Eur. Phys. J. B **80**, 137–145 (2011)
DOI: 10.1140/epjb/e2010-10604-0

THE EUROPEAN PHYSICAL JOURNAL B

Regular Article

Soliton-like excitations and solectrons in two-dimensional nonlinear lattices

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Received 4 August 2010 / Received in final form 10 November 2010
Published online 14 January 2011 –

Abstract. We discuss here the thermal excitation of soliton-like supersonic, intrinsic localized modes in two-dimensional monolayers of atoms imbedded into a heat bath. These excitations induce local electrical polarization fields at the nano-scale in the lattice which influence electron dynamics, thus leading to a new form of trapping. We study the soliton-mediated electron dynamics in such systems at moderately high temperatures and calculate the density of embedded electrons in a suitable adiabatic approximation.

1 Introduction

The properties of one-dimensional (1d) nonlinear lattices are well explored, starting with the Fermi-Pasta-Ulam models [1] and several analytical solvable other models like the Toda lattice [2]. Arevalo et al. [3,4] studied the influence of friction and noise on solitonic excitations in lattices with cubic and quartic anharmonicities as well as for a truncated Morse potential. Two types of damping were investigated: external friction of Stokes-type and internal friction (inelastic friction, also called hydrodynamic friction). It was shown that Stokes-type friction strongly influences the long-wave components of solitonic excitations and that solitons decompose after a time in the order of $1/\gamma_0$, where γ_0 (in our notation) is the characteristic collision frequency connected with Stokes friction.

Here we study soliton-like excitations in two-dimensional atomic layers which are weakly coupled to an external heat bath modeling the surrounding by a standard Langevin equation. We do not have in mind a concrete physical system but just for illustration one could think about the nonlinear excitations in atomic monolayers at a surface, or about the CuO_2 layers in cuprate-like lattices.

We are mostly interested in the influence of soliton-like excitations on electronic properties of the layer. As lattice solitons we denote here strong, localized compression-expansion waves (we shall focus on the compression) able to travel some time practically undeformed with, generally, supersonic velocity. In recent works we have discussed how electron trapping by solitons influences electric conduction on anharmonic 1d lattices [5–16]. In two-dimensional (2d) systems, nonlinear effects are expected to play also a similar role. We are aware that solitons in 2d-systems are difficult to rigorously define. However as in 1d systems we still may find compression waves or, in other words, intrinsic localized modes running approximately with sound or supersonic velocity. In the field of hydrodynamics, the existence of 2d solitonic excitations moving along surfaces and in falling films is known both in theory and experiment [17–20]. For optical lattices, the existence of soliton-like excitations in 2d-systems was also shown theoretically [21] and found experimentally [22,23].

Further, several authors [24–33] have shown the existence of soliton-like excitations in 2d molecular square, triangular and and hexagonal (honeycomb) lattices with in-plane displacements. Marin et al. [34] found in a 2d hexagonal lattice model propagating breathers, and recently Russell and Eilbeck reported about nonlinear excitations, they called *quodons* [35,36]. From the methodological viewpoint it is worth noting that several authors [21,24,26,28] have shown that for particular nonlinear lattices, a continuous description of the nonlinear excitations is possible by means of coupled nonlinear Schrödinger equations or by suitable generalizations of the soliton-bearing Kadomtsev-Petiashvili equation [37].

In the present work we study strongly nonlinear thermal excitations in 2d lattices of atoms with Morse interactions. We investigate here transient nonlinear structures at the nano-scale with wave fronts including not more than 10−100 atoms and lasting a time of the order of 10 time units (corresponding to the reciprocal basic oscillation frequency). In reference [16] we studied soliton-like excitations in 2d-lattices at zero temperature. Here we introduce temperature and explore features of 2d excitations in such *heated* lattices. Needless to say as temperature increases quite many static and dynamic excitations may appear provided a sufficient level of the mean

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thermal energy is reached [15]. Some evidence for the existence of thermally excited soliton-like compression waves comes from simulations for 2d Lennard-Jones systems at "moderate" temperatures [38–40]. For example the molecular dynamics calculations of the specific heat of thermal molecular systems on a plane show at moderately high temperatures a significant deviation from the ideal mean temperature Dulong-Petit plateau of a linear (harmonic) lattice thus pointing to the existence of nonlinear effects. At temperatures which are too low, only infinitesimal, linear excitations (phonons) are excited. On the other hand, at too high temperatures, the life-time of nonlinear excitations is too short and besides the anharmonic lattice approaches the hard sphere fluid limit. Accordingly, we are interested in a temperature range where lattice-excitation amplitudes are large enough for the nonlinearities to play a genuine role [41]. It is also known [38–40] that the scattering of the nonlinear excitations on embedded impurities involves soliton-like waves at non-zero temperature.

