THERMAL SOLITONS AND SOLECTRONS IN 1D ANHARMONIC LATTICES UP TO PHYSIOLOGICAL TEMPERATURES

M. G. VELARDE[*], W. EBELING[†] and A. P. CHETVERIKOV[‡]

Instituto Pluridisciplinar,
Universidad Complutense de Madrid,
Paseo Juan XXIII, 1, Madrid-28040, Spain
[*]mgvelarde@pluri.ucm.es
[†]ebeling@physik.hu-berlin.de
[‡]ChetverikovAP@info.sgu.ru

We study the thermal excitation of solitons in 1D Toda–Morse lattices in a wide range of temperatures from zero up to physiological level (about 300 K) and their influence on added excess electrons moving on the lattice. The lattice units are treated by classical Langevin equations. The electron distributions are in a first estimate represented by equilibrium adiabatic distributions in the actual fields. Further, the electron dynamics is modeled in the framework of the tight-binding approximation including on-site energy shifts due to electron-lattice coupling and stochastic hopping between the sites. We calculate the electron distributions and discuss the excitations of solectron type (electron-soliton dynamic bound states) and estimate their life times.

Keywords: Anharmonicity; Morse interactions; lattice solitons; solectrons; hopping conduction.

Since the work of Davydov and others, it is known that electrically charged solitons may travel along 1D lattices. Davydov conjectured that these electro-solitons are stable at finite temperatures and may persist even at physiological temperatures. Several authors [Christiansen & Scott, 1983; Lomdahl & Kerr, 1985; Scott, 1992] have checked Davydov's conjecture and have shown that the electro-solitons do not survive above 10 K lasting at most 2 ps. Davydov's work is based on electrical transport in a harmonic lattice, the nonlinearity comes in only due to the electron-phonon interaction as a polaronic effect. However, any "positive anharmonicity" in the underlying lattice could result in the appearance of very stable supersonic acoustic solitons [Zolotaryuk et al., 1996]. Following earlier work [Velarde, 2008; Velarde et al., 2005, 2006, 2008; Chetverikov et al., 2005, 2006a, 2006b; Makarov et al., 2006] we continue here exploring this line of thought and we show that taking into account the anharmonicity in the lattice together with the nonlinearity of the (polaron-like) electron-soliton interaction, the thermal stability of the electron-soliton dynamic bound states (called, for simplicity, solectrons) is considerably enhanced. The dynamics of the electrons is taken using quantum theory in the tight-binding approximation.

The 1D lattice system (length L) consists of N classical particles (all with equal mass m taken as lattice sites or lattice ions/ion cores/atoms with no internal dynamics) with periodic boundary conditions. The electrons (considered lighter than

the lattice units) occupy some volume in the 3D space surrounding the 1D lattice. For the *heavy* lattice particles, we assume that they obey classical Langevin dynamics. We include a phenomenological damping γ_0 and some external noise source. The lattice particles are described by coordinates $x_n(t)$ and velocities $v_n(t)$, $n = 1, \ldots, N$. The Hamiltonian consists of the classical lattice Hamiltonian H_a, the contribution of the electrons H_e, and the interaction of electrons with the lattice vibrations. We set

$$H = H_a + H_e, \qquad (1)$$

where the lattice part is

$$H_a = \frac{m}{2} \sum_n v_n^2 + \frac{1}{2} \sum_{n,i} V(x_n, \, x_i). \qquad (2)$$

The subscript denotes the lattice particle number and summation goes from 1 to N. Let us assume that the average distance between particles is σ ($\sigma = L/N$). At short distances, we consider that they repel each other with *exponentially* repulsive forces while at longer distances they attract each other with weak *dispersion* forces depending on their relative distance $r = x_{n+1} - x_n$. We will approximate the potential using the Morse model (akin to the Lennard–Jones potential and to the repulsive component of the Toda potential) $V = D\{\exp[-2B(r - \sigma)] - 2\exp[-B(r - \sigma)]\}$. For illustration in the computer simulations we shall use $N = 200$ and $B = 1/\sigma$. Then in the presence of random forces (hence nonzero temperature) and also external forces the evolution of lattice particles is given by the equations

$$\frac{d}{dt}v_n + \frac{1}{m}\frac{\partial H_a}{\partial x_n} = -\gamma_0 v_n + \sqrt{2D_v}\,\xi_n(t). \qquad (3)$$

The stochastic forces $\sqrt{2D_v}\,\xi_n(t)$ model a surrounding heat bath (Gaussian white noise). The parameter γ_0 describes the standard friction frequency acting from the bath. The validity of an Einstein relation is assumed $D_v = k_B T \gamma_0 / m$, where T denotes absolute temperature and k_B is Boltzmann's constant. For convenience, we use σ as the unit length and the inverse frequency of oscillations around the potential minimum ω_0^{-1} as the time unit. The unit temperature is $2D$. Typical values of the parameters for biomolecules are in the range [Hennig *et al.*, 2007] $\sigma \simeq 1$–$5A$; $B \simeq 1$–$5(A)^{-1}$; $D \simeq 0.1$–0.5 eV. This means that $B\sigma \simeq 1 - 25$ while $1/\omega_0$ is in the range of 0.1–0.5 ps.

