



From *polaron* to *solectron*: The addition of nonlinear elasticity to quantum mechanics and its possible effect upon electric transport

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ABSTRACT

A significant generalization of the *polaron* concept is given here. The building block of the new concept is the *anharmonicity* of the backbone lattice vibrations not considered by the earlier authors. Due to such (non-Hookean) *nonlinear elasticity*, solitons may appear in an one-dimensional Toda (and Toda–Morse) lattice (no electric charge is involved in the system). Then a discussion is provided about the interplay of an added, excess electron with these lattice excitations (including polaron-like effects) thus leading, in particular, to electron trapping by solitons and hence to the *dynamic* bound state called *solectron*. Also given here are features of the “truth and consequences” of introducing this new concept (and *quasiparticle*) when dealing with electric transport.

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1. Introduction

In a concise publication, Landau [1] discussed long ago the conditions under which an electron placed in a *periodic* field could be trapped by a crystal lattice *distortion*. His argument was taken up in [2,3] and by both in a joint [4] publication. They established that “the carriers in crystals with ionic lattices are not electrons from the conductivity band, but *polarons*”. Indeed “by its electric field, a conduction electron will dielectrically polarize the ionic crystal”. “At the very beginning of the process of polarization the polarized crystal already represents, for the electron, a potential well with a discrete spectrum. The electron having spent part of its energy on the polarization of the crystal, falls into one of the discrete levels, and is thus localized”. Then “the slow conduction electrons should continuously fall into *polaron* states”. Note that though, as already remarked by Landau and Pekar, the size of the *polaron* must be greater than the lattice constant, due to the discreteness of the lattice, the polaron is *pinned* unless a rather large number of ions are involved in the lattice excitation. The polaron should move in an electric field like a *negative* charge, the localized state as a whole being forced to move along the field. Landau and Pekar considered the crystal as a system undergoing small *harmonic* oscillations. Then they showed that the electrostatic induction of the electron (the interaction of the electron with the polarized crystal) forces oscillations of the ions which are *longitudinal* motions. Alongside their joint publication, the authors alerted, with no explicit details, about the needed role to be played by “a certain anharmonicity” on those forced oscillations and the expected ensuing “heat dissipation”. The *polaron* concept, due to the electron-lattice vibrations coupling, introduces nonlinearity in the dynamical description of electric conduction albeit preserving the linearity of Ohm’s law. Subsequent work done in [5–8] is worth mentioning. The latter coined the concept of *conformon* for a polaron-like entity (displacement of an electron probability density in a macromolecule causes a conformational rearrangement) propagating along an *aperiodic* macromolecule or along the secondary structure of an heteropolymer (in principle, with possible dissipation over large distances due to the inhomogeneity and aperiodicity of the backbone “lattice”). He did advance the possibility of taking advantage of such concept and transfer mechanism when dealing with artificial membranes where periodicity could be imposed.

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Later, Davydov [9–12] showed that if the on-site electron energy levels are taken depending on lattice displacements (to the linear approximation) then under certain other approximations the *polaron* evolution equations could be reduced to a soliton-bearing equation. First he got the (non-exactly solvable) discrete nonlinear Schroedinger equation that under further approximations leads to the (completely integrable) Ablowitz–Ladik equation. Subsequently, he proceeded further in accounting for the *longitudinal* lattice vibrations and also showed that when the *polaron* is sufficiently extended and the lattice discreteness can be overcome, the continuum approximation can be used and further particular conditions permitted, the *mobile* polaron could be found as a solitary wave solution or soliton (generally with *subsonic* velocity).¹ Davydov coined the concept of *electrosoliton* to describe the above-mentioned view of the *polaron* as a solitary wave (or soliton). Like the *polaron*, the *electrosoliton* can be considered as new physical entity (and electricity carrier). Both relative to the originally “bare” electron (particle) are “dressed” particles or “quasiparticles”, a concept also used by Landau in various other contexts. Recall that only *harmonic longitudinal* oscillations are demanded to the lattice units.²

The rest of this contribution is organized as follows. In Section 2 the *tight-binding* electron-lattice interaction is recalled together with the corresponding time evolution equations for the electron probability density. In Section 3 a sketchy account is given of the Toda (and imperfect Toda or adapted Toda–Morse) lattice model including its solitary and periodic (cnoidal) wave solutions (generally with *supersonic* velocity). Also discussed there are significant features of its specific heat and dynamic structure factor. Section 4 deals with the evolution of the compound electron-*anharmonic* lattice *longitudinal* vibrations leading to the introduction of the *solelectron* concept. Results about electron trapping by solitons are provided for various significant particular cases. In Section 5 the characteristics of the *solelectron*-mediated electric transport are discussed. Finally, in Section 6 a summary of results is provided.