Let us estimate now the region of interest, where the transition from the linear (phonon) region to the nonlinear (soliton) region occurs. In the 1d case this transition is well explored for Toda lattices [41] as well as for Morse lattices [9,12]. For Morse lattices it was shown that nonlinear excitations are found in the region $T \simeq (0.1{-}0.4)D$ where D is the depth of the potential well. In the 1d-case a molecule with one neighbor to the right and one to the left sits in a well with the depth $2D$. In the 2d case, assuming a triangular lattice the number of neighbors is 6 corresponding to a depth of the well $6D$. At temperatures corresponding to thermal amplitudes less than 10 percent of the well, we expect that phonon excitations dominate, whereas at higher temperatures, say between 10 and 60 percent of the depth of the well, we expect to see well-expressed nonlinear excitations. At still higher temperatures, we expect so many short-time excitations, that an identificaction of specific excitations like solitons is practically impossible. An estimate for the region of temperatures where we expect to see interesting effects is therefore $T \simeq (0.1{-}0.6)6D$. As temperature is measured in units of $2D$ then the (dimensionless) temperature regime of interest is around $T \simeq (0.5{-}2)$ in the 2d case.

Please note that here we shall not deal with excitations that can rigorously considered as solitons in the mathematical sense. Rather we shall consider whether these nonlinear-excitations, local compressions or intrinsic localized modes, run through the system with sound or supersonic velocity and last long enough to affect electron transfer or electric transport. Indeed the question which interests us is in particular the influence of nonlinear thermal excitations on the behavior of added "free" electrons in the system as earlier studied by Landau et al. [42–46]. It was shown that due to the nonlinearity induced by the electron-(acoustic) phonon interaction that is due to the Landau-Pekar polaron, or electron self-trapping process, soliton-like excitations, which Davydov called "electro-solitons", may travel along originally *harmonic* lattices. Davydov conjectured that for biomolecules these excitations could be stable at finite temperatures and could persist even at "physiological" temperatures. Unfortunately, however, several authors have found numerical evidence that Davydov's electro-solitons are destroyed already around 10 K and usually lasted only a few picoseconds (ps) [47–50]. If the underlying lattice dynamics is *anharmonic* like in the Toda and other nonlinear lattices then Davydov's conjecture is verified and the result is the appearance of quite stable (lifetime of the order of 10 time units) *supersonic* (acoustic) solitons [1,2,6,51]. We continue here with Davydov's idea making use of a truncated Morse potential and hence adding the *anharmonicity* of the lattice dynamics to the (nonlinear) electron-lattice interaction. Clearly these excitations bring a new form of "dressed" electrons formed as compounds of two different nonlinearities: (electro-soliton)-lattice soliton dynamic bound states. In the 1d case these bound states have been called, in short, "solectrons" to mark the difference with Davydov's original electro-solitons. Here in 2d Morse lattice systems we analyze the conditions for electrons to be also attracted to the local compressions thus calling them 2d- solectron excitations.

In 1d-systems the thermally excited solectrons are always disconnected. Therefore, with the kind of short-range interactions we consider in the lattice, we cannot have 1d-systems with spontaneously formed long range ordering hence highly conducting states. However, in 2d-systems the local compressions may eventually connect, thus leading to "wire-like" percolation trajectories.

The case of linear 2d lattices interacting with electron added has been studied by Brizhik et al. [52,53] where the self-trapping of electrons by lattice oscillations was shown. Our problem here can be considered as a follow-up of their work as we are including nonlinear lattice interactions. In the parameter range studied here, the trapping of electrons by solitonic excitations dominates in comparison to self-trapping effects. Adding temperature, the lattice units with Morse interactions are treated by classical Langevin equations, modeling the coupling of the atomic monolayer to the matter below and above by a weak coupling to a heat bath. For visualizations the densities of the core electrons are in a first approximation represented by Gaussian densities, thus permitting to follow the underlying lattice compressions. In a different approach the dynamic distributions of the (free) electrons is modeled using adiabatic approximations for the density of the (free) electrons based on Boltzmann-distributions.

In Section 2 we introduce our model for the description of 2d- atomic lattices based on a standard Langevin equation for the dynamics. We investigate the case of small Stokes friction and white noise, modeling weak coupling to an external heat bath with given temperature T. The simulations are carried out for relatively short times where the influence of the heat bath is small. According to Arevalo et al. [3,4] the Stokes damping does not permit the long wave packets to propagate for larger times of order $t > 1/\gamma_0$. We will concentrate therefore on short-time excitations for $t < 1/\gamma_0$. In Section 3 we develop the method of visualization of the non-uniformities in the lattice, which allows us to estimate the region of soliton-like excitations as well as their life times. Section 4 deals with the electron-lattice interaction thus describing how lattice deformations (or, more precisely, relative displacements between lattice units) affect added excess (free) electron motions and hence we also discuss polaron-like effects.

