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Properties of nano-scale soliton-like excitations in two-dimensional lattice layers

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ABSTRACT

Nano-scale soliton-like supersonic, intrinsic localized excitations in two-dimensional atomic anharmonic lattice layers are here considered. We study the propagation, the velocity and other soliton-like features at head-on collisions of such lattice excitations created by using suitable initial mechanical and thermal conditions. Noteworthy is that narrow, highly-energetic solitons moving along one lattice row are very robust, accompanied by weak anti-phase oscillations in the lateral direction.

1. Introduction

It is known that some nonlinear one-dimensional (1d) lattice systems can support localized excitations such as solitons and discrete breathers [1–7]. These excitations are well characterized including the influence upon them of friction and noise effects [8–12]. Following Davydov's and Scott's results [13–15] making use of the Morse potential we have studied the consequences of two superposed nonlinearities, one underlying the Davydov electro-soliton in originally harmonic lattices and the other underlying the originally anharmonic lattice soliton [16–23].

We shall consider here the excitations of lattice solitons in two-dimensional (2d) lattices, modeling mono-atomic layers. This work was stimulated by recent studies of nonlinear excitations in cuprate-like lattice layers and related materials [24–27]. Most of the mentioned works dealt with the study of breathers pinned or moving. Here our attention is devoted to soliton-like excitations, moving generally with supersonic velocity. As lattice solitons we denote strong (structure-less), localized compression waves able to travel practically undeformed. In hydrodynamics [28–41], in gas dynamics [42], in reaction–diffusion systems [5,43], in optics [44–51], in acoustics [52,53], and in Bose–Einstein condensates [54,55], 2d soliton excitations have been predicted and/or observed experimentally.

Several authors studied also soliton-like excitations in 2d molecular *square*, *triangular* and *hexagonal* lattices [24,56–60]. Eilbeck and colleagues [24–26] found propagating *breathers* in 2d hexagonal lattices and searched for high-temperature superconductance in layers of cuprate-like systems. Newns and Tsuei [27] investigated nonlinear excitations arising from bistable fluctuating bonds. We are using here a related model with Morse-type atomic interactions, neglecting however for simplicity on-site vibrations. The soliton-like excitations could be initiated either through suitable initial conditions (by adding momentum to chosen lattice units) or by heating the lattice with an appropriate thermal bath. The latter permits modeling the dynamics by Langevin equations for N atoms arranged in a plane.

2. Triangular lattice with Morse interaction and heat bath

The lattice particles or "atoms" in the layer repel each other with exponentially repulsive forces and attract each other with weak dispersion forces. The characteristic distance determining the repulsion between the particles in the lattice is σ, the equilibrium interparticle mean distance which is used as the length unit. Further a parameter b defines the strength of the repulsion between particles, otherwise called the lattice stiffness constant. Assuming that the forces depend only on the relative distance $r = |r_n - r_k|$ and derive from a suitably modified Morse potential with a smooth cut-off at 1.5σ, to avoid over representation of neighbors, we can write:

$$V(r) = 2D\left\{\exp\left[-2b(r-\sigma)\right] - 2\exp\left[-b(r-\sigma)\right]\right\} \times \left\{1 + \exp[(r-d)/2\nu]\right\}^{-1}. \quad (1)$$

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For the particular case of a *triangular* lattice, the evolution of the coordinates of particles are obtained by solving the Newton's equations of motion with the Morse forces (1) augmented with weak friction and random forces accounting for the surrounding thermal bath in which the atomic layer is embedded, thus leading to the earlier mentioned Langevin's equations. For illustration in our computations we use (1) with $b\sigma = 4, d = 1.35\sigma$ and $\nu = 0.025\sigma$. We use complex coordinates $Z = x + iy$, where x and y are Cartesian coordinates. Then we can write

$$\frac{d^2Z_n}{dt^2} = \sum_k F_{nk}(|Z_{nk}|)z_{nk} + \left[-\gamma_0\frac{dZ_n}{dt} + \sqrt{2D_v}\left(\xi_{nx} + i\xi_{ny}\right)\right], \tag{2}$$