In order to visualize the solitons in a first approach we focus attention on the "atomic" density. We assume that each lattice particle is surrounded by a Gaussian electron density providing a screened ion core of width $s = 0.35\,\sigma$. Then the total atomic electron density is given by

$$\rho(x) = \sum_n \frac{1}{\sqrt{2\pi}s} \exp\left[-\frac{(x - x_n(t))^2}{2s^2}\right]. \qquad (4)$$

Hence we assume that the atom is like a spherical object with continuous (valence) electron density concentrated around each lattice site. In regions where the atoms overlap, the electron density is enhanced. This permits easy visualization of solitonic excitations based on the colors in a density plot. This is of course a rough approximation. Figure 1 shows the result of simulations for the temperatures $T = 0.005$ and $T = 1$. The diagonal stripes correspond to regions of enhanced density which are running along the lattice. This is a sign of solitonic excitations. Checking the slope, we see excitations which over 10 time units move with *supersonic* velocity. These pictures are quite similar to solitonic excitations described by Lomdahl and Kerr [1985] albeit with life times of at most 2 ps and stable only up to 10 K. Here we have solitonic excitations living about 10–50 time units corresponding to 1–3 ps. Besides, they survive even at $T = 1$ which is well above the physiological temperature (about 300 K which is above $T \approx 0.1$ with $D \simeq 0.1$ eV). This confirms an earlier finding of stable solectrons up to such temperatures [Hennig *et al.*, 2006].

We have computed both potential energy, U, and kinetic energy, T_{kin}, and hence the internal energy E ($E = U + T_{\text{kin}}$) and the corresponding specific heat (at constant volume/length) C_v. They appear plotted in Fig. 2. As the energy unit we use the oscillation energy $m\omega_0^2\sigma^2 = 2D(B\sigma)^2$ (recall that for illustration we use $B\sigma = 1$). Accordingly, the region where the nonlinearity plays a major role is $0.95 > C_v/k_B > 0.75$. As we see in Fig. 2, the corresponding temperatures are in our energy units between $T \simeq 0.1$ and $T \simeq 1$, thus justifying the pre-eminent role of solitons shown in Fig. 1. We may bring this to a more physical picture by introducing the binding strength of the Morse interaction. Then solitons are to be expected stable in the range $T_{\text{sol}}^M \simeq 0.2$–$2.0D$ or in electron-volts $T_{\text{sol}}^M \simeq 0.02$–$0.2$ eV. Thus for biological macromolecules, this estimated range includes physiological temperatures.
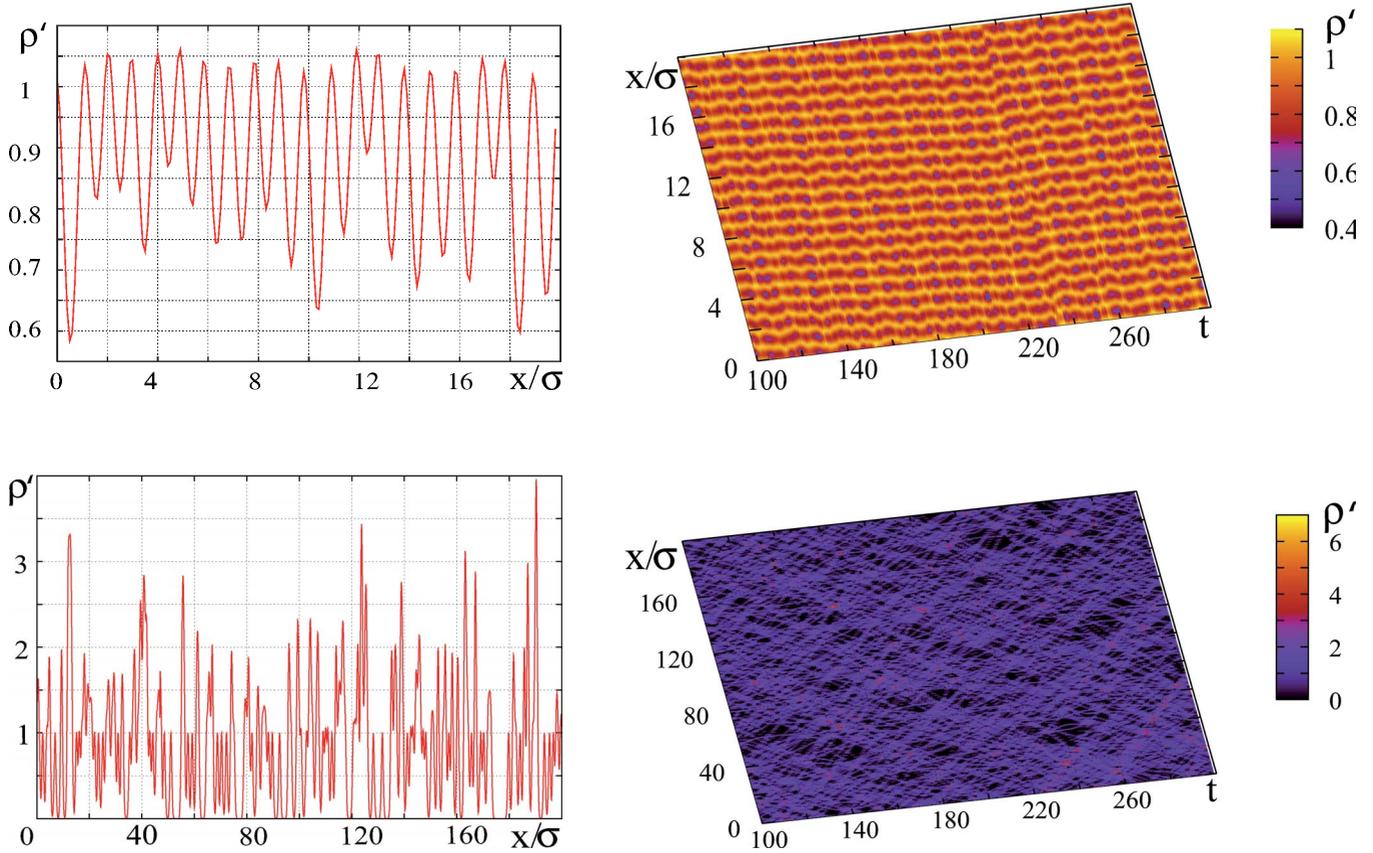
Fig. 1. Visualization of running excitations on 1D anharmonic lattices. Density $\rho' = \rho\sqrt{2\pi}s$ refers to valence-like electrons in lattice atoms (color coding in arbitrary units). $N = 200, B\sigma = 1, s = 0.35\,\sigma$. For two temperatures (given in units of $2D$) we have: Upper set of figures: (i) $T = 0.005$: Only harmonic lattice vibrations show up with no evidence of soliton-like excitations; and bottom set of figures: (ii) $T = 1$: Besides many excitations also a few strong solitons appear running with velocity around $1.3v_{\text{sound}}$. In both cases on the left figure there is a snapshot of the distribution for a certain time instant and on the right figure the actual time evolution of the distribution is displayed.