2 Two-dimensional model of the dynamics

The Hamiltonian consists of a classical lattice component H_a, and the contribution of the electrons H_e, which includes the interactions with the lattice deformations. Focusing on the lattice part, the Hamiltonian is

$$H_a = \frac{m}{2}\sum_n v_n^2 + \frac{1}{2}\sum_{n,j} V\left(r_n,\, r_j\right). \qquad (1)$$

The subscripts locate lattice sites and the summations run from 1 to N. The characteristic length determining the repulsion between the particles in the lattice is σ. We shall assume that the lattice particles repel each other with exponentially repulsive forces and attract each other with weak dispersion forces. We limit ourselves to nearest-neighbors only using the relative distance $r = |r_n - r_k|$. Then using the Morse potential (see Fig. 1) we set:

$$V = D\left\{\exp\left[-2b(r-\sigma)\right] - 2\exp\left[-b(r-\sigma)\right]\right\}. \qquad (2)$$

The peculiarity of 2d systems demands modifications of the potential in the long-range part, in order to avoid unphysical cumulative interaction effects. By imposing a suitable cut-off this rules out a stronger interaction than due arising from the influence of particles outside the first neighborhood of each particle. In fact, rather than a cut-off we consider the interaction with a smooth decay to zero as distance increases [38–40]. Hence rather than (2) for the 2d lattice we take

$$V(r) = D\left\{\exp\left[-2b(r-\sigma)\right] - 2\exp\left[-b(r-\sigma)\right]\right\} \times \left\{1 + \exp\left[(r-d)/2\nu\right]\right\}^{-1}. \qquad (3)$$

As a rule the cut-off "interaction radius" is supposed to be equal to 1.5σ, together with parameter values $d = 1.35\sigma$ and $\nu = 0.025\sigma$. In Figure 1 the original Morse potential (2) is shown in green and the modified one (3) in red. Beyond the cut-off radius the potential is set to zero. To study, at varying temperature, the nonlinear excitations of the lattice and the possible electron transport in a lattice in the simplest approximation it is sufficient to know the lattice (point) particles coordinates at each time and the potential interaction of lattice deformations with electrons. Coordinates of particles are obtained by solving the equations of motion of each particle under the influence of all possible forces. The latter include forces between particles which are supposed to be of the Morse kind and the friction and random forces accounting for a Langevin model bath in the heated lattice. The physical model behind our Langevin equations is the following: we consider a layer of atoms and electrons which is embedded into an external heat bath of temperature T, which creates

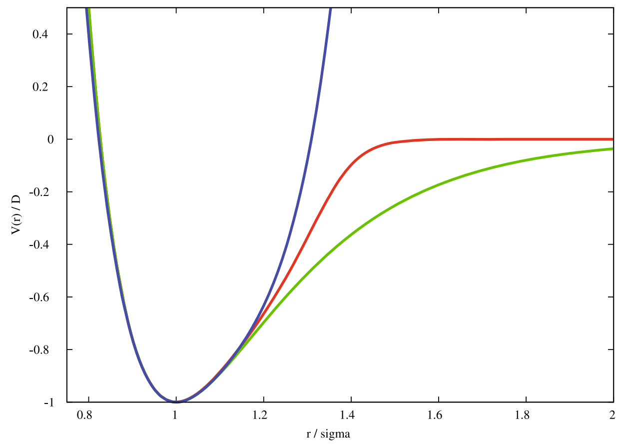

Fig. 1. (Color online) Interaction between lattice particles: comparison of the original Morse potential (green dotted line) with the "truncated" Morse potential used by Arevalo et al. [3] (blue line) and our "truncated" (and modified) Morse potential (solid red line) used for our computer simulations (parameter values $b\sigma = 4$, $d = 1.35\sigma$, $\nu = 0.025\sigma$).

some noise and Stokes friction. Both of these external factors should obey the Einstein relation. This way we are working within the canonical ensemble. We are well aware that beside Stokes friction exist alternative possibilities for modeling dissipation. Arevalo et al. [3,4] studied solitonic excitations in 1d-systems with cubic and quartic anharmonicities comparing two models of dissipation: Stokes (outer) friction and hydrodynamic (internal) friction. It was shown that the Stokes damping does not permit the long wave components of the wave packet to propagate, while the hydrodynamic friction allows this under certain conditions. We understand that according to this result, the hydrodynamic friction is in certain respect more favorable for the excitations of solitons than the Stokes friction. However our aim is here to model a physical problem, namely the excitations in an atomic layer coupled to a reservoir in thermal equilibrium. In this physical situation we consider the Stokes friction, which is an outer friction generated by the reservoir as the more appropriate physical model.