where an index n identifies a particle among all N particles of the ensemble, γ_0 is a friction coefficient with the dimension of a reciprocal frequency, D_v defines the strength of stochastic forces, with $T = D_v/\gamma_0$ (Einstein's relation) defining the corresponding temperature. The quantity $\xi_{nx,y}$ denotes statistically independent generators of the Gaussian white noise, $Z_{nk} = Z_n - Z_k$. Further $z_{nk} = (Z_n - Z_k)/|Z_n - Z_k|$ is a unit vector defining the direction of the interaction force F_{nk}, between the n-th and the k-th particles, corresponding to (1). In view of the above, only those lattice units with coordinates Z_k, satisfying the condition $|Z_n - Z_k| < 1.5\sigma$, are taken into account. Time is normalized by the inverse frequency of linear oscillations near the minimum, depth D, of the Morse potential well (1) denoted by ω_M^{-1}. The energy is scaled with $2D$. In the computer simulations, with periodic boundary conditions, the evolution of particles is considered to take place inside a region with $N = 400$ particles initially defining a *triangular* lattice $20\sigma \cdot 20\left(\sqrt{3}/2\right)\sigma$.

3. Numerical experiments

After making a choice for the temperature we started the simulations with a strong coupling to the thermal bath. When the system reaches thermal equilibrium with the bath, i.e. when the kinetic energy is constant in time, we lower the coupling to a very small value using *friction* parameter values in the range $\gamma_0 = 10^{-5} - 10^{-2}$. The *friction* starts being so small that no influence on the properties is observed, the system is still *canonical* but already at the border of a *micro-canonical* ensemble. The influence of Stokes-type friction which we use in our model on solitons has also been studied in detail by Arevalo et al. [8,9] for truncated (at fourth-order term) 1d Morse lattices. According to their estimates the Stokes damping does not permit the long wave components of wave packets to propagate for $t > 1/\gamma_0$. In our time units this means that for $t > 10^2 - 10^5$ the solitons may be strongly influenced by Stokes friction. For that reason we limited our computer runs to short enough albeit significant time intervals, $t = 10 - 10^2$, to ensure that soliton excitations are not significantly influenced by the Stokes friction.

In a first series of computer experiments we generate initially nearly *planar* excitations having locally the profile of a Toda soliton [2] with (reciprocal) width χ. The estimated velocity of the excited wave depends on χ as depicted in Fig. 1. As it can be seen, the velocity of the excitations appears in the range from about to significantly above the (linear) sound velocity. To visualize the space and time evolution of compressions along the lattice we first use the method of tracking atomic electron densities [12,61] as the lattice units or atoms are modeled as little spheres formed by the "atomic" electrons. Each of these atomic electrons are represented by a Gaussian distribution, with width $\lambda = 0.3$, centered on each lattice site. Noteworthy is that the electrical structures we study here are in the nano-scale range since at the macroscopic scale screening effects make such structures impossible.

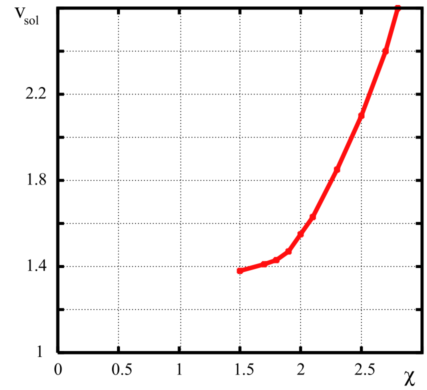

Fig. 1. Triangular Morse lattice. $N = 400$ (20×20) atoms or lattice sites. Velocity of soliton-like excitations in units of the 1d (linear) sound velocity represented as a function of the soliton (reciprocal) width.

