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LOCALIZED LUMP-SOLITON-LIKE EXCITATIONS IN TRIANGULAR MORSE LATTICES

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Abstract. Localized supersonic long-living nonlinear modes excited in triangular lattices of point particles interacting via potential Morse bonds are studied in a frame of a model with appropriately chosen bonds to rule out redundancy bonds. Numerical simulations on a base of Newtonian equations are performed to define configurations (coordinates and velocities of all particles) of steady-state (meta-stable) modes and their characteristics including in particular excitations being lump soliton-like.
Keywords: 2D Morse lattice; solitons in adjacent rows; meta-stable states; track length; life time.

1. Introduction

Molecular lattices with nonlinear particle interactions and possessing rather simple structure are able to support long-lasting, high-energy localized excitations of both immobile and mobile type. They may be interpreted as waves of deformation which influence mechanical properties of materials. Also the mobile excitations (waves of deformation) can be considered as potential carriers of charged particles, electrons or holes (positive charges). Due to this, problems of excitations and dynamics of nano size localized modes in both one-dimensional (1d or quasi 1d chains or molecular wires) and two-dimensional (2d) nonlinear lattices are of great interest, in particular when excitations are supersonic.

The 1d nonlinear lattice dynamics problem has been studied extensively by many researchers, following the pioneering work by Fermi-Pasta-Ulam [1], and subsequent works by Zabusky and Kruskal [2] and Toda [3]. The characteristics of fast solitonic waves have been analyzed in details. One should mention that soliton-like excitations (in short solitons) having supersonic velocities are expected to emerge on the background of low-frequency phonons. Other localized modes, so called discrete breathers (a.k.a. intrinsic localized modes), can be excited in a 1d lattice mainly when having on-site potential, with the exception of some special cases. In 2d lattices both discrete breathers and solitons may be excited as mobile modes in lattices without on-site potential. The characteristics of discrete breathers have been studied intensively (see, e.g. [4-12]). A peculiar type of high-energy supersonic solitons called crowdions [13] can be excited in a simple way, just by kicking a single particle along one of the crystallographic axes. However excitation of a crowdion carrying both energy and mass concentrated on the extra particle is associated with formation of a topological lattice defect. In order to avoid defect formation one can excite a quasi-1d soliton in one crystallographic direction of a 2d-lattice by assuming an initial excitation in a lattice with a form close to a

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soliton in the underlying 1d lattice [14]. Such excitations do not cause emergence of permanent topological lattice defects. However, a supersonic soliton "radiates" energy to adjacent atomic rows. In case of high soliton velocity its energy has relatively small values due to the fact that the spectrum of frequencies of lateral excitations is located predominantly outside of the lattice phonon band [15-17] and small lateral perturbations are localized along the soliton path. Generally the track length of a quasi-1d soliton is limited to a few dozens of interatomic distances. In order to increase such length we may think about exciting solitonic modes in some (M) adjacent atomic rows. In such way a front of M-solitons is expected moving transverse to the given main direction of soliton motion.

2. Model description

A triangular lattice of point particles interacting via potential Morse bonds is studied by means of computer simulation. A molecular-dynamical ensemble model with complex variables $Z_n=x_n+iy_n$ is used. The latter are introduced to describe a position of n-th particle in the (x,y)-plane. The Newtonian or Langevin equations of motion are solved in computer simulations to describe the lattice dynamics at 0 K or at elevated temperatures [14-17]:

$$\ddot{Z}_n = \sum_k F_{nk}(|Z_{nk}|) z_{nk} + \left[-\gamma \dot{Z}_n + \sqrt{2D_v}\left(\xi_{nx} + i\xi_{ny}\right)\right] \tag{1}$$