For convenience in the 2d lattice dynamics we use complex coordinates $Z = x + iy$, where x and y are Cartesian coordinates. Then the Langevin model brings the equation for the lattice units

$$\frac{d^2 Z_n}{dt^2} = \sum_k F_{nk}\left(Z_{nk}\right) z_{nk} + \left[-\gamma_0 \frac{dZ_n}{dt} + \sqrt{2D_v}\left(\xi_{nx} + i\xi_{ny}\right)\right], \qquad (4)$$

where an index n identifies a particle among all N particles of the ensemble, γ_0 is a friction coefficient, D_v defines the intensity of stochastic forces, $\xi_{nx,y}$ denotes statistically independent generators of the Gaussian 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}, corresponding to the Morse potential, between the nth and the kth particles. To have dimensionless variables we consider the spatial coordinates normalized to the length σ used in the Morse potential (2) or (3). Time is normalized to the inverse frequency of linear oscillations near the minimum of the Morse potential well, ω_M^{-1}. As earlier noted, the energy is scaled with $2D$, where D is the depth of the Morse potential well. Further the (dimensionless) parameter b defines the strength of the repulsion between particles. The interaction force F_{nk} is given by

$$F_{nk} = F_{nk}\left(|Z_{nk}|\right) = - \left.\frac{dV(r)}{dr}\right|_{r=|Z_{nk}|}. \quad (5)$$

In view of the above only those lattice units with coordinates Z_k, satisfying the condition $|Z_n - Z_k| < 1.5$, are taken into account in the sum in equation (4). In computer simulations the interaction of particles is considered to take place inside a rectangular cell $L_x L_y$ with periodic boundary conditions and $L_{x,y}$, depending on the symmetry of an initial distribution of units and their number N. For illustration we consider a distribution corresponding to the minimum of potential energy for an equilibrium state of a *triangular* lattice $10\sigma \times 10\sqrt{3/2}\sigma$ for $N = 100$ or $20\sigma \times 20\sqrt{3/2}\sigma$ for $N = 400$. The positions on a triangular lattice at zero temperature ("cold" lattice) are used as initial conditions. Then the lattice is heated by the stochastic source (white noise) to the temperature $T = mD_v/\gamma$. This corresponds to the mean kinetic energy of a particle $\langle T_{kin}\rangle$ reaching the value T. The obtained values of Z_n and $V_n = dZ_n/dt$ are subsequently used as new initial values $Z_n(0)$ and $V_n(0)$ for the lattice at corresponding temperature while setting $D_v = 0$. Notice that by varying $Z_n(0)$ and $V_n(0)$ it is possible to specify a localized excitation in a lattice. Using data about trajectories of particles $Z_n(t)$ and the evolution of velocities $V_n(t)$ we can calculate: (a) the mean kinetic and potential energies of the particles; (b) the temperature of the ensemble; and (c) the particle distribution $\rho(Z,t)$ using a formula introduced in the following section.

Technically speaking the simulations are carried out in two steps:

Step 1: we make a choice for the temperature and start simulations with a strong coupling to the heat bath. When the system reaches the thermal equilibrium with the heat bath, i.e. if the kinetic energy is constant in time, we switch off the coupling and go to the next step.

Step 2: the friction is now zero or so small, that no influence on the properties is observed. Now we start the observations, all pictures given are from this second phase of the simulations, in which the system is still canonical but already at the border to a micro-canonical ensemble.

We checked that the described properties do not depend on the value of the friction parameter γ_0. If this value is small enough, the relaxation time $1/\gamma_0$ is much larger than the characteristic time of the dynamics of a lattice which is unity in our scale, so we require that $1/\gamma_0 \gg 1$ is fulfilled. In our simulations used friction in the range $\gamma_0 = 0.0001{-}0.001$ and checked carefully that the assumed value does not influence the results. In this case the amplitudes of the stochastic forces are small for the temperature values considered. Therefore the noise and the friction act in our simulations only as negligibly small perturbations to a Newtonian dynamics. Of course, if both of these factors (noise and friction) are switched off completely for step 2 the condition mentioned is in every respect satisfied. We mentioned already that the influence of Stokes-type friction which we used in our model on solitons has been studied in detail by Arevalo et al. for truncated (at the fourth order term) one-dimensional Morse lattices [3]. 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 $t > 1000{-}10000$ the solitons may be strongly influenced by Stokes friction. Since our runs are for time intervals $t = 10{-}100$ we believe that we have some guaranty that solitonic excitations are not strongly influenced by the Stokes friction used in our model.