4. Head-on collision of soliton-like excitations

The propagation of two oppositely moving soliton-like excitations is depicted in Fig. 2. Their velocity is obtained by observing that the lattice excitation moves a distance of 16 units in a time interval of $t = 8$ units. Hence the velocity is $16/8 = 2$ in units of the (linear) sound velocity in 1d lattices. Note that $v_{\text{sound}} = 1$ in 1d lattices and slightly above unity in 2d *triangular* lattices. Since this soliton-like excitation moves with velocity 2 it is clearly supersonic. Besides as Fig. 1 shows the observed wave velocity increases with the (reciprocal) width parameter χ. Fig. 2 also illustrates a *head-on* collision of such lattice excitations quite similar to the case of 2d solitons in fluid flows [31–38]. The density distribution (left column) and the "electric" potential landscape (right column) are displayed for three time instants. We observe a transformation of the initial piece of a *plane* wave, embracing a few rows, to a *horseshoe*-shaped soliton-like supersonic excitation [62–64]. The transverse size of the wave reduces to just one or a few rows of atoms excited at a time. An apparently different type of soliton and another head-on collision event is depicted in Fig. 3 where we see in six consecutive snapshots the propagation of two very narrow bell-shaped solitons with rather high energy. It seems to be a nano-size genuine soliton for discrete lattices. The moving fronts are now moving little hills which propagate with a very high velocity, around 2.8 times the (linear) sound velocity. This special form of highly-energetic and fast (quasi one-dimensional) "bell-shaped solitons" appears very robust. We see in Figs. 2 and 3 that the moving soliton-hills run over hundreds of lattice sites and cross each other without any appreciable change of shape. This is a "signature" of solitons as it is also for the hydrodynamic case and for other systems (for further details see also [33–35,65]). This seems remarkable since they move in a heated medium of moderate temperature and hence are subject to noise and friction. Of course, they are not solitons in a strict mathematical sense originating from a lattice Hamiltonian integrable system.

Noteworthy is that the life-time of the soliton-like excitations though long is always finite and depends on the initial front length. Of special interest are the fast and highly-energetic solitons shown in Fig. 3. These narrow (quasi one-dimensional) excitations comprise of just very few lattice sites and are more affected by the discrete character of the lattice. We see some similarities to moving breathers found by other authors [24–26] as, e.g., the small extension in all directions and the shape of a little hill. On the other hand, our narrow solitons are very fast, with velocities about 2–3 times the (linear) sound velocity in the lattice and carry rather high energies. It appears that the transverse oscillations in the vicinity of our narrow highly-energetic solitons exhibit similarity with finite size optical modes. In our case, at variance to

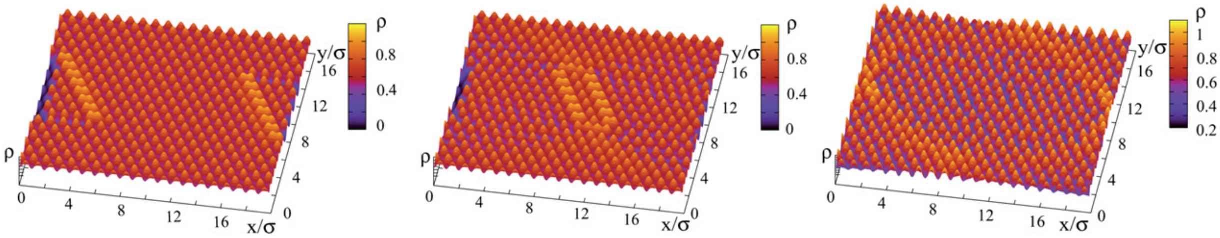

Fig. 2. Triangular Morse lattice. Head-on collision of two oppositely moving solitons: $t = 0$ (initial configuration; left panel), $t = 4$ (near collision; center panel) and $t = 8$ (after collision; right panel). All dots correspond to peaks in Gaussian atom core electron densities as indicated in the main text. We see the enhanced overlapping of the densities which is a signature of the underlying local mechanical lattice compressions. Parameter values: $N = 400$, $b\sigma = 4$, $\lambda = 0.3$, $\gamma_0 = 10^{-5}$ and $T = 0.01$ (note that this temperature corresponds to quite a "cold" lattice hence to a practically purely mechanical problem).