2. Electron dynamics on a lattice

In order to illustrate the above given picture and in view of what follows let us recall how the electron-lattice interaction and electron transfer along a lattice brings nonlinearity using the *tight-binding* approximation (electrons are *localized* on atomic/lattice sites and only occasionally hop to neighboring sites). Thus to account for electron *hopping* from one lattice site to another use can be made of creation (a_n^\dagger , creates an electron at site “ n ”) and annihilation (a_n , annihilates or lowers an electron at site “ n ”) operators (anticommutation relations $\{a_m, a_n^\dagger\} = \delta_{mn}$, $\{a_m, a_n\} = \{a_m^\dagger, a_n^\dagger\} = 0$; $a_n^\dagger a_n$ provides electron number operator) in *second quantization* formalism [16]. Then the Hamiltonian operator is

$$\mathcal{H} = \sum_n [E_n a_n^\dagger a_n - a_n^\dagger (V_{n,n-1} a_{n-1} + V_{n+1,n} a_{n+1})]. \tag{1}$$

The transfer matrix elements, $V_{n,n-1}$, etc indicate intersite transfer energy exchange (overlap integrals related to the probability of electron *hopping* from site to site; more on this is given further below). The first term accounts for the on-site electron (levels) having in mind an *excess* electron added to the originally undistorted lattice.

The single electron wave function under tight binding approximation is $|\Psi(t)\rangle = \sum_n c_n(t) a_n^\dagger |0\rangle$, ($|n\rangle = a_n^\dagger |0\rangle$), with appropriate *inner* product and normalization, $\langle \Psi(t) | \Psi(t) \rangle = \sum |c_n|^2 = 1$. It evolves according to Schroedinger equation

$$i\hbar |\dot{\Psi}(t)\rangle = \mathcal{H} |\Psi(t)\rangle, \tag{2}$$

where $\hbar = h/2\pi$, h is Planck’s (universal) constant. An overdot denotes derivative with respect to time. The complex quantity $c_n(t)$ permits one to define electron probability density relative to the corresponding site “ n ”. To obtain its time evolution use can be made of the Lagrangian formulation, with

$$\mathcal{L} \equiv \langle \Psi | i\hbar \frac{\partial}{\partial t} - \mathcal{H} | \Psi \rangle = \sum_n c_n^* (i\hbar \dot{c}_n - E_n c_n + V_{n,n-1} c_{n-1} + V_{n+1,n} c_{n+1}). \tag{3}$$

With $\partial \mathcal{L} / \partial \dot{c}_n = i\hbar c_n^*$, $\partial \mathcal{L} / \partial c_n^* = d/dt (\partial \mathcal{L} / \partial \dot{c}_n = 0)$ defining conjugated momenta, the least action principle $\delta \int_{t_1}^{t_2} dt \mathcal{L}(c_n, \dot{c}_n, \dots) = 0$ yields

$$i\hbar \dot{c}_n = E_n c_n - (V_{n,n-1} c_{n-1} + V_{n+1,n} c_{n+1}), \tag{4}$$

where the coupling of electron (normalized) probability density (amplitude, c_n) to lattice variables (lattice displacements or vibrations, implicit in the $V_{n,m}$) appears. Then the (symmetrized) electron Hamiltonian or energy is

¹ The approximations used by Davydov brought mathematical beauty and “transparent” understanding (kind of “simplicity”) of the dynamics. But was it not a bit too much simplification?

