse chain without on-site motions ($N = 200$, $\kappa = 0.5$, $t = 0$–200), with periodic boundary conditions. Upper panel: for clarity note that the velocity ordinate runs from -0.01 to 0.09 as indicated in the vertical scale on the right. Three other panels: left to right: time evolution $t = 10, 20, 50$ of velocity distribution $v_i(t)$. Soliton velocity: $v_{\text{sol}} = 1.05$ in units of the sound velocity v_{sound}. What matters for a soliton is velocity, which depends on amplitude/energy while 'frequency' is meaningless (otherwise said $\omega = 0$).

with the nonlinearity of the inter-site potential brings the soliton as a solitary wave. If we have in mind the continuum limit and a transformation to the moving frame, the soliton corresponds to a homoclinic trajectory of the underlying dynamical system.

2. (Pinned) DB. In the simplest case when on-site oscillations dominate over inter-site motions (with η_b and η_D, both large enough) we may assume that a 'highly' energetic oscillation with frequency significantly smaller than the low critical frequency is localized on a single lattice site. Then it can be described by the on-site component of Eq. (3): $\frac{d^2 q_n}{dt^2} = \eta_b \eta_D \left[1 - e^{\eta_b q_n}\right] e^{\eta_b q_n}$ with $q_n = v_n = 0$ as the initial condition for all units save one, here $n = 50$ for which $q_{50} = 0$, $v_{50} \neq 0$. Its space–time evolution is depicted in Fig. 3. Here we have a collection of (on-site, Einstein) nonlinear oscillators whose closed trajectories, prescribed by the given initial conditions, correspond to the energy levels of a centre fixed point. We have in mind the so-called anticontinuum limit, which is the starting point for the rigorous proofs [11,12] of the existence of DB when on-site oscillations are 'perturbed' by inter-site potentials linking together the otherwise free units. Such sufficient conditions refer to frequencies below ω_{cr1} (in the band gap) or above ω_{cr2}, both outside the phonon band as earlier mentioned.

In what follows, contrary to the approach starting from the anticontinuum limit, we explore the passage from case 1 (solitons) to case 2 (DB) by perturbing the Debye lattice with the on-site oscillations.