3 Visualization of nonlinear lattice excitations by representing the evolution of core densities

Following the Boltzmann-Gibbs approach we may expect that, when heating the lattice, in principle, all possible static and dynamic excitations may spontaneously appear with some non-vanishing probability. The probability may however be quite low, to find structures with higher energy and, further, to identify them in the sea of fluctuations. We need therefore an appropriate method to see and to identify the dynamic structures we are searching for. Let us discuss a method of visualization tracking the core electron densities. The lattice units, molecules or atoms may be modeled as points on a plane which are surrounded by little spheres formed by the "atomic" electrons. We will assume that these atomic electrons may be represented by a Gaussian distribution centered on each lattice site:

$$\rho(Z,t) = \sum_{|Z-Z_i(t)|<1.5} \exp\left[-\frac{|Z - Z_i(t)|^2}{2\lambda^2}\right]. \quad (6)$$

The evolution of the density (6) in a cold lattice $T = 0.01$ is illustrated in Figures 2, 3 and 4 by focusing on individual densities and on their overlapping regions. The latter provide unambiguous signature of the excitations in the 2d system of Morse molecules. In Figures 2 and 3 we show the evolution of a solitonic excitation with a front extended over about 10 sites in time. In Figure 4 we see the propagation of a very narrow soliton with rather high energy which moves with 2.8-sound velocity. This special form of high-energetic and fast two-dimensional solitons appears very robust.

The evolution of the density (6) in a heated system ($T = 0.1$) is illustrated in Figure 5. For a generic Hamiltonian, H, the probability of occurrence of an

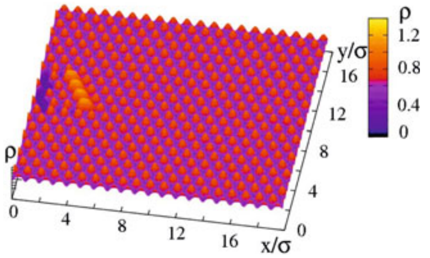

Fig. 2. (Color online) Triangular Morse lattice. The mean density of atomic electrons of $N = 400$ particles. In order to study the evolution of perturbations we changed the initial density at $t = 0$ in a small region creating this way a supersonic soliton-like excitation ($b\sigma = 4$, $\lambda = 0.3$, $T = 0.01$).

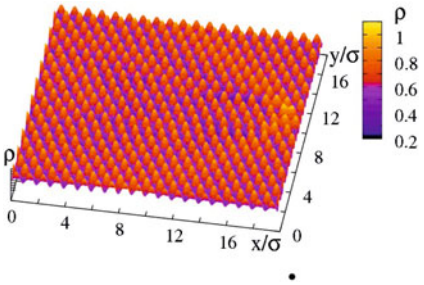

Fig. 3. (Color online) Triangular Morse lattice. Density at the time $t = 8$ resulting from the evolution of the initial perturbation at $t = 0$ ($N = 400$, $b\sigma = 4$, $\lambda = 0.3$, $T = 0.01$).

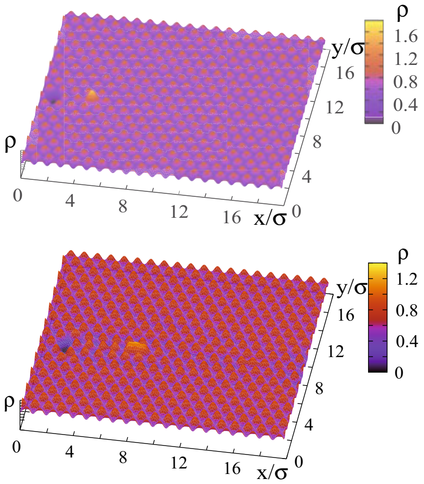

Fig. 4. (Color online) Triangular Morse lattice. We initiated a high-energy narrow soliton propagating in x-direction with 2.8-sound velocity. The upper panel shows the density at time $t = 1$, the lower panel presents the soliton density at time $t = 6$ after passing the right boundary, returning to initial position and moving further. Note that the soliton had passed in time 6 a distance of 24 units. ($N = 400$, $b\sigma = 4$, $\lambda = 0.3$, $T = 0.01$).

