## Contents

# Chapter 1

# Thermal solitons in 1D and 2D anharmonic lattices — solectrons and the organization of non-linear fluctuations in long-living dynamical structures

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We study the thermal excitation of intrinsic localized modes in the form of solitons in 1d and 2d anharmonic lattices at moderately high temperatures. Such finite-amplitude fluctuations form long-living dynamical structures with life-time in the pico-second range thus surviving a relatively long time in comparison to other thermal fluctuations. Further we discuss the influence of such long-living fluctuations on the dynamics of added excess free electrons. The atomic lattice units are treated as quasi-classical objects interacting by Morse forces and stochastically moving according to Langevin equations. In 2d the atoms are initially organized in a triangular lattice. The electron distributions are in a first estimate represented by equilibrium adiabatic distributions in the actual polarization fields. Computer simulations show that in 2d systems such excitations are moving with supersonic velocities along lattice rows oriented with the cristallographic axes. By following the electron distributions we have also been able to study the excitations of solectron type (electron-soliton dynamic bound states) and estimate their life times.

## 1. Introduction

In the linear approximation the fluctuations in condensed matter are mainly determined by the spectral distribution of phonons and other infinitessimal modes [1,2,3,4,5]. Nonlinear finite-amplitude fluctuations are less explored. There are however several interesting cases which are well studied [6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29]. Nonlinear fluctuations are of interest in view of their potential for possible novel electronic properties of materials, because of the strong interactions of the state of the atoms with embedded electrons. There is also the claim that nonlinear excitations may be of relevance for the transport phenomena observed in copper oxide layers [30,31]. Furthermore experiments have shown that the collective vibrations of the atomic lattice of certain superconducting copper oxides behave in a manner that is hard to explain unless one assumes that motions characteristic of the presence of "stripes" are shaking the ion lattice [32,33,34,35,36].

The electron distributions are in a first estimate represented by equilibrium adiabatic distributions in the actual polarization fields offered by the classical lattice dynamics. Here, in particular, we show the existence of strong dynamical excitations forming stripes which are soliton-like and have a Toda-like shape [37,38]. These entities are moving with supersonic velocities along the cristallographic axes of the lattice over about 10 - 100 atomic distances and have a lifetime of a few picoseconds.

The dynamics of the electrons is here not studied in detail, instead we are using simple adiabatic approximations assuming that the electron density suitably follows the running lattice soliton compressions. This is just a first approximation which we feel is enough for the purpose of this communication.

## 2. Solitonic Excitations in Morse Lattices

The Hamiltonian of the atomic lattice system which we consider here, e.g. in 1d, is

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

The subscripts locate lattice sites and the summations run from 1 to $N$ with periodic boundary conditions. The characteristic length determining the repulsion between the particles in the lattice is the equilibrium distance $\sigma = L/N$ for a lattice of length $L$. We 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 their relative distance $r = |r_n - r_j|$. For the interaction we use the Morse potential

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

where $b$ is a stiffness parameter. For 2d systems appropriate modification of the potential is to be done in the long-range part, in order to avoid unphysical cumulative interaction effects. We manage this by imposing a suitable cut-off at $1.5\sigma$.

We take all $N$ units with equal masses $m$ considered as lattice atoms with no internal dynamics. The electrons occupy some volume in the 3d space surrounding the 1d lattice. As we want to account for heating for the *heavy* lattice particles we assume that they obey classical Langevin dynamics appropriately augmenting (1). We include a phenomenological damping $\gamma$ and some external noise source. For illustration in the computer simulations we shall use $N = 200$. Then in the presence of random forces (hence at non zero temperature) and also external forces the evolution of atomic lattice units is given by the Langevin equations

$$\frac{d}{dt}v_j + \frac{1}{m}\frac{\partial H_a}{\partial x_j} = -\gamma v_j + \sqrt{2D_v}\,\xi_j(t), \tag{3}$$

where $v_j(t)$ denotes velocity of unit $j$. The stochastic forces $\sqrt{2D_v}\,\xi_j(t)$ model a surrounding heat bath (Gaussian white noise). The parameter $\gamma$ describes the standard friction frequency acting from the bath. The validity of an Einstein relation is assumed $D_v = k_B T\gamma/m$, where $T$ denotes absolute temperature and $k_B$ is Boltzmann's constant. For convenience, we use the inverse frequency of oscillations around the potential minimum $\omega_0^{-1}$ as the time unit. The unit temperature is 2D. Typical values of the parameters for biomolecules are in the range $\sigma \simeq 1-5A$; $b \simeq 1-5(A)^{-1}$; $D \simeq 0.1-0.5eV$. This means that $b\sigma \simeq 1-25$ while $1/\omega_0$ is in the range of $0.1-0.5ps$ [11,15,39,40,41,42,43].