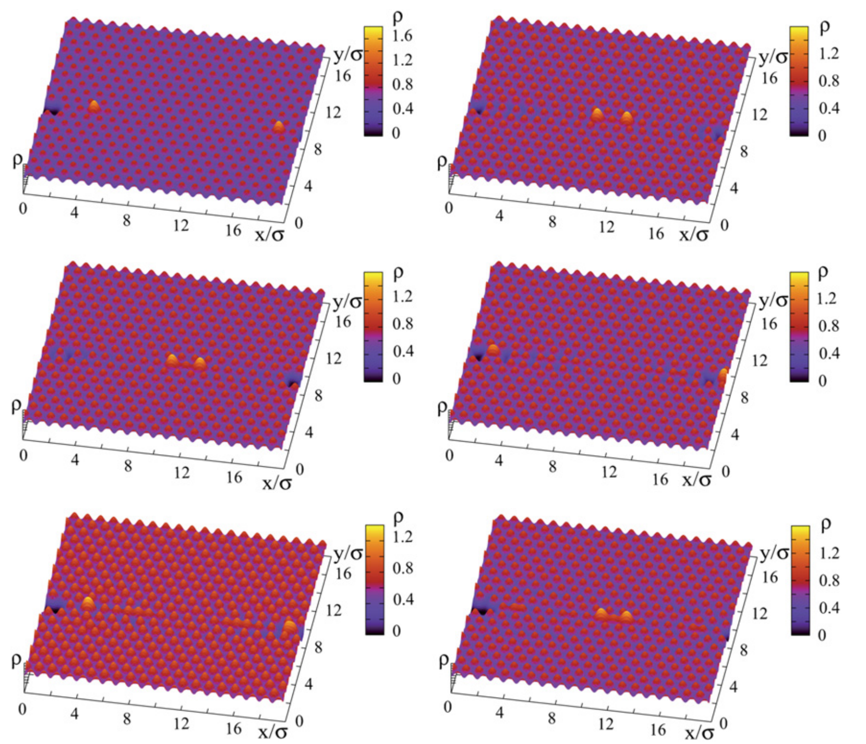

Fig. 3. Triangular Morse lattice. Head-on collision of two initially and subsequently unaltered highly-energetic nonlinear soliton-like excitations moving in opposite directions with supersonic speed at six consecutive time instants: $t = 2, 3, 4, 5, 6, 7$ in left-to-right, top-to-bottom zig-zag reading. Note that the solitons cross several times the boundaries, with weak transverse size. Parameter values: $N = 400$, $b\sigma = 4$, $\lambda = 0.3$, $\gamma_0 = 10^{-5}$ and $T = 0.01$.

breathers, the nonlinear effects are concentrated in just one lattice row. To further analyze our nonlinear excitations, we studied also the evolution of the transverse motion as shown in Fig. 4. The transverse oscillations are in anti-phase to motions in adjacent rows and have a dimensionless frequency a bit below 3. Recall that the dispersion law for a 1d lattice is

$$\omega = 2\omega_M \left|\sin\frac{k\sigma}{2}\right|, \tag{3}$$

where ω_M is the oscillation frequency of an atom sitting at the minimum of the Morse potential which is 1 in our units. The maximal frequency value is $\omega_{\max} = 2$ and the corresponding period is $\tau = 2\pi/\omega_{\max} = 3.14$. A *triangular* 2d lattice is asymptotically equivalent (from the point of view of forces acting on a particle along of main axes) to a 1d lattice with twice the stiffness. The corresponding maximal frequency value is then $\omega_{\max} \simeq 2\sqrt{2}$ and the period is around 2.2. Though an asymptotic approximation this result leads us to expect that the (inverse) oscillation frequencies are in the range $2.2 < \tau < \pi$. The period estimated from the computer experiment is $\tau \simeq 2.9$.