Let us study now the interaction between the lattice units and the surrounding added free (conduction) electrons. In a first semiclassical approach we assume that all lattice atoms which are near to each other by $1.5\,\sigma$ or less contribute to the local potential $V(x)$ acting on each electron

$$V_e(x) = \sum_n V_0(x - x_n), \quad r = |x - x_n| < 1.5\sigma.$$

(5)

For illustration we take

$$V_e(x) = \frac{-U_e \sum_n h}{[(x - x_n)^2 + h^2]^{1/2}},$$

(6)

where U_e is a parameter which fixes the "depth" of the potential and h another parameter which estimates its range. For typical 1D systems we

expect that the binding energy is in the range $U_e \simeq 0.05$–0.1 eV. The binding energy U_e is a second (independent) energy unit of the system. This characteristic energy is in general smaller than the binding energy between lattice units which in our model is D. Let us consider $U_e \simeq 0.02$–$0.2D$ and $h = 0.3\,\sigma$. The field acting on an electron in the lattice can be thought as the sum of all fields created by the neighboring atoms in the range $\pm 1.5\,\sigma$. The value U_e is taken such that the electrons are only weakly bound to the atoms and may transit from one side to the other of a lattice unit. Accordingly the electrons are able to wander through the lattice eventually creating an electron current. To place a pair of electrons between two lattice particles is in general not favorable in energetic terms, since the energy of repulsion $e^2/\epsilon_0 r$ has to be overcome; ϵ_0 denotes dielectric constant.
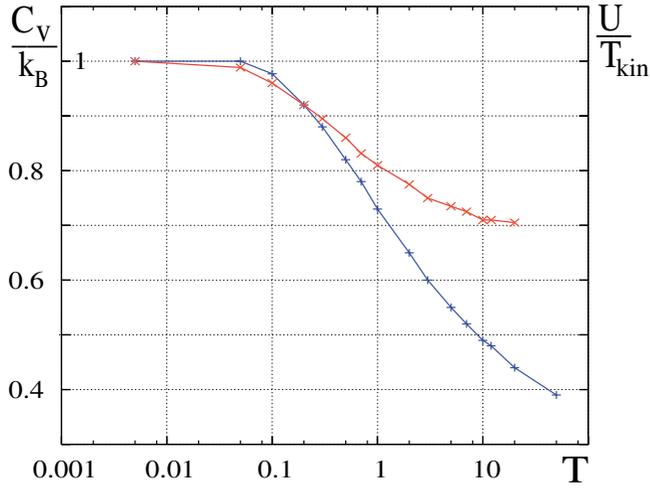
Fig. 2.   Specific heat at constant volume/length (C_v, upper curve) and ratio of potential energy to kinetic energy (U/T_{kin}, lower curve) for the 1D lattice with Morse interactions. T is in dimensionless units. Note that in the low-T range there is no Debye part ($\sim T^d, d = 1$ here) as we have *classical* lattice dynamics only. The flat part corresponds to the Dulong–Petit law.