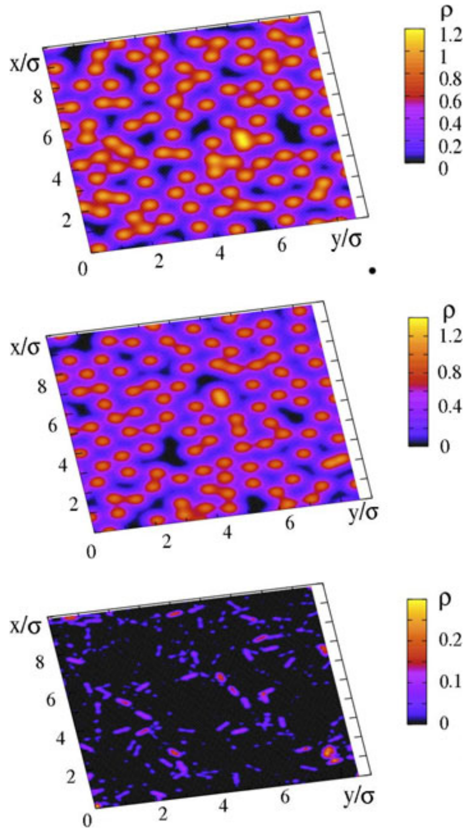

Fig. 5. (Color online) Triangular Morse lattice with $N = 100$ units heated to the temperature $T = 0.1$ (in units of $2D$) ($b\sigma = 2$, $\lambda = 0.25$) with periodic boundary conditions. Visualization of excitations (phonons and solitons) leading to local increases of density of the atomic electrons. The first two pictures illustrate the evolution of the density distribution at subsequent times and exhibit moving density waves. In the third, bottom picture appears the time evolution of the highest peaks in a cumulative representation of the amplitude-filtered density peaks for a time interval of about 50 time units. In particular the strongest compressions show the features of high-energy solitons, as these compression waves, or intrinsic localized modes, move with velocity around $1.2v_{sound}$ and have a lifetime of a many time units. Here v_{sound} is the sound velocity in a 1d lattice.

excitation is proportional to $\exp(-H/k_BT)$. Excitations which are "favorable" with respect to this measure are expected to occur more often. The first two pictures of Figure 5 show the evolution of the density distribution by snapshots at two subsequent time instants separated by 2 time units. In order to see running density waves the third, bottom picture provides the time evolution of the highest peaks of the density in a cumulative representation. From the distance between the peaks and the time interval between the snapshots we may estimate the velocity. It appears that the strongest thermally initiated compressions move with velocity about $1.2v_{sound}$ and have a lifetime of a few time units. These features point to soliton-like behavior as for the 1d lattice [6]. Indeed, they move a few picoseconds with nearly unaltered profile and just this robustness is the reason that we can identify them with the proposed visualization method. We have shown here just one example of our simulations. In general we observed that initial plane wave excitations with finite length transform within a few time units into horse-shoe-like wave-structures which move with velocities up to $2v_{sound}$. Recalling that the sound velocity in a 2d-triangular lattice is $\sqrt{2} \simeq 1.4$ the sound velocity in 1d-lattices we see that our horse-shoe structures have a speed near to the sound velocity, sometimes they are supersonic. In several experiments we have studied 2 waves moving against each other and have observed that when colliding they indeed cross each other unaltered, much like other 2d-solitons are doing [17–20]. Let us emphasize that our intrinsic localized modes appear at the nanoscale and they include no more than 10−100 atoms. The nanosize of our 2d-structure makes possible the existence of electric structures due to polarization effects, similar as those shown earlier for the 1d-case. In view of screening effects we cannot expect to see similar electric structures at the macroscale, i.e the electrical structures we found are specific for the nanoscale.

4 Adding excess electrons into the lattice and soliton-mediated electronic effects

Let us now consider that one or several non-interacting electrons are embedded into the atomic lattice, maybe as a result of doping effects. The atoms generate – in the field of charges – a polarization potential as long ago studied by Landau and Pekar [42,43]. Let us assume that the electron is located at the position $\mathbf{r}$ and several atoms are located at nearby positions $\mathbf{r}_j$. Let h be a characteristic distance of polarization and U_e the maximal polarization energy. For the potential generated by the atom number j at the origin we assume

$$U_e\left(r_j\right) = -U_e\left[\frac{h^4}{\left(r_j^2+h^2\right)^2} - \frac{h^4}{\left(r_0^2+h^2\right)^2}\right], \qquad (7)$$

$$U\left(r_j\right) = 0 \qquad \text{if} \qquad r_j > r_0 \qquad r_0 = 1.5\sigma. \qquad (8)$$

In accordance with our model potential we also here truncate the polarization potential at the cut-off distance $r = 1.5\sigma$. The distribution of the total electrical potential generated by all the atoms at place $\mathbf{r}$ is then given by

$$U(\mathbf{r}) = \sum_j U_j\left(\mathbf{r} - \mathbf{r_j}\right). \qquad (9)$$

This generates some distribution of the potential acting on the added excess electrons due to the interaction with the lattice units. Looking at the formula (9) we see that any cluster of atoms generates a potential hole in which the electron density might be concentrated. Further any displacement of the atoms changes the polarization energy. The electron will try to follow up these changes. This is the basic effect leading to the solectron formation to be considered later. The feedback of the electron distribution on the lattice dynamics is neglected here. This rather complex effect, which in general leads to an enhancement of solectron effects, will be studied in detail in a subsequent work. Here we work in a parameter region, where the feedback effects do not exceed a few percent.