As the energy unit we use the oscillation energy $m\omega_0^2\sigma^2 = 2D(b\sigma)^2$ (recall that in particular we use $b\sigma = 1$). Accordingly, the region where the anharmonic nonlinearity plays a major role is $0.75 < C_v/k_B < 0.95$. In the 1d case the corresponding dimensionless temperatures are in the range $T \simeq 0.1-1$. Thus solitons are to be expected stable in the range $T_{sol}^M \simeq 0.2D - 2.0D$ or in electron-volts $T_{sol}^M \simeq 0.02-0.2eV$. Clearly for biological macromolecules this estimated range includes physiological temperatures (ca. 300K).

Let us now add *excess free* electrons, as a form of doping, and consider their interaction with the lattice units [44]. Hence consider that one or several non-interacting electrons are embedded into the atomic lattice. The lattice atoms generate –in the field of charges– a *polarization* potential. Let us assume that the electron is located at 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

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

$$U_j(r) = 0 \qquad \text{if} \qquad |r-r_j| > r_0 \qquad r_0 = 1.5\sigma. \tag{5}$$

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

$$V_e(\mathbf{r}) = \sum_j U_j(\mathbf{r} - \mathbf{r_j}). \tag{6}$$

We are interested in the *dynamic* phenomena initiated by solitonic excitations in the lattice and neglect feedback effects. However we are aware that both phenomena, the local compression by a static process (polaron formation) and by a running compression hence the consecuences of soliton excitation are intimately connected [45,46,5]. The choice $h \simeq 0.3\sigma$ provides shallow minima at the location of the lattice atoms with significantly deep local minima at the location of a compression.

In a thermal system the lattice units perform quite complex motions, we may expect therefore a rather complex structure of the polarization field acting on the added excess free electrons. A snapshot of the polarization field landscape created by the lattice atoms is presented in Fig. 1. The potential energy has been given in units of the binding energy $U_e$ (4). Taking into account the energy unit $2D(b\sigma)^2$ this means the scale is given by the ratio $\eta = \frac{U_e}{2Db^2\sigma^2} = \frac{1}{2b^2\sigma^2}\frac{U_e}{D}$. For $b\sigma = 1$ the energy scale is therefore $\eta = \frac{U_e}{2D}$. Thus for calculating any physical quantity the actual value taken by $\eta$ is significant.

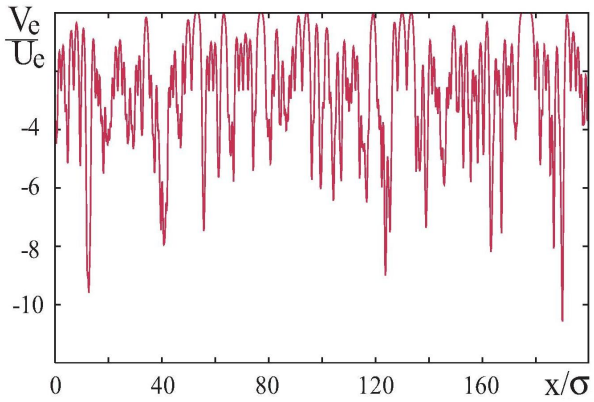


Fig. 1. Morse lattice. Snapshot of the local atomic lattice field potential landscape $U(x)$ acting on electrons in 1d. Many weak excitations and a few very strong solitons clearly appear. For units see main text. Parameter values: $V_e = U, N = 200, h = 0.3\sigma, T = 1$ and $b\sigma = 1$.