However, the electron may attract more than two lattice particles thus forming a deep potential hole akin to a *polaron* state which is a *static* structure corresponding to favorable energetic configurations. Here, we are rather interested in the *dynamic* phenomena initiated by solitonic excitations in the lattice. However, we have to take into account that both of these phenomena, the local compression by a static process (polaron formation) and by a running compression (soliton excitation) are intimately connected. 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 field acting on the electrons. Let us give now several examples of the fields created by the atoms. Two snapshots are presented in Fig. 3. The potential energy has been given in units of the binding energy U_e. Taking into account the energy unit $2D(B\sigma)^2$ this means the scale is given by the ratio $\eta = U_e/2DB^2\sigma^2 = (1/2B^2\sigma^2)(U_e/D)$. For $B\sigma = 1$ the energy scale is therefore $\eta = U_e/2D$.

The potential $V(x)$ is time-dependent and gives at each time a snapshot of the actual situation. The potential changes quickly and the distribution of the electrons tries to follow them as fast as possible hence electrons are "slaved" accordingly, thus permitting an *adiabatic* approximation. We have a situation similar to that described for free electron statistics in semiconductor theory [Blakemore, 1962]. When the electron density $n(x)$ is sufficiently low, so that the electrons are still non-degenerated, we may approximate the Fermi statistics by the Boltzmann statistics. The Boltzmann approach is often a rather good approximation which connects in a simple way the distribution with the landscapes of the local potential. Then, we take

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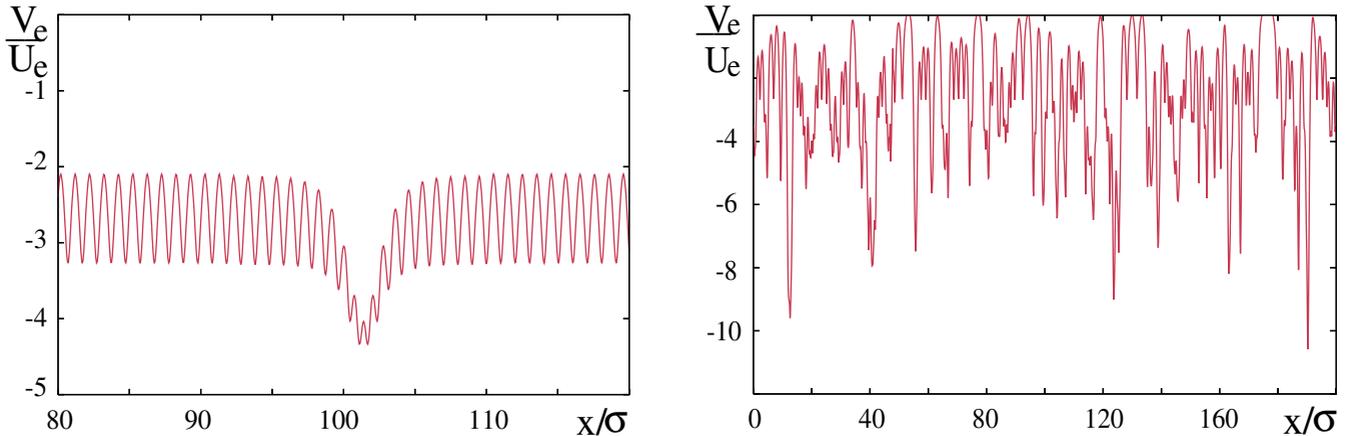

Fig. 3.   Snapshot of the local field potential $V(x)$ acting on electrons in the anharmonic lattice ($N = 200, h = 0.3\,\sigma$ and $B\sigma = 1$). (Left) At $T = 0$ we observe one running soliton which was excited by an external perturbation. (Right) At $T = 1$ we observe many weak and a few very strong solitons. For units see main text.

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. 4 (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) then getting off it and eventually finding another soliton once more to surf-on and so on. For $T = 0.1$ we observe several rather stable running excitations (diagonal stripes) with velocity around $1.2v_{\text{sound}}$. For $T = 1$ (not shown in the figure) one can observe many weak and only a few very stable excitations moving with *supersonic* velocity $1.4v_{\text{sound}}$. The probabilities estimated from the Boltzmann distribution are strongly concentrated at the places of minima. This means that most of the electrons are concentrated near solitonic compressions.

Let us use the tight binding approximation allowing the potential landscape to be nonuniform. As a consequence, using second-quantization formalism we take

$$H_e = \sum_n \{E_n(x_{n-1}, x_n, x_{n+1})c_n^+ c_n - V_{nn-1}(x_n, x_{n-1})(c_n^+ c_{n-1} + c_n c_{n-1}^+)\}, \quad (8)$$

where c_n, c_n^+ are destruction, creation operators endowed with appropriate anticommutation relations. In our approximation these are c-numbers. To lowest order the energy levels E_n are all taken equal, i.e. they do not depend on n and then the first term in (8) can be scaled away. Let

us go a step forward. Assuming that the interaction depends exponentially on the distance of the ions [Hopfield, 1974; Gray & Winkler, 2003] we can set

$$H_e = \sum_n \{(E^0 + \delta E_n)c_n^* c_n - V_0 \exp[-\alpha(q_n - q_{n-1})](c_n^* c_{n-1} + c_n c_{n-1}^*)\}, \quad (9)$$

where E^0 refers to the unperturbed (uniform) lattice without excitations and δE_n is the perturbation due to the nonlinear lattice excitations (relative displacements of lattice units). We define $x_n = n\sigma + q_n/B$. Then the probability to find the electron at the lattice site or atom located at x_n is $p_n = c_n c_n^*$.