Let us emphasize that our intrinsic localized modes are in the nano-scale range and they include no more than 10–100 atoms. The nano-size of our 2d soliton excitations makes possible the existence of electric structures due to electric *polarization*

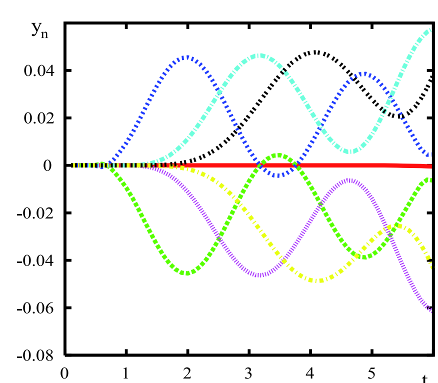

Fig. 4. Triangular Morse lattice. Time evolution in the atomic rows adjacent to the (central) one in which a high energy soliton-like excitation is running (red: soliton row; dark blue and green: nearest row; light blue and pink: next-nearest row, etc.). The (dimensionless) period of oscillations is below 3. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

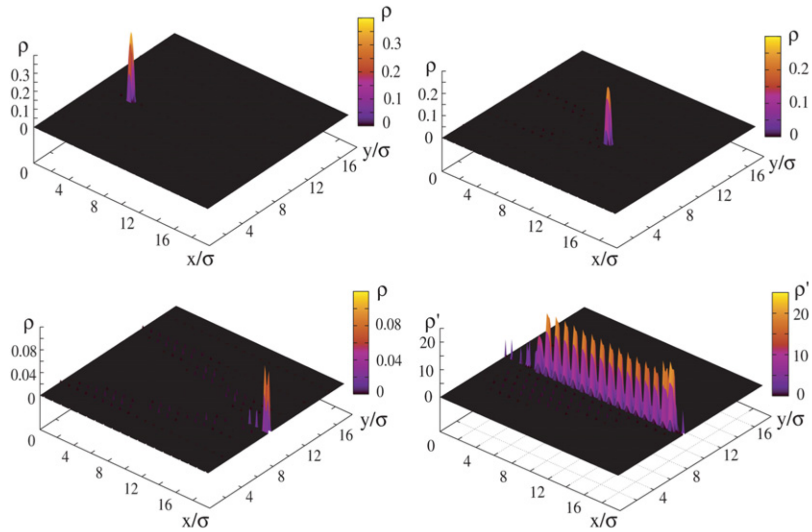

Fig. 5. Triangular Morse lattice with atoms as units. Density of atom core electrons after retaining only the highest peaks. The sequence of three snapshots, corresponding to three time instants, illustrates the long lasting quasi-1d solitonic excitations running along a crystallographic axis. The initial condition is an "optimized" Toda profile as explained in the main text. The last figure is a "bubble-chamber-representation" (including memory), i.e., a cumulative plot of many consecutive snapshots for the given time interval at the prescribed final time instant. Parameter values: $N = 400$, $b\sigma = 4$, $\lambda = 0.3$ and $T = 0.01$.

effects. These electrical polarization fields may influence electron dynamics and be accompanied by the corresponding electron waves at the nano-scale. This may lead to electron trapping by moving polarization waves if excess electrons are added to the system.

5. Long lasting quasi-one-dimensional solitons

In the preceding section we have provided features of quasi-onedimensional solitons in two-dimensional lattices. Their shape is Toda-like in the direction of propagation and Gaussian-like in the transverse one. By changing the initial coordinates and velocities in a wide range we found that in the family of quasi-one-dimensional soliton-like excitations there is one of particular (numerical) high stability which is running along one of the crystallographic directions, whose longitudinal profile is determined by Toda solitons with an effective stiffness b_{eff} replacing the original Toda stiffness.

Indeed, here we denote by a "Toda-like" soliton a lattice excitation

$$x_{n+1}(t) - x_n(t) = 1 - \frac{1}{b_T}\left[\ln \frac{\sinh^2(\kappa)}{\cosh^2(\kappa n - \beta_0 t)}\right], \tag{4}$$

measured in units σ in a Toda lattice with stiffness b_T described for deviations from unit equilibrium distances (in units σ). The parameter κ is related to the energy of the soliton. Further ω_0 is the frequency corresponding to the minimum of the Toda potential. Besides the parameter β_0 denotes the reciprocal characteristic time