Here $Z_{nk}=Z_n - Z_k$, $z_{nk}=(Z_n - Z_k)/ |Z_n - Z_k|$, $F_{nk}(|Z_{nk}|)$ is an interaction force between n-th and k-th particles, γ is a friction coefficient, D_v is intensity of the chaotic force, $\xi_{nx,ny}$ are independent sources of Gaussian white noise. D_v and γ connect with the noise by a fluctuation-dissipation relation, D_v equals to zero in a case of the cold lattice considered here. γ=0 stands for natural losses in a lattice not taken into account. Forces of interaction are described by modified Morse potential:

$$V^{M\,\mathrm{mod}} = 2D\left\{\left[e^{-2b(r-\sigma)} - 2e^{-b(r-\sigma)}\right] * \frac{1}{1+e^{\frac{r-d}{2\nu}}}\right\}, \tag{2}$$

where $r = |Z_{nk}|$, parameters D and b reflect the values of potential minimum depth and stiffness coefficient respectively, σ is an equilibrium radius of the Morse potential, parameters d and ν are chosen to provide negligibly small values of both potential and force at distances larger than a cut-off radius. Usually in our simulations the cut-off radius $r_{cut} = 1.5\sigma$ is chosen in order to provide interaction of each particle only with particles of the first coordination sphere.

Both zero deviations of particles from equilibrium positions and zero velocities of all particles, excluding those involved in initial excitations are used as initial conditions. Simulations are performed in a cell with lengths $L_{x,y}$ corresponding to geometry of a lattice and a number of particles N. Soliton-like excitations are defined initially in one or several atomic rows in accordance with the standard shape of solitonic excitations [2]

$$q_n = q_{n+1} + A\frac{1}{3}\ln\left(1+\frac{sh^2\kappa}{ch^2\left(\kappa\left(n-n_{centr}\right)-shk*t\right)}\right), \qquad v_n = \dot{q}_n, \tag{3}$$

where q_n is a dimensionless displacement from an equilibrium position of n-th particle along one of crystallographic axes, v_n is a corresponding velocity. Periodic boundary conditions are used. The characteristics of a soliton-like excitation are specified by parameters κ (where $1/\kappa$ corresponds to soliton width at mid-height) and amplitude A. In our simulations narrow high energetic supersonic solitons are considered (κ = 2, A = 1.5 – 2.4). One should note that for a soliton in 1d chain A=1 but in case of higher dimensionality the values of A should consider the compensation of bonds with particles in adjacent lattice rows.

3. Results of simulations

First of all we should take into account that in case of high initial amplitude of a quasi 1d soliton-like excitation its “radiation” to adjacent rows is low because frequencies of the perturbations spectrum of the fast running soliton are higher than the critical frequency of the phonon band [15-17]. For this reason, initially excited soliton (Fig. 1a, b) first moves with low energy losses.