The Hamiltonian (8) leads to the equations of motion for the quantities c_n. The corresponding equations for the lattice particles become in this approximation

$$\ddot{q}_n = -p_n \frac{\partial \delta E_n(q_{n-1}, q_n, q_{n+1})}{\partial q_n}$$
$$+ \{1 - \exp[-(q_{n+1} - q_n)] \exp[-(q_{n+1} - q_n)]\}$$
$$- \{1 - \exp[-(q_n - q_{n-1})]\} \exp[-(q_n - q_{n-1})]$$
$$+ \alpha V_0 \{\exp[-\alpha(q_n - q_{n-1})](c_{n-1}^* c_n + c_{n-1} c_n^*)$$
$$- \exp[-\alpha(q_{n+1} - q_n)](c_n^* c_{n+1} + c_n c_{n+1}^*)\}. \quad (10)$$

Solving numerically the Schrödinger equation in the tight-binding model the occupation numbers p_n are obtained. This procedure works well at zero and near zero absolute temperatures. As known
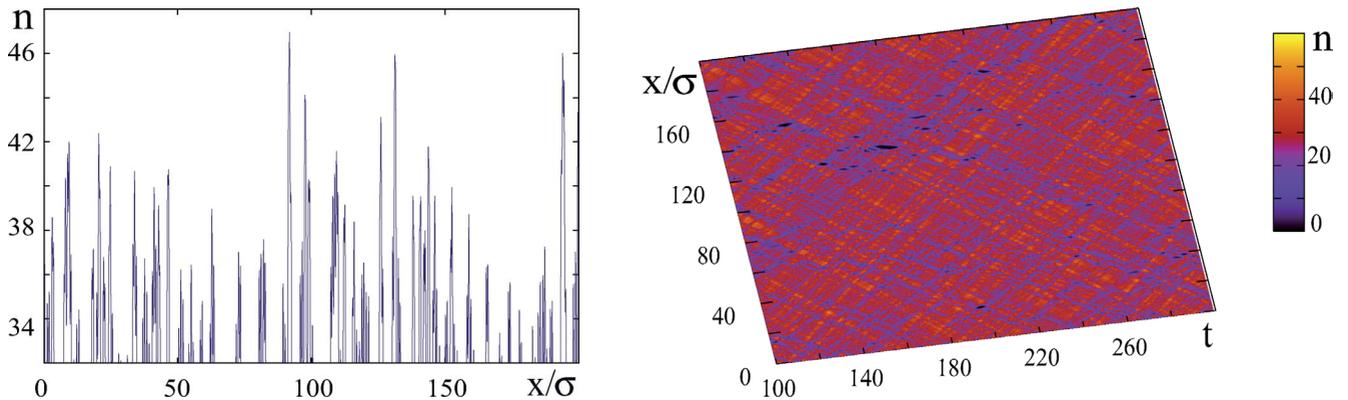

Fig. 4. Probability distribution of an electron in a heated anharmonic lattice in the *adiabatic* approximation according to local Boltzmann distribution. (Left) A snapshot of the distribution is given for a certain time instant. (Right) The actual time evolution of the distribution is displayed. The temperature is $T = 0.1$. Parameter values: $B\sigma = 1, h = 0.3\sigma$, $N = 200$.

from quantum molecular dynamics, at higher temperatures the treatment of thermal systems using the Schrödinger equation leads to difficulties in the computer simulations. There are several ways to overcome these difficulties, one follows Pauli's [1928] master equation approach and another uses path integral Monte–Carlo calculations [Filinov *et al.*, 2004]. We follow here Pauli's method and proceed from the Schrödinger equation to a master equation for the occupation probabilities p_n. To first-order approximation we can write

$$\frac{dp_n}{dt} = \sum [W_{nn'}p_{n'} - W_{n'n}p_n]. \tag{11}$$

For simplicity we consider only one-step transitions $n' = n \pm 1$. The transition probabilities contain two factors, the symmetric transition probabilities which are proportional to the square of the interaction potential and an unsymmetrical thermal factor $E(n, n')$ which is not unique. Introducing the second-order transition probabilities $|V_0 \exp[-\alpha(q_n - q_{n'})]|^2$ Eq. (11) takes the form

$$\frac{dp_n}{dt} = \frac{2\pi}{\hbar}V_0^2 \{\exp[-2\alpha(q_{n+1} - q_n)]$$
$$\times [E(n, n+1)p_{n+1} - E(n+1, n)p_n]$$
$$+ \exp[-2\alpha(q_n - q_{n-1})]$$
$$\times [E(n, n-1)p_{n-1} - E(n-1, n)p_n]\}. \tag{12}$$