² Although electric conduction is possible in a charged ionic *harmonic* lattice, to account for equipartition, heat transport and thermal expansion the *anharmonicity* in the potential must be invoked (or, alternatively, doping, etc.) [13,14]. However not all anharmonicities ensure this as the lattice ought to be able to sustain a temperature gradient and not a mere temperature difference alone [15].

$$H = \sum_n E_n |c_n(t)|^2 - \sum_n V_{n,n-1} (c_n^* c_{n-1} + c_n c_{n-1}^*), \quad (5)$$

and thus

$$i\hbar\dot{c}_n = \partial H / \partial c_n^*. \quad (6)$$

For the nearest-neighbor interaction model the on-site electron energy, in general, depends on the distance between the n th-lattice unit and its left ($n - 1$) and right ($n + 1$) units. Then the simplest approximation corresponds to assuming that it is independent of the lattice site number so that the corresponding term $a_n^\dagger a_n$ can be scaled away from the Hamiltonian (1) by an appropriate choice of the “zero” (reference) energy level. Clearly if account is to be done of electron–electron interaction permitting, for instance, electron-pairing then the diagonal elements must be taken into consideration, together with their Coulomb repulsion (for which a simplified form was proposed in [16,19,20]).³ As a very first-approximation, only the off-diagonal transfer matrix elements are considered to significantly contribute to electric transport (with a single electron).

3. Solitons and the paradigmatic Toda anharmonic lattice

3.1. Solitons

The study of anharmonic lattices owes much to the seminal work done in [21–29]. FPU tried numerically albeit with no success to explain *equipartition* of energy (of paramount importance in statistical mechanics) by using the first few non-Hookean corrections to linear elasticity in the form of *cubic* and *quartic* anharmonic potentials as a mechanism to allow energy sharing and exchange between harmonic modes otherwise non-interacting. The difficulty was clarified by Zabusky and Kruskal who studied solitary waves and solitary-wave (overtaking) collisions in such anharmonic lattices and their continuum counterpart. In view of their remarkable particle-like behavior, these waves reappearing unaltered following collisions, the hallmark of their dynamics, Zabusky and Kruskal denoted them by *solitons* (*solit/solitary* wave; *on*/like in *electron*, *proton*, etc.).⁴ In fact, before the discovery of the soliton, Visscher and collaborators numerical computations had revealed “soliton-like” mediated behavior and enhanced heat transport. Solitary waves and solitons found also in other realms of science appear as potential “universal” carriers of almost anything [30] (like surf waves/non-topological solitons in the ocean or bores/topological solitons in rivers).

Let us recall how solitons appear in the *anharmonic* Toda lattice. Consider an one-dimensional (1D) lattice of units (mass, m or $m = 1$ for simplicity) interacting with their nearest-neighbors via a potential $U(r)$. Then, classically, for the displacement of the n th-lattice unit/particle from its equilibrium position, Newton’s equations are

$$\ddot{r}_n = U'(r_{n+1} - r_n) - U'(r_n - r_{n-1}), \quad (7)$$

where r_n denotes displacement (vibration or elongation; depending on circumstances it is of interest to focus on local lattice deformations or on gradient of displacements) of the unit at site “ n ”. A dash indicates a derivative with respect to the argument (corresponding space variable).⁵ No on-site dynamics or structure is considered. There are cases of, e.g., biological interest where an intra-unit dynamics is added, like an oscillator unit (units with such internal structure coupled to the other degrees of freedom in the system have been considered by Fröhlich [large polaron], Davydov, Holstein [small polaron] and others). If rather than actual unit-displacements, relative displacements, $\xi_n = r_{n+1} - r_n$, are considered, then Eq. (7) becomes