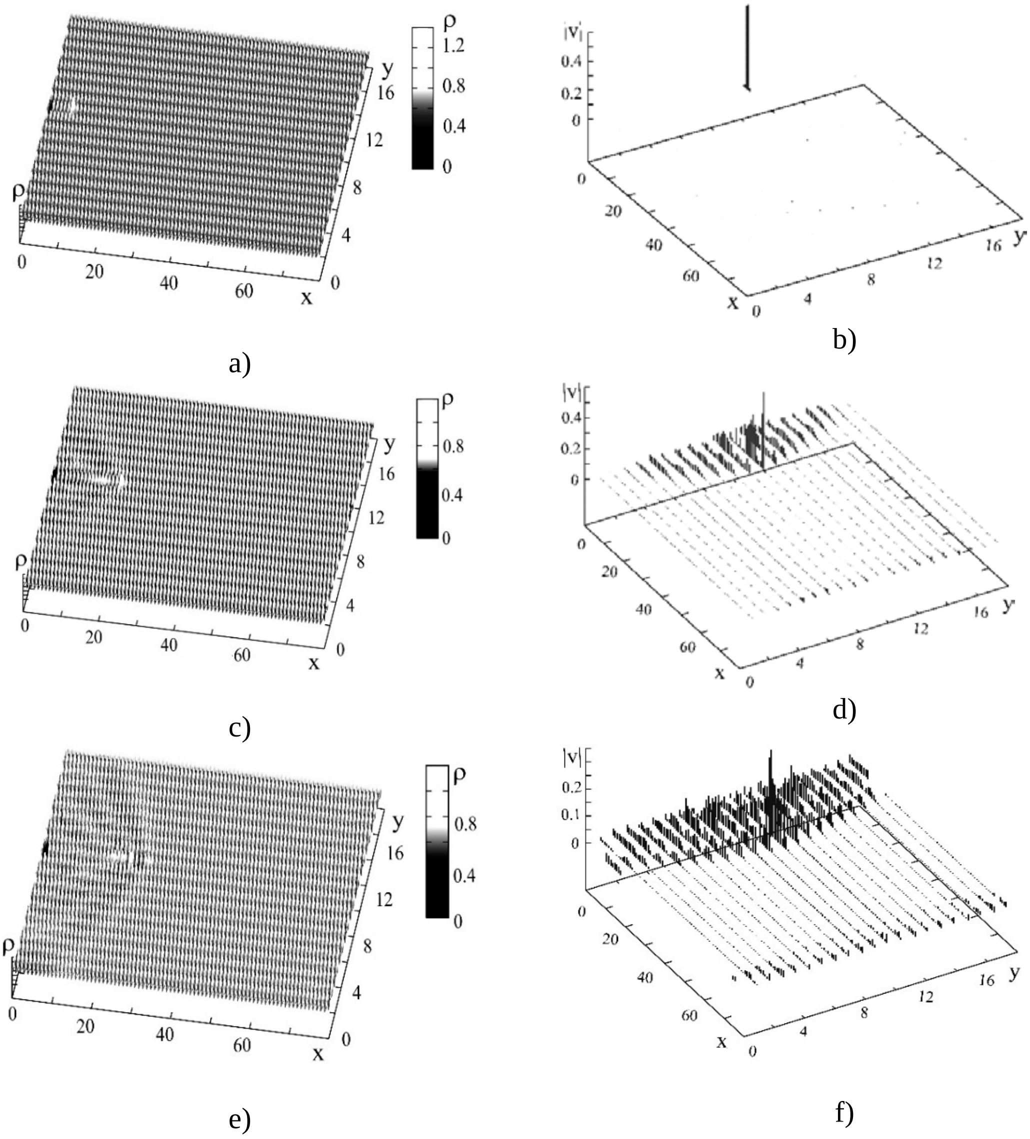

Fig. 1. Triangular Morse lattice. Distributions of density ρ (x,y) (a, c, e) and velocity modulus $|v_n|$ (b, d, f) at initial time t = 0 (a,b), at intermediate time instant t = 5 (c,d) and at the time instant before disintegration of the quasi 1d soliton t=10 (e,f). N = 1600, $b\sigma$ = 4, A = 2, κ = 1.5. The value $b\sigma$ = 4 is chosen to be optimal one in a range of possible values of the stiffness coefficient b.

Nevertheless as it moves the soliton velocity v_{sol} decreases significantly. The radiation intensity increases with decreasing v_{sol} value. The formation of a new localized excitation behind a soliton in the same atomic row has been observed (Fig. 1c, d). In 1d lattice this phenomenon of splitting of initial excitation which is not an exact soliton of the equation of motion defines a solitonic train. However in the considered case such splitted part of the initial excitation is breather-like. The process is terminated when the whole soliton disintegrates without the formation of any topological lattice defect (Fig. 1e, f). One should note that the path length of such quasi 1d excitation is not too long. It increases with the energy of the initial excitation (amplitude *A*), see Fig. 2. However this pattern works in a limited amplitude range because of increase of lattice strain at high *A* values.

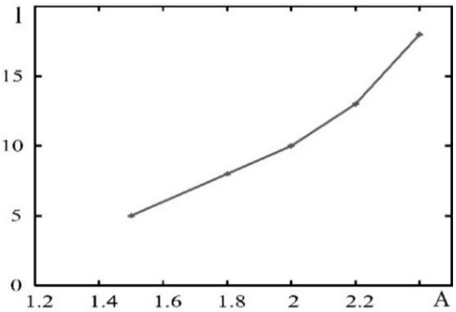

Fig. 2. Triangular Morse lattice. Dependence of the localized solitonic excitation track length on its amplitude *A*. N = 1600, $b\sigma$ = 4, κ = 1.5.

One can increase the path length by exciting initial solitons in adjacent atomic rows in such a way that a fragment of a plane wave with a front transverse to the direction of solitons velocity can be formed (Fig. 3a, b). In this case first only external solitons affect the lattice significantly while the transverse motion of internal solitons is collapsed between external rows.