The factor $(2\pi/\hbar)V_0$ is the reciprocal electron relaxation time scale (or relaxation rate). The ratio between the mechanical (lattice) relaxation and the electron scale is τ_P (adiabatic parameter) that in our computations here we set to unity though generally the electron dynamics is by far the fastest one. The thermal factor obeys detailed balance [Lebowitz & Bergmann, 1957]

$$\frac{E(n', n)}{E(n, n')} = \frac{\exp[\beta E(n)]}{\exp[\beta E(n')]}. \tag{13}$$

The simplest, and most used way, to satisfy this condition is the Monte–Carlo procedure which distinguishes between "uphill" and "downhill" transitions [Binder, 1979]. Here for "downhill" transitions we take $E(n, n') = 1$ for $n' = n \pm 1$, if $E_n = E'_n$ or $E_n < E'_n$. In all other cases when the transitions to states of the neighbors are "uphill", a Boltzmann factor weighs them, $E(nn') = \exp[\beta(E_{n'} - E_n)]$. The Monte–Carlo procedure guarantees that in thermal equilibrium the canonical distribution

$p_n^0 = \text{const} \exp[-\beta E_n]$ is a solution of the master equation. Further, it may be shown that there exists an (Boltzmann) entropy theorem which guarantees the convergence of any initial distribution to the canonical distribution, with stationary external conditions [Lebowitz & Bergmann, 1957]. Details about the thermal factor, can be found elsewhere [Binder, 1979; Filinov *et al.*, 2004; Böttger & Bryksin, 1985]. In order to get an equation for the coordinate which depends only on p_n we neglect the phases in Eq. (10) and set

$$\ddot{q}_n = -p_n \frac{\partial \delta E_n(q_{n-1}, q_n, q_{n+1})}{\partial q_n}$$
$$+ \{1 - \exp[-(q_{n+1} - q_n)]\} \exp[-(q_{n+1} - q_n)]$$
$$- \{1 - \exp[-(q_n - q_{n-1})]\} \exp[-(q_n - q_{n-1})]$$
$$+ 2\alpha V_0 \{\exp[-\alpha(q_n - q_{n-1})]\sqrt{p_{n-1}p_n}$$
$$- \exp[-\alpha(q_{n+1} - q_n)]\sqrt{p_n p_{n+1}}\}. \tag{14}$$

Let us discuss now the eigenvalue problem for the energy states taking into account the influence of the lattice deformations on the on-site electron energy levels (9). The simplest assumption is the Holstein model $\delta E_n = \chi r_n$, where $r_n = q_n/B$ is the shift. In [Kalosakas *et al.*, 1998, 2003] the constant χ is denoted as "electron-phonon coupling constant" leading for large values of χ to the formation of polarons. Following these authors we take the coupling constant in the range $0.5 < \chi < 2\,\text{eV/Angstrom}$.

In fact, we shall assume that the energy shifts depend on the deviations q_n only in a symmetric way. A reasonable ansatz is

$$\delta E_n \simeq \frac{\chi}{2B}[(q_{n+1} - q_n) + (q_n - q_{n-1})] + \cdots \tag{15}$$

To simplify the computer work we have used in most simulations instead of (15) the local potential V as calculated above by assuming for the deviations, $\delta E_n = V(x = x_n)$. In other words, we assume that the shifts are proportional to the (classical) shift of the potential energy which is due to the lattice deformations. To a first approximation we have

$$\delta E_n \simeq \frac{U_e \sigma h}{B(\sigma^2 + h^2)^{3/2}}[(q_{n+1} - q_n) + (q_n - q_{n-1})]. \tag{16}$$

Taking the typical values of the parameters used above we arrive at $\chi \simeq 0.01\text{–}0.1\,\text{eV/Angstrom}$ which is a bit below the earlier noted values used in the literature though not a serious shortcoming
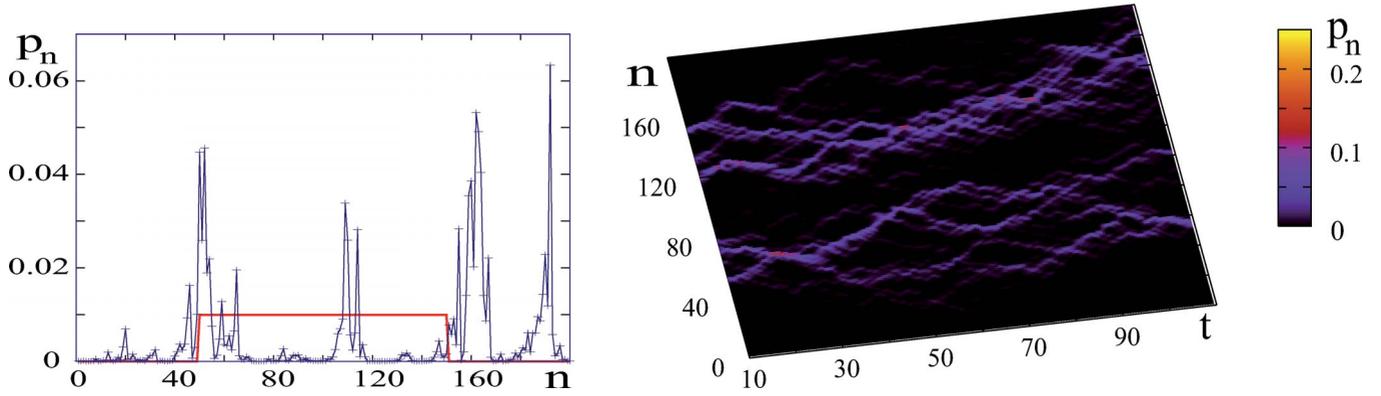
Fig. 5. Time evolution of the electron probability distribution in a heated anharmonic lattice according to Pauli's equation and hence beyond the adiabatic approximation. (Left) The initial (rectangular) distribution as well as the distribution at a (dimensionless) time instant $t = 120$ are plotted. (Right) The actual time evolution of the distribution is displayed. The temperature is $T = 1$ and the parameter values are: $B\sigma = 1, h = 0.3\sigma, N = 200, U_e = 0.01, \alpha = 1$.