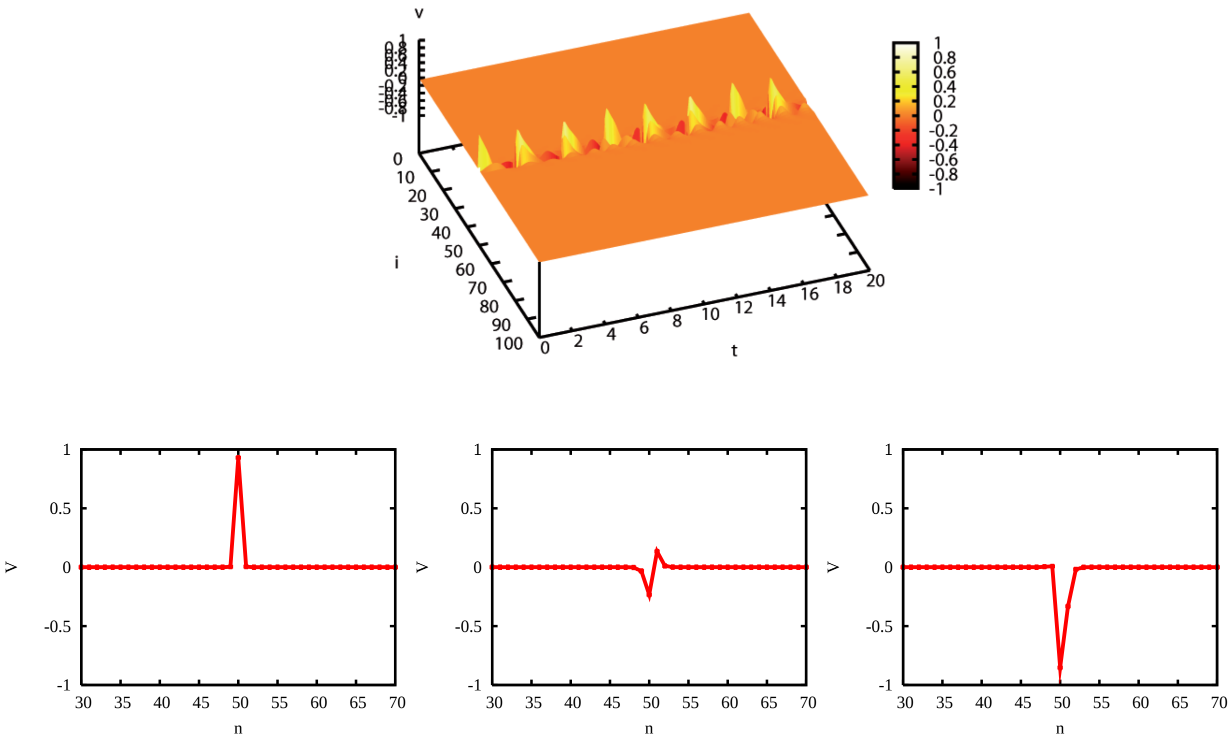


Fig. 3. ‘Low frequency’ DB. Upper panel: for clarity note that the velocity ordinate runs from -1 to 1 as indicated in the vertical scale on the right. Three other panels: left to right: time evolution of velocity distribution $t = 0$–20, $t = 0.1, 1.2, 2$ for a lattice with $N = 100$. What matters for a DB is frequency, which depends on energy. There is no motion in space.

4. WAVE EXCITATIONS IN THE ANHARMONIC LATTICE. GENERAL APPROACH AND THE PASSAGE FROM LATTICE SOLITONS TO DB

Lattice solitons and DB can be excited by appropriate albeit different initial conditions. However, in order to see the passage from one mode to the other we have used the same, i.e. $q_n = v_n = 0$ save one where $q_{n_0} = 0$, $v_{n_0} \neq 0$. We carried out a series of computer experiments by fixing the value of η_D and varying the parameter η_b. We have also carried out another series of computer experiments where the opposite was done by holding fixed the value of η_b and varying the parameter η_D, but here we shall not reproduce results of this second series. For reference we first show a ‘high’ energetic and supersonic soliton along the lattice in Fig. 4 as a more realistic variant of that exhibited in Fig. 2.

Having in view Fig. 4, Fig. 5 provides results for three computer runs. When $\eta_D = 0.4$ (or any other value) and $\eta_b = 0.5$ we have on-site potentials with a stiffness constant half that of the inter-site oscillators. The influence of the former is being felt in the appearance of a complex structure in the local excitation (centre panel to be compared to Figs 2 and 4). Yet the latter retains from the soliton its moving feature with still supersonic velocity. The panel on the right in Fig. 5 is a zoomed picture of the 120–160 range of sites along the lattice. As for the centre panel it is a snapshot taken at time $t = 100$ in the dimensionless units, assumed to be a long time interval. We erased the noisy background to clearly identify a local structure that does not remain rigid in the course of time. Rather maxima and minima give way to new maxima and minima as the local excitation progresses along the lattice as time goes on. This process occurs with the period decreasing with increasing relative influence of the on-site potential as measured by η_b (and/or η_D). Indeed, a similar behaviour can be observed in the two other sets of panels going from supersonic to subsonic velocity ($\eta_b = 1$) and eventually zero value ($\eta_b = 8$). The latter is genuinely a pinned DB.