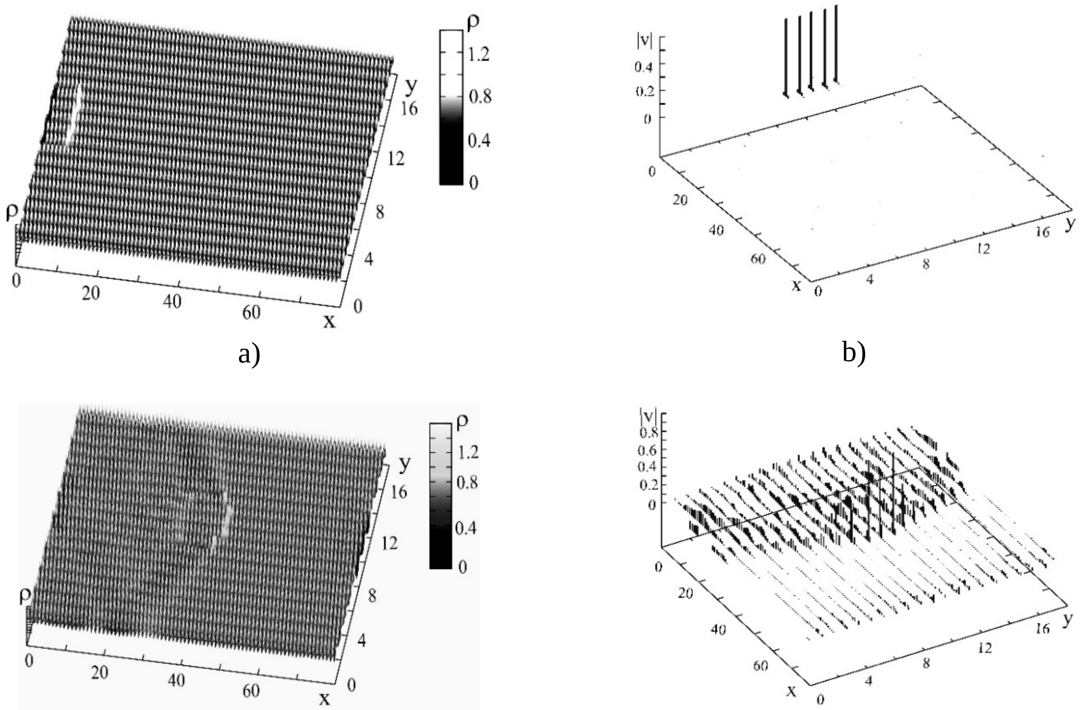

Fig. 3. Triangular Morse lattice. Distributions of density ρ (x,y) (a, c) and velocity modulus $|v_n|$ (b, d) at initial time t = 0 (a,b) and at an intermediate time instant t = 15 (c,d) with the excitation of M=5 solitons in adjacent rows. N = 1600, $b\sigma$ = 4, A = 2, κ = 1.5.

When external solitons loose considerable part of their energy and slow down, the next two internal solitons increase energy loss. It takes place while the initial excitation transforms to a state of quasi 1d soliton followed by further dissintegration. Of course the larger is the number of initially excited rows, *M*, the longer is the path length (Fig. 4).

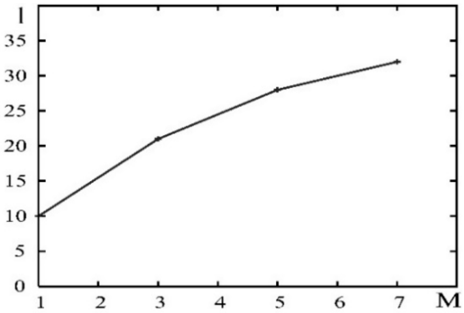

Fig. 4. Triangular Morse lattice. Dependence of the localized solitonic excitation track length on the number, M, of excited solitons in adjacent rows. $N = 1600$, $b\sigma = 4$, $A = 2$, $\kappa = 1.5$.

4. Conclusion

A numerical study of quasi one-dimensional supersonic soliton-like excitations and soliton-like supersonic modes involving *M* adjacent atomic rows (M-solitons) propagating in a triangular Morse lattice has been performed. Solitons in adjacent atomic rows were excited in such a way that a solitary wave front is transverse to the close-packed direction along which the main soliton excitations move. It appears that the maximal distance the solitons can travel grows with increasing soliton amplitude, which in 2d must be higher than in 1d lattices. The maximal distance is not too long due to losses of energy, mainly, from the edges of the soliton-like wave front. Noteworthy is that such maximal distance travelled by the solitons increases with increasing *M* (the number of excited solitons).

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