here. In such parameter range, polaronic effects are rather weak.

The results of computer simulations are presented in Figs. 5 and 6. The differences with earlier reported results [Hennig *et al.*, 2006, 2007]

are due to the addition here of the coupling of lattice displacements to the on-site energies. On the other hand, the differences with the results of the adiabatic approximation presented above are due to the relaxation of the electronic distribution.
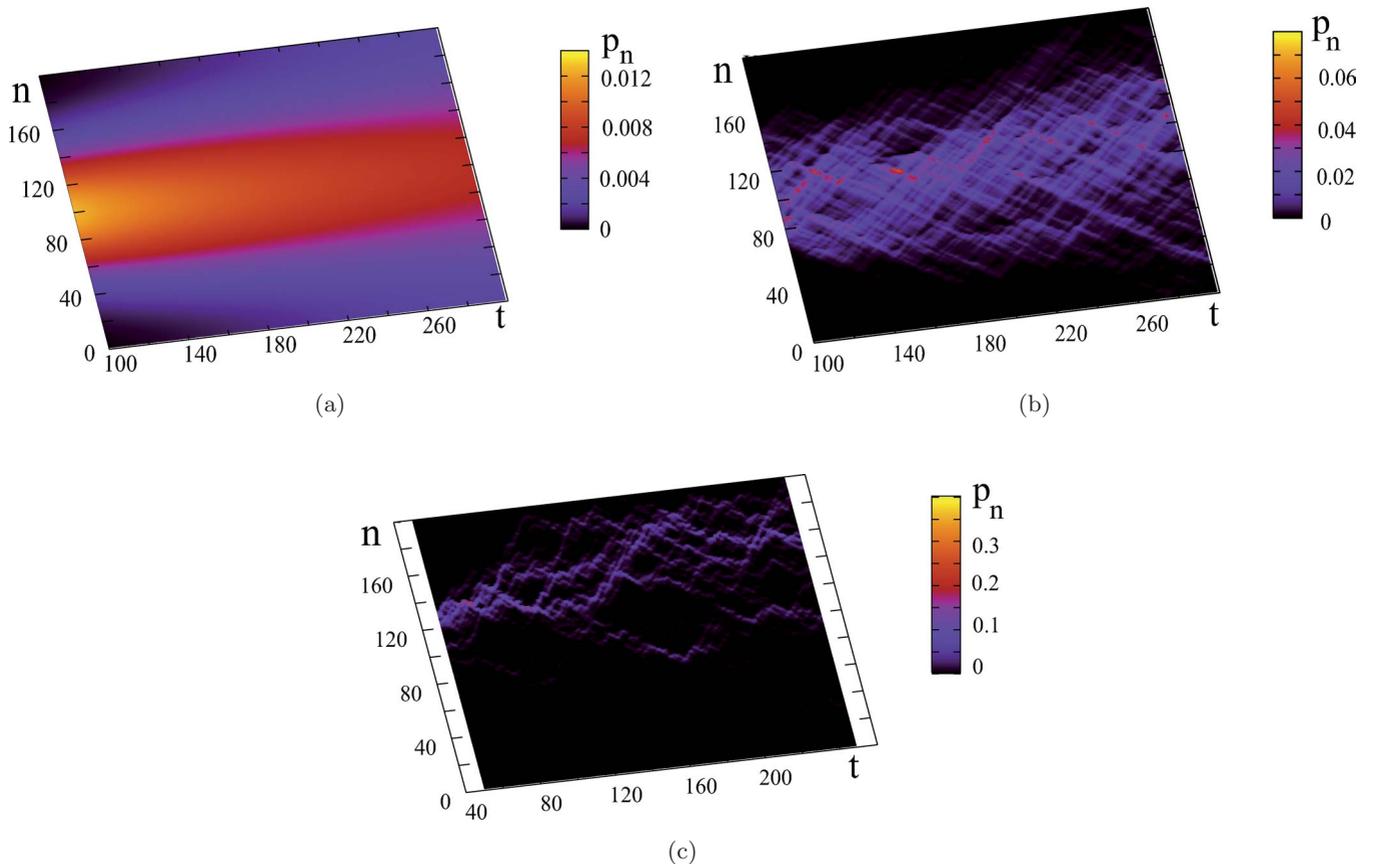

(a)

(b)

(c)

Fig. 6. Actual time evolution of the probability distribution of the electrons (according to Pauli's equation) in a rather "cold" lattice: (a) $T = 0.005$, and in a "heated" lattice: (b) $T = 0.1$ and (c) $T = 1$. Parameter values: $B\sigma = 1, h = 0.3\sigma, N = 200$.