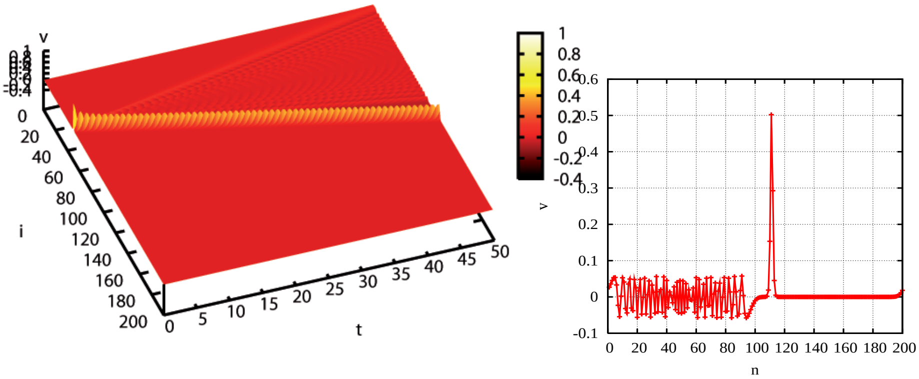


Fig. 4. 'High' energetic soliton (embracing eight lattice atoms) for $\eta_D = 0$ (no on-site oscillations), $\eta_b = 0$, $v_{50}(t = 0) = 1$. The left panel shows lattice with $N = 200$ for the time interval $t = 0$–50. For clarity note that the velocity ordinate runs from -0.4 to 1 as indicated in the vertical scale on the right. The right panel depicts velocity at $t = 50$. Compared to Fig. 2, here the choice of the initial profile is not as good an approximation to the 'exact' solution as in the previous case. This leads to the appearance of linear phonon radiation (moving with sound velocity) observed lagging behind left of the (supersonically moving) maximum.

(a)

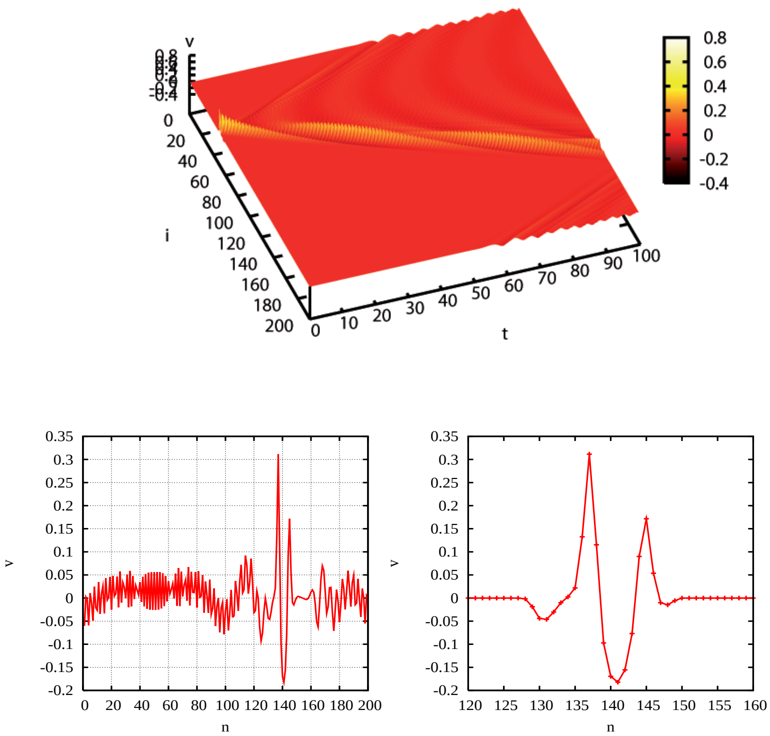
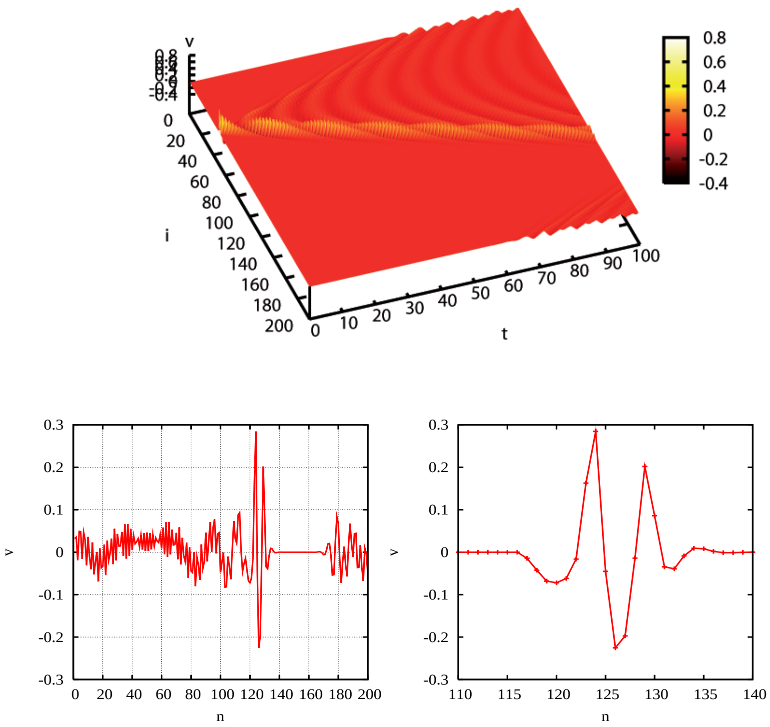