Worth noting is that the potential $U(x)$ is time-dependent and changes quickly so that the distribution of the electrons tries to follow it as fast as possible and hence the added excess free electrons are "slaved" accordingly, thus permitting an *adiabatic* approximation. We have a situation similar to that described for the free electron statistics in semiconductors [47,48]. When the electron density due to doping is sufficiently low, so that the electrons are still nondegenerated we may approximate the Fermi statistics by the Boltzmann statistics. This is often a rather good approximation connecting in a simple way the distribution with the landscapes of the local polarization potential. Then, we take

$$n(x) = \frac{\exp[-\beta U(x)]}{\int dx' \exp[-\beta U(x')]}\,, \tag{7}$$

with $\beta = 1/k_B T$. Here $x$ denotes the linear coordinate along the lattice. An example of the estimated density is shown in Fig. 2 (not normalized and given in logarithmic scale). The (relatively high) peaks correspond to the enhanced probability of a soliton to meet and trap an electron. This defines the solectron, i.e. an electron "surfing" on a soliton for about 10-50 time units (i.e. a few picoseconds) eventually getting off it and finding another soliton to surf-on and so on, in a kind of "promiscous" quantum dynamics evolution [49,50]. For $T = 0.1$ we observe several rather stable running excitations (diagonal *stripes*) with velocity around $1.2v_{sound}$. For $T = 1$ (not shown in the figure) one can observe many weak and only a few very stable and high level excitations moving with *supersonic* velocity $1.4v_{sound}$. The probabilities estimated from the Boltzmann distribution are strongly concentrated at the places of polarization potential minima. This means that most of the electrons are concentrated near to solitonic compressions. We wonder about the possible role of such

solectrons in electron transfer (ET) in biomolecules or molecular wires found at long distances [51,39,40,52]

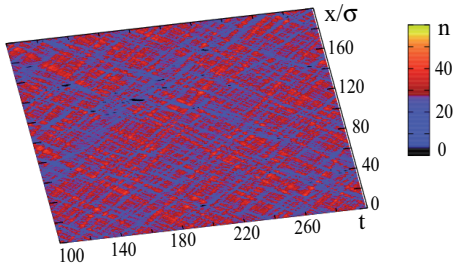


Fig. 2. Morse lattice. Probability distribution of an electron in a heated anharmonic lattice in the *adiabatic* approximation according to local equilibrium distributions. Parameter values: $N = 200, h = 0.3\sigma, T = 0.1, \sigma = 1$ and $b\sigma = 1$.

## 3. Solitonic Excitations in 2d Layers

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

$$\frac{d^2 Z_n}{dt^2} = \sum_k F_{nk}(|Z_{nk}|)z_{nk} + \left[-\gamma\frac{dZ_n}{dt} + \sqrt{2D_v}\,(\xi_{nx} + i\xi_{ny})\right], \tag{8}$$

where an index $n$ identifies a particle among all $N$ particles of the ensemble, again $\gamma$ 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 n-th and the k-th particles. To have dimensionless variables we consider the spatial coordinates normalized to the length $\sigma$ used in the Morse potential. As earlier noted, time is scaled by the inverse frequency of linear oscillations near the minimum of the Morse potential well, $\omega_0^{-1}$ and energy is scaled with $2D$, where $D$ is the depth of the Morse potential well. Further the (dimensionless) parameter $b$ defines the lattice stiffness, i.e. the strength of the repulsion between particles. The interaction force $F_{nk}$ is given by

$$F_{nk} = F_{nk}(|Z_{nk}|) = -\frac{dV(r)}{dr}|_{r=|Z_{nk}|}. \tag{9}$$

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 in the sum in Eq. (8). In computer simulations the interaction of particles is considered to take place inside a rectangular cell $L_x \cdot L_y$ with periodic boundary conditions and $L_{x,y}$ , depending on the symmetry of the 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 $10\sigma \cdot 10\sqrt{3/2}\sigma$ for $N = 100$ or $20\sigma \cdot 20\sqrt{3/2}\sigma$ 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 $T = mD_v/k_B\gamma$. This corresponds to the mean kinetic energy of a particle $< T_{kin} >$ 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 new 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 the lattice. Using data about trajectories of particles $Z_n(t)$ and the evolution of velocities $V_n(t)$ we can calculate the mean kinetic and potential energies of the lattice particles, the temperature of the ensemble, and the particle distribution $\rho(Z, t)$ using a Boltzmann-like approximation.