The relaxation effects increase with increasing $\tau = (2\pi/\hbar)V_0$; for $\tau \to 0$ the simulations for the Pauli equation correspond to the adiabatic approximation. The Pauli-like approach goes beyond the adiabatic approximation since the lattice dynamics and the electron dynamics are treated independently including their coupling. Indeed, in the master equation approach we take into account that the electrons need time to follow the atomic motions which leads to certain delay in their response and to some deviations from the stationary solution. Qualitatively, however, solving Eq. (11) simultaneously with Eq. (10) the picture remains the same as in Figs. 5 and 6 show.

In Fig. 5 we show the solution of the master equation for a rectangular initial distribution (constant distribution between 50 and 150). In the left figure, we see the resulting distribution after time $t = 120$ exhibiting a remarkable structure reflecting the solitonic excitations. In the right figure, appears the evolution of the distribution in time. The Pauli equation is solved simultaneously with the lattice dynamics and then the evolution of the occupation density i.e. of the components $p_n(t)$ is obtained.

In Fig. 6 we show the evolution of an electron distribution which is initially (at $t = 0$) peaked at the center of the lattice with $N = 200$ atoms. Recall that the electrons are treated as independent particles, their Coulomb interaction is neglected. We considered a few typical cases: (a) The electrons are disconnected from the lattice ($\alpha = 0$). The electron probability density spreads in time following Pauli's equation; (b) At higher temperatures $T = 0.1$ we observe the beginning of nonlinear regimes and the formation of low-energetic solitons. The electron distribution is localized near the few excited solitons which are still rather weak. The solitons form quite stable solectrons; (c) At a still higher temperature $T = 1$ only one rather strong soliton dominates in the lattice. The electron distribution is localized near this strong soliton. We observe also that due to the presence of an oppositely moving soliton the electron probability density distribution splits into two parts thus confirming a result earlier found in a simpler approach [Velarde *et al.*, 2008]. Note that the effects are even more pronounced due in part to not so weak but rather strong polaronic effects. Note also that the values of U_e and α cannot be fixed *a priori* since they depend on the physical nature of the lattice under study.

In summary, we have shown that for sufficiently high electron density, most of the electrons tend to form clusters (droplets) around solitonic compressions [Schneider & Stoll, 1975]. The electrons within the clusters may be degenerated. In 1D-systems the droplets are always disconnected. Electricity can be carried only by moving droplets. Therefore, we cannot expect that a 1D-system goes under the influence of solitonic compressions to metal-like or even superconducting-like states. However the situation may change drastically in 2D- or quasi-2D systems. Then with increasing density of the solitonic droplets, percolation becomes possible, a question to be discussed elsewhere.

We have shown that thermal excitations may exist at physiological temperatures (about $300\,\mathrm{K}$) with life times of several picoseconds. Assuming that the dissipative dynamics of the charged species is characterized by an *effective* relaxation time τ, we can write

$$v(t) = v(t_0) \exp\left[-\frac{t - t_0}{\tau}\right], \qquad (17)$$

where v denotes the velocity and $1/\tau$ is a "collision frequency". These life times determine transport properties like the electrical conductivity, the self-diffusion coefficient and the mean square displacement. We have estimated the life times from the wandering landscapes for different temperatures as shown in Figs. 1, 3–5. Computer simulations were carried out for $T = 0.005$, 0.1 and 1. At low temperatures ($T = 0.005$) phonons dominate and potential wells of individual atoms have maxima and minima of width 0.5. They do not move and the slopes of the lines are zero. At $T = 0.1$, when the solitonic regime is expected to show up the simulations yield a background mostly red. Solitons are excited already but the number of solitons is small and they are relatively low energetic (in the snapshot we see 3–4 solitons of a width 2 which can be identified on the length 30 separated by long pieces of an almost flat lattice). The soliton velocity is about 1.1–$1.2 v_{\mathrm{sound}}$. Noteworthy is that these solitons have a long life-time: about 10% of blue solitonic excitations appear with a life time $\tau_{\mathrm{blue}} \simeq 5$–40. The minima are not very deep. Then at $T = 1$, which is already at the upper border of the solitonic regime (and, say, at the edge of melting in the system), outside the yellow regions we only see red areas. The situation is close to the ideal one, the density of solitons is about 10% again. In one of the simulations, we observe two less energetic and two more energetic (narrower and with higher velocity) solitons. At a later time, we can identify one

high energetic soliton and three weaker ones, and so on. The solitons are rather stable with a velocity in the range 1.2–$1.4v_{\text{sound}}$. For the earlier given parameter values of biomolecules these velocities (and supersonic electric current) are in the range of few Angstroms per picosecond (hence about Km/s).

Acknowledgments

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