For the distribution of the free electrons on the polarization potential field we start by assuming a Boltzmann law for the electron density

$$n_{el}(\mathbf{r}, t) = C \exp[-\beta U(\mathbf{r}, t)], \qquad (10)$$

where $\beta = 1/k_B T$. For illustration we have studied the distribution of the polarization potential and the densities in the Boltzmann (10) approximation at several temperatures. Figure 6 illustrates the case of $T = 0.01$. The minima of the polarization potential and the corresponding maxima of the density of free electrons are well separated. Figure 7 corresponds to the "intermediate" temperature $T = 2$. Here the specific heat is $C_v = 0.9$, significantly smaller than the Dulong-Petit value and we expect that solitons are excited. Two more representations of electronic densities are shown in Figures 8 and 9. We see that with increasing temperatures the electronic densities are getting much broader spreading over the lattice and we may get *percolation*. These effects depend on the temperature, the electron density and the values of the parameters b, h, and ν. Beyond a percolation threshold the conductivity is expected to rise due to the transition from a hopping process to some band-like conductivity. The effect is transient and changes quickly in time, it will be studied in a subsequent paper.

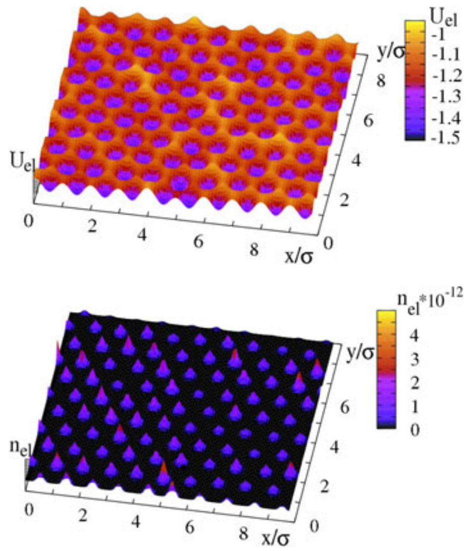

Fig. 6. (Color online) Triangular Morse lattice at very low temperature. Snapshot of the distribution of the polarization potential equations (7, 8) (upper panel) and the Boltzmann distribution of electrons equation (10) (lower panel) which show isolated wells and corresponding peaks of electronic density ($N = 100$, $T = 0.01$, $b\sigma = 3$, $U_e = 0.1$, $h = 0.7$).

5 Concluding remarks

By means of numerical experiments we have shown in the present work the existence of localized nonlinear excitations, or intrinsic localized modes, at the nano-scale in 2d layers of Morse atoms at *moderately* high temperatures, where the atomic oscillations in the mean do not

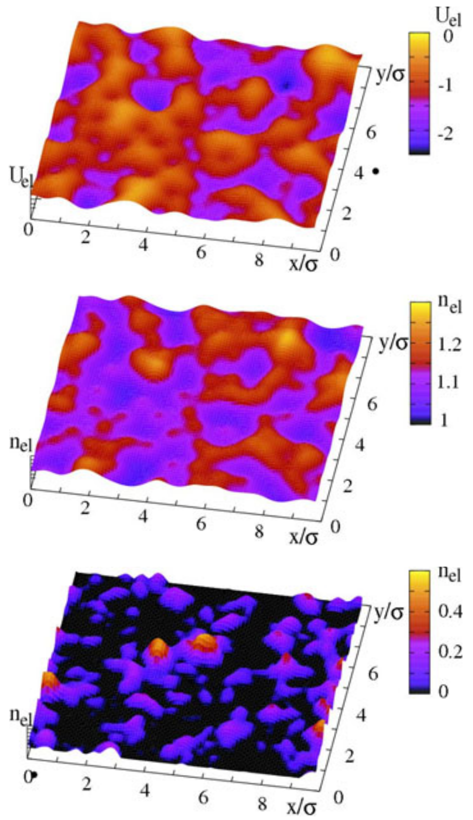

Fig. 7. (Color online) Triangular Morse lattice at intermediate temperature. The snapshots of the distributions of the polarization potential and the Boltzmann density of the free electrons show "percolating" regions. Upper picture: polarization potential; center picture: Boltzmann density; bottom picture: cumulated representation of the highest densities ($N = 100$, $T = 2$, $b\sigma = 3$, $U_e = 0.1$, $h = 0.7$).