$$\ddot{\xi}_n = U'(\xi_{n+1}) - 2U'(\xi_n) + U'(\xi_{n-1}). \quad (8)$$

³ Taylor expanding yields $E_n = E_0 + J_L(\xi_n - \xi_{n-1}) + J_R(\xi_{n+1} - \xi_n)$, where E_0 is the electron energy when the lattice is undistorted and hence all lattice units are at their equilibrium positions; $J_L, J_R > 0$. Further one can assume $J_L = J_R = J$. A warning on such simplifications seems pertinent. On the one hand, scaling away the diagonal terms does not permit one to see in a straightforward way the classical counterpart of the problem as we lose the energy landscape offered to the electron. On the other hand, if *nonlinear elasticity really matters* care should be taken in having consistency not jeopardizing the relevance of its role. Accordingly, linearizations may turn out not being self-consistent simplifications. From the perspective of a *classical* mechanics approach, the case of conducting polymers (following Ohm’s law) described by the so-called SSH Hamiltonian model [17,18] is one where solitons (in particular deformation *topological* solitons) come from the degeneracy of the ground state (and mismatch of two configurations) and not from genuine *anharmonic* lattice dynamics as the interaction invoked is harmonic. In such a case linearization as above expressed is relevant and enough to have theory describing experimental data. Formally, and even conceptually, from the *quantum* mechanics perspective once the Hamiltonian is written the output, hence the soliton, comes from the dynamics, including the lattice dynamics. For conducting polymers an open question is the possible role of *nonlinear elasticity* enhancing electron transport to non-Ohmic level but, at present, no experimental evidence seems to exist giving relevance to that question.

⁴ Anecdote: as Zabusky has indicated their first idea not pursued for reasons alien to science – there was a company with such a trademarked name – was to call them *solitrons*. As recently found, a similar case is that of *solelectron* which is the trademarked name of an electronic company. There is also a beauty product called *soltron* and the word *surfon* designates a web site... so it is difficult to find a truly original, not trademarked word for the concept and quasiparticle originated in the dynamic bound state of an electron to a soliton.

⁵ If one searches for traveling solutions then one may set $r_n(t) = r_{n-m}(t - m\tau)$; $m = 1$ defines the *soliton* whereas $m \geq 2$ can be used to define *breathers* aka *intrinsic localized modes* (ILM), i.e. pulsating traveling waves which are exactly translated by “ m ” sites after a fixed propagation time “ $m\tau$ ”, which are allowed to oscillate as they propagate on the lattice. “Breathers” seem to having first been observed in lattices of (on-site) nonlinear oscillators *loosely* or weakly coupled among themselves.

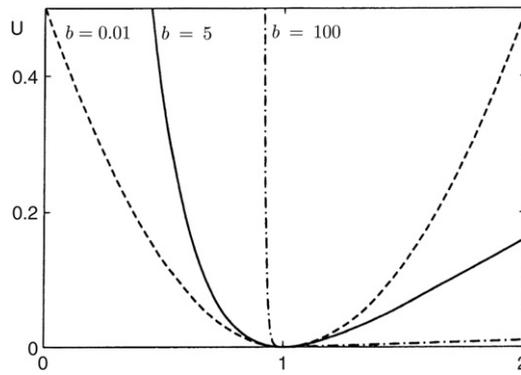


Fig. 1. Toda potential (9) with $\omega_0 = \sigma = 1$ and $b = 0.01$ (practically, the harmonic limit, indicated by a dashed line), $b = 5$ (solid line), and $b = 100$ (practically, the hard sphere limit, indicated by a dash-dotted line). Along the abscissa there is interparticle distance, r , centered around the potential minimum.

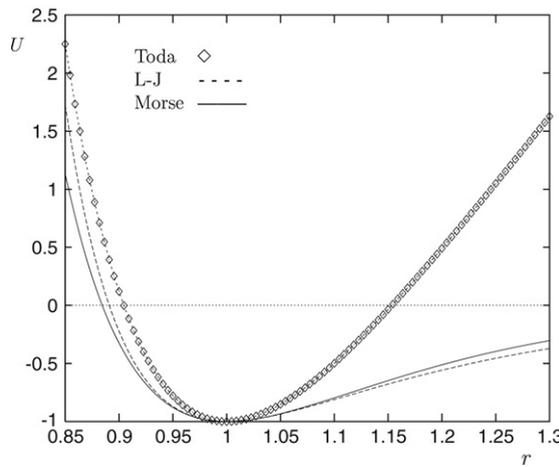


Fig. 2. Toda potential ($U = U^T = \frac{a}{b} [e^{-b\sigma(r-1)} + b\sigma(r-1) - 1]$), Morse potential ($U = U^M = \frac{a}{2b} [(e^{-b\sigma(r-1)} - 1)^2 - 1]$) and Lennard-Jones potential ($U = U^{L-J} = U_0 [\frac{1}{r^{12}} - \frac{1}{r^6} - 1]$). In order to have all the three minima of the potential functions at the same location (1, -1) the parameters have been adjusted with the basic frequency the same. It clearly appears that Toda’s interaction (upper curve) captures the repulsive core well whereas its attractive part becomes unphysical for large values of the displacement. The abscissa is, like in Fig. 1, denoted by $r \equiv \xi_n/\sigma$.