In our computer simulations we used $\gamma = 0.0001 - 0.001$ and checked carefully that the assumed value does not significantly influence the results. In this case the amplitudes of the stochastic forces are small for the

temperature values considered. Therefore the (Langevin) noise and the friction act in our computer simulations only as small albeit significant perturbations to the deterministic Newtonian dynamics.

We restrict here consideration to an isolated system (without influence from the bath), and follow the time evolution of quasi-1d excitations running along special lattice rows (similar as in the 1d-case) which may be analytically described as *effective* or *adapted* Toda solitons [37,38,24,53,54,55]. These soliton-type excitations run in just one characteristic row which is embedded into the 2d layer in the form

$$x_{n+1}(t) - x_n(t) = \sigma - \frac{1}{b_{eff}} ln \left[ 1 + \frac{\sinh^2 \kappa}{\cosh^2(\kappa n - \beta t)} \right] , \tag{10}$$

where $b_{eff}$ is the dimensionless lattice stiffness. Further the parameter $\kappa$ is defined by the energy of the soliton and $\beta$ is the reciprocal characteristic time

$$\beta = 1/\tau = \omega_0 \sinh \kappa \, . \tag{11}$$

Such analytical formulae provide a solution of the equation of motion in 1d-lattices of atoms interacting by Toda forces. It appears that the Toda formulae may also be used for an approximate description of soliton-like excitations in Morse lattices [54,55]. The idea is to use the free constants as tunable quantities, in particular by playing with the stiffness $b_{eff}$. A very good approximation for the solitons in 1d Morse lattices is obtained with the choice $b_{eff} = 3b$ were $b$ is the Morse stiffness. For excitations in 2d-systems we shall use (10) albeit treating the effective stiffnes as a free adjustable parameter. We fixed in one row the initial coordinates and momenta according to (10) and optimized the value of $b_{eff}$ giving the most lasting unaltered structures. In the particular case $b_{eff} = 1.5b$, the excitation remains localized and soliton-like for quite a long time (see Fig. 3). By studying numerous other examples we come to the conclusion that the quasi-one-dimensional "adapted

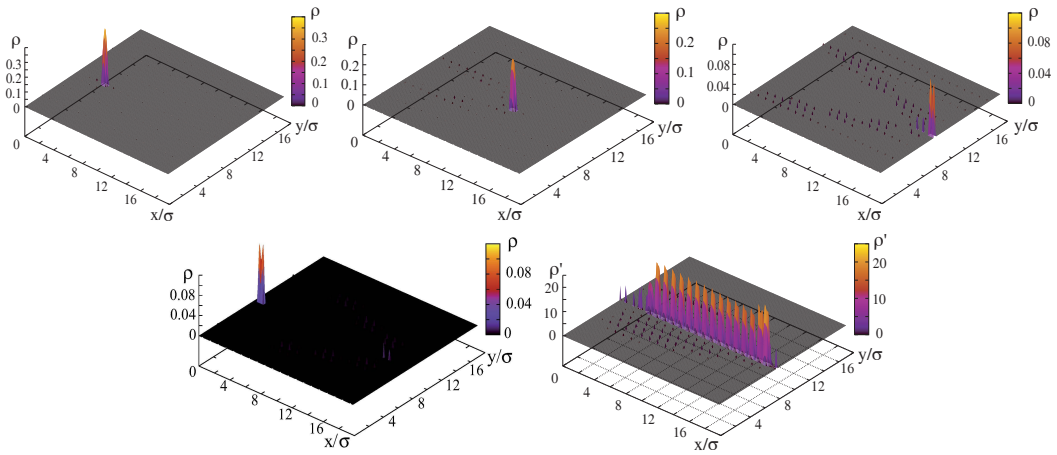


Fig. 3. Morse 2d-lattice. Quasi-1d solitonic excitation running in a 2d triangular Morse lattice along a chosen row. The initial condition is an "optimized Toda profile" that survives practically unaltered quite long time; $b\sigma = 4$. The figure shows four snapshots in sequence and the last panel is a composite cumulating pictures along the complete time sequence.

Toda solitons" with stiffness $b_{eff} = 1.5b$ which are running along rows aligned with the main crystallographic directions are localized excitations in triangular lattices with particular long lasting high stability. (We profit to alert the reader about an unfortunate typo in [54], where rather than $1.5b$ appears $6b$ which is not correct). We expect that this property holds also for other symmetries, as e.g. in $NaCl$ crystals.