$$\beta_0 = 1/\tau = \omega_0 \sinh\kappa. \tag{5}$$

In earlier publications [16,21,66–68] it has been shown that the analytical expressions obtained by Toda may be used to describe the solitons obtained by simulations for 1d-Morse chains, if the Toda stiffness is replaced by, e.g., three times the Morse stiffness i.e. by the replacement $b_T \to 3b$, where b is now the stiffness of the Morse potential defined by Eq. (4). This way, an appropriate analytical description for the soliton-like deformations running in 1d-Morse lattices is

$$x_{n+1}(t) - x_n(t) = 1 - \frac{1}{3b}\left[\ln \frac{\sinh^2(\kappa)}{\cosh^2(\kappa n - \beta_0 t)}\right]. \tag{6}$$

In order to find an appropriate description for the solitons which we have observed along crystallographic axes of 2d lattices we have used again this formula (6) for the initial conditions. However it occurred that we fail to describe the narrow solitons in 2d-Morse lattices. We found out empirically that in order to get stable running solitons, we had to increase the compression by a factor two, that means we used instead of the factor $1/3b$ in Eq. (6) the factor $2/3b$, which was like using $b_{\mathrm{eff}} = 1.5b$. Then we used b_{eff} as a free parameter trying to find out the minimal level of additional excitations both along the trajectory of a soliton and transverse to it. In most cases the initially localized excitation spreads as time proceeds, as expected. Our numerical experiments clearly show that the value b_{eff} corresponds to the longest lasting excitations (Fig. 5). We may conclude that for the above mentioned conditions the analytical Toda formula for the one-dimensional chains with Toda interactions may be used also for the description of quasi-onedimensional soliton-like excitations in 2d triangular Morse lattices after the procedure of changing the compressions by some factor as described above. From the point of view of physics, the changes in describing a two-dimensional Morse lattice are due to the influence of the rows parallel to the active chain where the soliton runs. The neighboring rows create additional forces which change the effective forces acting along the active chain and change the amplitudes. This requires some changes to find the excitations which have optimal stability against perturbations and the longest lifetime. After numerous computer runs we came to the conclusion that the quasi-one-dimensional "adapted" or better "optimized" Toda solitons with some adapted compression which may run on rows along the main crystallographic directions are of particular high stability and have a quite long lifetime. Illustrations of the results are depicted in Fig. 6 where we show the velocity distribution of the particles in the direction of the soliton propagation and transverse to it. A high peak appears in the direction of soliton motion representing the motions in the "active" row and a small spreading in the transverse direction corresponding to oscillations of the lattice neighbors perpendicular to the soliton propagation.

We have cross-checked that this type of excitation is similarly long lasting and stable also along all other crystallographic axes. We expect that this property holds also for other symmetries, e.g., in the case that rectilinear chains of atoms are realized, as, e.g., in *NaCl* crystals.

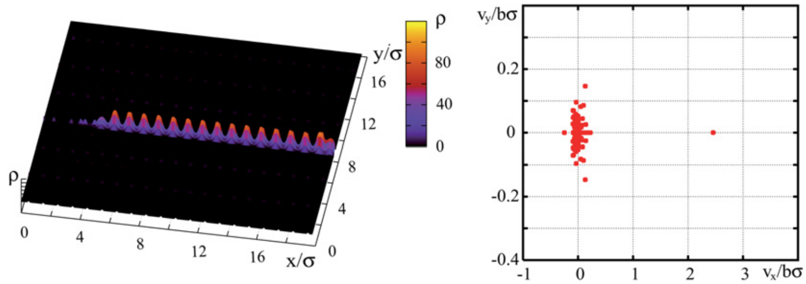

Fig. 6. Triangular Morse lattice. Cumulative picture of the peaks of atom core electron density illustrating long lasting and hence highly stable soliton-like excitations running along a crystallographic axis in a 2d triangular Morse lattice ("bubble chamber representation"). The right picture shows the velocity distribution of the lattice units. The peak in the x-direction corresponds to the propagating soliton, the lateral distribution in y-direction corresponds to oscillations transverse to the direction of the soliton propagation. Parameter values: $N = 400$, $b\sigma = 4$, $\lambda = 0.3$ and $T = 0.01$.

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