Then let us consider a *paradigmatic* interaction potential introduced by Toda,

$$U(\xi_n) = \frac{a}{b} [e^{-b(\xi_n - \sigma)} + b(\xi_n - \sigma) - 1], \tag{9}$$

where σ is the mean interparticle distance; $a > 0$ and $b > 0$ are parameters; b accounts for the non-Hookean stiffness of the “springs” in the lattice; the last term (-1) is added for computational convenience and need not to be included.⁶ Note that with ab finite for $b \rightarrow 0$, the function (9) becomes the harmonic potential (linear Hookean, “springs” for a standard crystal lattice) and $\omega_0^2 \equiv ab/m$ defines the angular frequency of vibrations in such harmonic limit (via Taylor expansion) of (9). [N.B. $\frac{a}{b}e^{-br} + ar - \frac{a}{b} = \frac{ab}{2}(r^2 - \frac{b}{3}r^3 + \dots)$.] In the extreme opposite case $b \rightarrow \infty$, the potential (9) approaches the hard-rod/sphere limit (fluid-like system). Fig. 1 illustrates the form of (9) for several values of the stiffness parameter (anharmonicity) and Fig. 2 shows its relative form when adequately compared with Morse and Lennard-Jones potentials [31,32].

In what follows consideration will be given only to strong interparticle compressions such that $\xi \leq \sigma/2$ (below $r = 1$ in Fig. 1). [N.B. Materials are usually stronger when compressed and weaker when stretched.] In view of this, the fact that the attractive part of Toda’s potential (9) is unphysical is of no concern to the study here.

For any finite value of b , in the infinite lattice, the equations of motion (8) possess a one-parameter family of soliton solutions

$$\xi_n = \sigma - (1/b) \ln [1 + \sinh^2 \kappa \operatorname{sech}^2 (\kappa n \mp \sinh \kappa) \omega t]. \tag{10}$$

⁶ Note also that under an external force or for finite temperatures the lattice constant is not equal to the minimum of the potential well since $U(9)$ does not depend on lattice site coordinates but on relative lattice displacements.

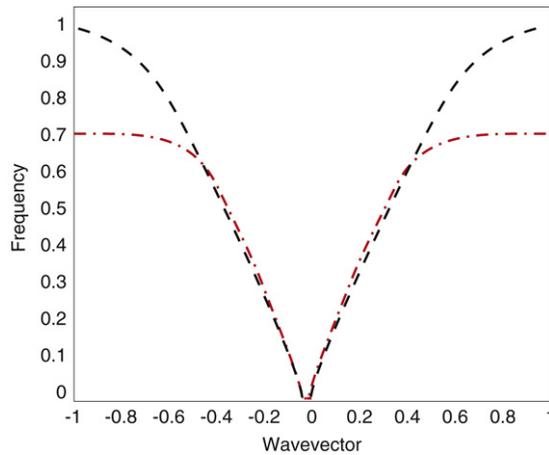


Fig. 3. Dispersion relation (frequency vs wavevector; first Brillouin zone) for *cnoidal* waves (solitons; lower, dash-dotted curve) and the limiting case of harmonic waves (phonons; upper, dashed curve) as the modulus of the Jacobian elliptic function approaches zero. Ordinate units, ω_0 ; abscissa units, π/σ .

[N.B. Inverting the logarithm it is just the sech^2 for $e^{-b(\xi_n - \sigma)}$. This exponential is related to the force (9) and characterizes the strength of the solitonic pulse.] The parameter κ controls the wave velocity and by the same token the wave amplitude (higher solitons travel faster),