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 problem which arises is however that the probability may be quite low to find structures with high energy and, further, to identify them in the sea of fluctuations. We have observed quite many localized soliton-like modes which live some 10 - 20 time units, most of them oriented along the three basic crystallographic directions of

the triangular lattice. We may conclude that many excitations we see in the heated system have the character of the localized quasi-one-dimensional modes described in the previous Section.

At low temperature ($T = 0.1$) small oscillations of lattice atom-particles near equilibrium states are observed. Then at a higher temperature ($T = 0.5$) particles are able to leave equilibrium states traveling for quite long distances though elongations of bonds are small. At a still higher temperature $T = 1$ some tracks of short-life-time excitation modes are observed. Both front profile and front velocity, show these excitations as soliton-like.

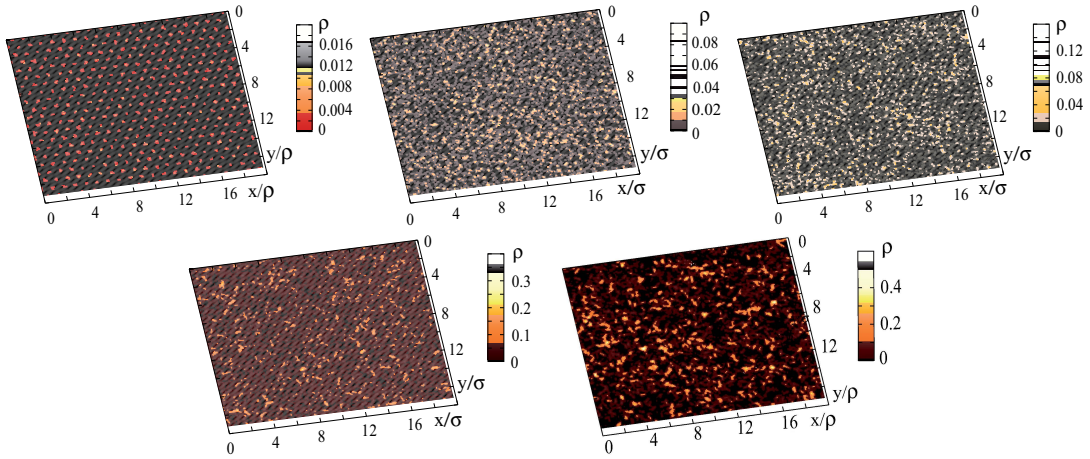


Fig. 4. Morse 2d lattice. Thermal excitation of long-living solitons at different temperatures in a triangular lattice at different temperatures with $b\sigma = 4(\gamma = 0.04$ in a)-d), $\gamma = 0.2$ in e), noise is not switched off for simulation procedure) Evolution of filtered density for a long time $\Delta t$ is presented. Note that the picture shows the time evolution of the highest peaks in a cumulative representation of the amplitude-filtered density peaks for several time intervals.

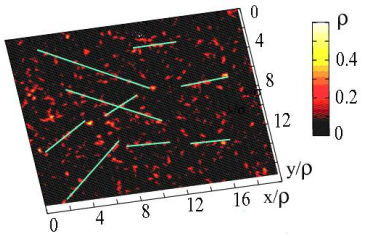


Fig. 5. Morse 2d lattice. Snapshot of the local soliton traces like *stripes* we see in computer simulations of 2d lattices. The electrons are expected to follow this intrinsic localized mode time and space evolution.

## 4. Conclusion and outlook

In conclusion we feel that intrinsic localized modes behaving as soliton-like excitations in 1d and 2d anharmonic lattices are worth exploring further for they may very well be of significance to experiment. Indeed, on the one hand, in 1d crystal lattices, there is the possibility, yet to be fully explored, of soliton-mediated supersonic (Angstroms per picosecond), fast electron transfer (ET) over long distances (thirty nm and beyond) which only recently has been explored [39,40,26,43,52]. On the other hand, in 2d systems, our computer simulations show that thermal soliton-like excitations may exist at least up to temperatures of the order of 100 K with life times of several picoseconds. Some of them are organized in stripes reminiscent of those seen in several experimental studies [32,33,34,35,36]. Another process, which we observed in our 2d computer simulations is

reminiscent of percolation [56,53,54,55], which bears qualitative similarity to dynamical structures observed in cuprates [27].

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