Fig. 5. Space–time evolution ($N = 200$, $t = 0$–100) of velocity for localized excitations ($\eta_D = 0.4$): (a) $\eta_b = 0.5$. Upper panel: for clarity note that the velocity ordinate runs from -0.4 to 0.8 as indicated in the vertical scale on the right. Two other panels: the right panel is a zooming of the lattice interval $n = 120$–160 in order to see the internal structure of the localized excitation. It appears as a two/three-peak structure moving along the chain with oscillations alternating maxima and minima. The first peak goes down as the second one grows higher. Subsequently this second peak becomes the first and in turn goes down and so on. Velocity at $t = 100$.

(b)



(c)

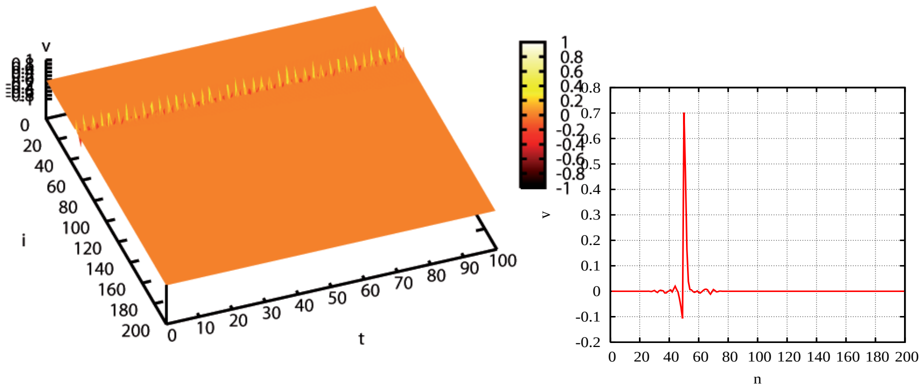


Fig. 5. *Continued.* (b) $\eta_b = 1$. Upper panel: for clarity note that the velocity ordinate runs from -0.4 to 0.8 as indicated in the vertical scale on the right. Two other panels: the right figure is a zooming of the lattice interval $n = 110$–140. Before the peaked structure we see that the DB do not interact with the background. Clearly, increasing η_b the velocity of the DB becomes more and more subsonic and eventually becomes pinned. Velocity at $t = 100$; (c) $\eta_b = 8$. Left panel: for clarity note that the velocity ordinate runs from -1 to 1 as indicated in the vertical scale on the right. Right panel: velocity at $t = 100$ (pinned DB).

5. SUMMARY OF RESULTS

From the computer simulations, the overall behaviour extracted is depicted in Fig. 6 by plotting the velocity of the localized excitation vs one or the other of the parameters of the dynamics. It can be seen that the weaker the inter-site oscillations (η_b going up), the greater is the tendency of DB to become very fast pinned from $\eta_b = 0$ to around $\eta_b = 4$ where there is an apparent dramatic passage from genuine (lattice) soliton to genuine DB. There appears a wide range of values of η_b where the localized excitation can be considered as a nonlinear periodic (soliton-like) wave modulated by a narrow envelope to be interpreted as a moving DB.

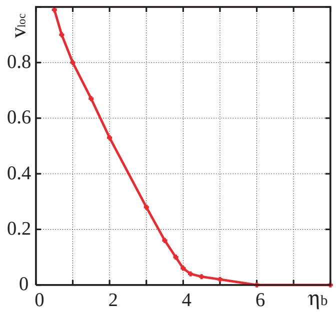


Fig. 6. Terminal velocity vs η_b at const $\eta_D = 0.4$. Similar results are obtained for a wide range of values of the latter parameter.

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Lainelevi mittelineaarsete potentsiaalidega võres

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On vaadeldud lainelevi ühemõõtmelises võres, kus nii võrepunktide kui ka võrepunktidevahelised potentsiaalid on mittelineaarsed. Tähelepanu on koondatud kaht tüüpi lokaalsete ergastuste, võresolitonide ja diskreetsete briiserite tekkemehhanismi selgitamisele. On näidatud, kuidas vaadeldavate potentsiaalide suhtelise tugevuse muutumine võimaldab üle minna ühelt lokaalse ergastuse tüübilt teisele.