$$v_{\text{soliton}}(\kappa) = \pm \omega_0 (\sinh \kappa) / \kappa, \tag{11}$$

which shows its *supersonic* character as the linear sound velocity is given by $v_{\text{sound}} = \omega_0$ (positive and negative signs merely give direction of wave propagation). Note that the value of ξ_n accounts for the local lattice *compression* experienced by two neighbor units. In *dynamical systems* terminology the solitons (10) are *homoclinic* orbits [33]. Although the soliton tends at infinity to a constant value, $\lim \xi_n = \sigma$ as $n \rightarrow (+\infty)$ or $(-\infty)$ [for sech^2 the asymptotic value is zero], the flatness of the soliton wings yields easily to a new hump thus appearing as having a long range (albeit exponentially decaying) influence, a feature with consequences to be illustrated later on. This can be easily seen, when a periodic hence finite lattice is considered. Then the exact solution of the equations of motion is the periodic “cnoidal” wave

$$\xi_n = \sigma - (1/b) \ln [1 + (2\nu K(k)/\omega)^2 \text{dn}^2(2K(k)[(n/\lambda) \mp \nu(\lambda, k)t])] - E(k)/K(k), \tag{12}$$

where dn denotes the Jacobian elliptic function with modulus k ($0 < k \leq 1$) [34]. The functions $K(k)$ and $E(k)$ are complete elliptic integrals of the first and second kind, respectively.⁷ The Jacobian elliptic functions sn , cn and dn are related to each other and both sn and dn can be written in terms of cn (short word for *cnoidal*). It can be shown that in the *continuum* limit the solution (12) of the discrete lattice can be approximated by the *cnoidal* solution of the Boussinesq–Korteweg de Vries equation [24,28,29,33] and on another limit by the solitary wave solution in the form of sech^2 . It can also be shown that indeed the B-KdV equation and the Toda lattice do have much in common. By analogy with the linear, harmonic case the exact dispersion relation is

$$\nu(\lambda, k) = \omega_0 / 2K(k) [sn^{-2}(2K(k)/\lambda) + E(k)/K(k) - 1]^{1/2}. \tag{13}$$

Clearly when k gets small one recovers the harmonic wave whereas as k grows the *cnoidal* wave (12) gets more and more *localized* and eventually goes into the solitary wave (10) if the lattice length is allowed to also increase. Note that by analogy with the harmonic Fourier modes (phonons in the quantum terminology) in a linear lattice, here the solitary or *cnoidal* waves (or solitons) are the corresponding eigenmodes of the lattice with non-Hookean “springs” (Fig. 3). In what follows advantage will be taken of the knowledge of the exact solutions, (10) or (12), of the Toda lattice. There is, however, a shortcoming. The Toda lattice cannot sustain a thermal gradient although it permits a temperature difference, hence it is “transparent” to heat and is not a heat conductor (solitons with exponential interaction like (9) run freely in the Toda lattice). This problem does not arise with Lennard–Jones interactions.⁸ In view of this, use is to be done of an *imperfect* Toda lattice and, recalling that interest here focused only on high lattice compressions, this can be achieved by substituting (9) with the rather similar and physically motivated Morse interaction (Fig. 2) [31] thus considering an *adapted* (non-integrable, hence imperfect) Toda–Morse lattice whose solutions and corresponding features should not differ significantly from the exact Toda solutions given above.

⁷ As Toda has indicated it was his knowledge of elliptic functions that gave him clues to propose the potential function (9) in order to have exactly solvable Hamiltonian nonlinear model dynamics, *rara avis* in many-body physics.

⁸ Peierls was the first to explain heat conduction in a lattice by identifying two types of phonon–phonon interaction: one preserving momentum and energy flow not contributing to heat, and the other, called *umklapp* (bending-back) process in that a three-phonon interaction transfers momentum to the lattice as a whole, contributes to thermal resistivity and hence to heat. An unambiguous understanding of such process demands appeal to *anharmonicity* in the lattice dynamics.

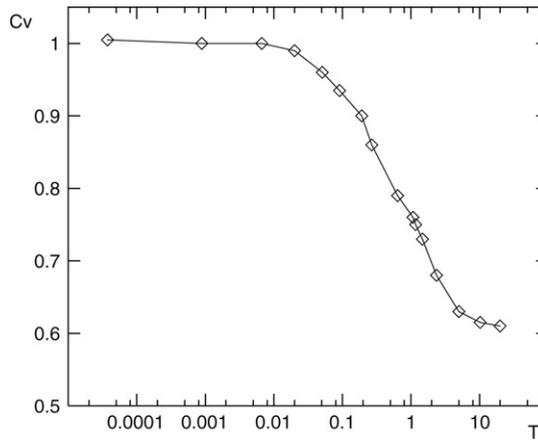


Fig. 4. Typical plot of the (numerically computed) specific heat at constant length/volume in k_B units. $T_{transition} = 1$, for which $C_L \equiv C_v = 0.75$. $C_v = 1$ is the Dulong–Petit value (solid phase; harmonic interaction) and $C_v = 0, 5$ corresponds to the fluid-like phase (hard-rod interaction). Missing in the figure is the low temperature values arising from genuinely quantum mechanics (T^n Debye law), dimension $n = 1$.