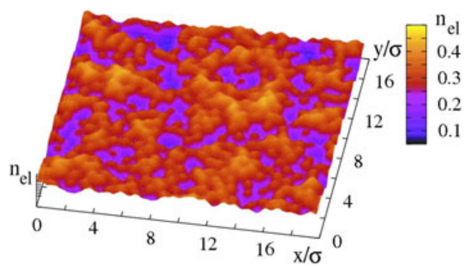

Fig. 8. (Color online) Triangular Morse lattice at a temperature, where nonlinearity starts to influence the excitations. Snapshot of a percolating Boltzmann distribution of electrons in the polarization potential ($N = 400$, $T = 0.5$, $b\sigma = 3$, $U_e = 0.1$, $h = 0.7$).

exceed 50 percent of the wells. Nonlinear waves (anharmonic phonons) arise as thermal excitations, made visible in an appropriate way that we have specified. Both front profile and front velocity, show these excitations as soliton-like. They propagate in general with slightly supersonic velocity. Therefore these excitations bear similarity to the soliton solutions for 1d Toda – lattices and

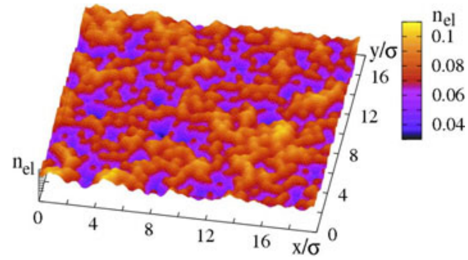

Fig. 9. (Color online) Triangular Morse lattice at intermediate temperature with developed nonlinear excitations. Snapshot of a percolating Boltzmann distribution of electrons in the polarization potential ($N = 400$, $T = 2.0$, $b\sigma = 5$, $U_e = 0.1$, $h = 0.7$).

the corresponding soliton – like excitations we have observed in cold and in thermal Morse lattices [6]. However in 2d-systems the nonlinear excitations show several differences. At first we see in Figures 2 and 3 that the distance between the ends of an initially finite front decreases in the course of evolution, the front boundaries seem to attract each other. The above implies that the life-time of the excitations is always finite and depends on the initial front length. The excitations with a minimal front length which run in just one chain of atoms have a short time life. However if we increase the energy (the amplitude) of this type of solitonic excitations we find a much longer life time as demonstrated in Figure 4. These excitations with minimal front length are quite robust and appear therefore quite frequent in thermally excited systems as shown in Figure 5.

In some respect the soliton-like excitations in two-dimensional atomic systems arising at the nano-scale level, are analog to the macroscopic soliton excitations at fluid surfaces [17,18,20]. We have shown that the excitations in atomic layers induce electrical polarization fields which may influence electron dynamics thus leading to a kind of electron trapping process similar to the Landau-Pekar process [42,43]. We have studied the soliton-mediated electron dynamics in such systems at the above mentioned *moderately* high temperatures and have calculated the density of embedded electrons in an adiabatic Boltzmann approximation. Leaving aside mathematics, what is significant to our purpose here is that the excitations are connected with a moving local density enhancement and with local polarization fields. They are indeed local compression waves running with velocities typical of expected soliton-like excitations.

Let us insist on the electron trapping process, in that local compressions may deform the potential landscape in which the electrons are moving. We neglected here the feedback of the concentration of electron density on the lattice deformation. In our case, for the given sets of parameters, the feedback is small, changes of deformations and polarization energies are usually less than a few percents. The electrons tend to be trapped in the regions of maximal density of lattice points created by the local compressions and then forced to move dynamically bound to the soliton-like compressions. This generalizes earlier findings of Brizhik et al. [52,53] who demonstrated the possibility of self-trapping of electrons in 2d lattices. The excitations which we have detected in Morse lattices are the analog to the solectron phenomena observed in 1d-systems. Under appropriate conditions, in 1d- as well as in 2d-systems, the electronic density is rather concentrated in regions near to solitonic compressions. The electrons are attracted to the local compressions and form bound states thus justifying the concept of 2d-solectron excitations. In 1d-systems the electronic clusters are always disconnected. Electricity may be carried only by moving clusters. Therefore we cannot expect that 1d-systems go under the influence of soliton compressions to highly conducting states. However as we have shown here, this situation may change drastically in 2d- or quasi-2d systems. In 1d case the local compressions are like Toda solitons. In 2d they are more complicated running compressions. However they are always intrinsic localized modes connected with local density enhancements and with the corresponding local potential wells. Then with increasing density of the solectron droplets, as shown by snapshots from computer experiments, percolation of the regions of enhanced density becomes possible. An open question is the generalization of our semi-classical description of the electrons to a proper quantum-statistical approach.

The authors acknowledge fruitful discussions with Larissa Brizhik, Leonor Cruzeiro, Sergej Flach, Dirk Hennig, Hartmut Linde, Gerd Röpke, F. Michael Russell, Erkki Brändas, Sven Larsson and Georges Vinogradov. This research was supported by the Spanish *Ministerio de Ciencia e Innovacion*, under Grant EXPLORA-FIS2009-06585-E. The authors also acknowledge the hospitality of the *International Center for Nonlinear Dynamics and Complex Systems* in Pescara (Italy), where part of this research was carried out.

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