3.2. Morse potential and the imperfect Toda potential or the adapted Toda–Morse lattice

As earlier noted, the Toda lattice was constructed in such a way as to possess solitons made of elliptic functions. It did not originate in the study of a realistic, experimentally related physical problem. Yet it has reached a *paradigmatic* status as all features are known exactly, including thermodynamic quantities like partition function, the specific heat (at constant volume/length), etc [27,28,35–38]. To overcome the lack of heat transfer possibility one could suitably redefine it thus making an *imperfect* Toda lattice in the spirit of Van der Waals imperfect gas theory, which allows condensation (a phase transition) while maintaining the perfect gas formalism, i.e., formally the same equation of state. This approach can be followed in a drastic way by simply disregarding the attractive part in the computations or better by “adapting” the Toda potential [31,32] to be a Morse one. As earlier noted the Morse potential is practically equivalent to the Lennard-Jones potential (Fig. 2) though its attractive part is a bit less realistic,

$$U_M(\xi) = D [e^{-B(\xi-\sigma)} - 1]^2, \tag{14}$$

to be matched by the Toda potential

$$U_T(\xi) = \left(\frac{a}{b}\right) [e^{-b(\xi-\sigma)} + b(\xi - \sigma) - 1], \tag{15}$$

placing together the minima of both potential functions. This can be achieved by defining $a_{TM} = a = \frac{2}{3}BD$ and $b_{TM} = 3B$. Then both potential functions share in common up to a third-order Taylor expansion term with fourth-order terms approximately equal. Then this adapted Toda–Morse potential (or imperfect Toda potential in the sense of Van der Waals) is a *local* approximation to the Morse potential with implicit density dependence through ω_0 and b . It offers the possibility of heat conduction and “phase transitions”-like phenomena as discussed elsewhere [38].

3.3. Specific heat, and solitons at the “edge of melting”

The specific heat at constant length/volume of the Toda lattice was obtained long ago [37,39].⁹ First, one computes the free energy $F = k_B T \lg Z$, where Z is the normalization factor of the corresponding *canonical* distribution $\rho_N = e^{-H/k_B T} / Z$, where H is the corresponding Toda (or imperfect Toda) Hamiltonian, T and k_B denote, respectively, absolute temperature and Boltzmann’s (universal) constant. The specific heat is the second derivative of F with respect to T at given constant lattice length. Fig. 4 depicts in semi-log plot C_L versus T , in k_B -units. Needless to say, the $C_L(T)$ function does not account for low temperatures where a T^n Debye law applies (n , dimension). It only captures the Dulong and Petit law, here $C_L = 1$, in the chosen units.

The high-temperature limit $C_L = 0, 5$ corresponds well with the fluid-like, hard-sphere phase. Then around $T = 1$, $C_L \approx 0, 75$ it is the *soliton* range. Well below $T = 1 = T_{transition}$, phonons control the thermodynamics (and dynamics) of the system. Similar phenomena can be observed in the dynamical structure factor (DSF) as shown in Fig. 5 in a log–log plot. The DSF (typical for *inelastic* thermal neutron scattering experiments, $4 \text{ \AA} \sim 5 \text{ meV} \sim 60 \text{ K}$) gives the frequency spectrum

⁹ When the lattice has fixed constant length, as expansion is not permitted, experiences internal stress (pressure). If, however, the lattice length is free but no external force to it is applied (like compression or stretching at a free end), it can be shown that the lattice ($a, b > 0$) expands as it vibrates. The solitary wave is a *compression* pulse, and cnoidal waves cause expansion with, however, high compression at each periodic wave “peak” (or maximum).

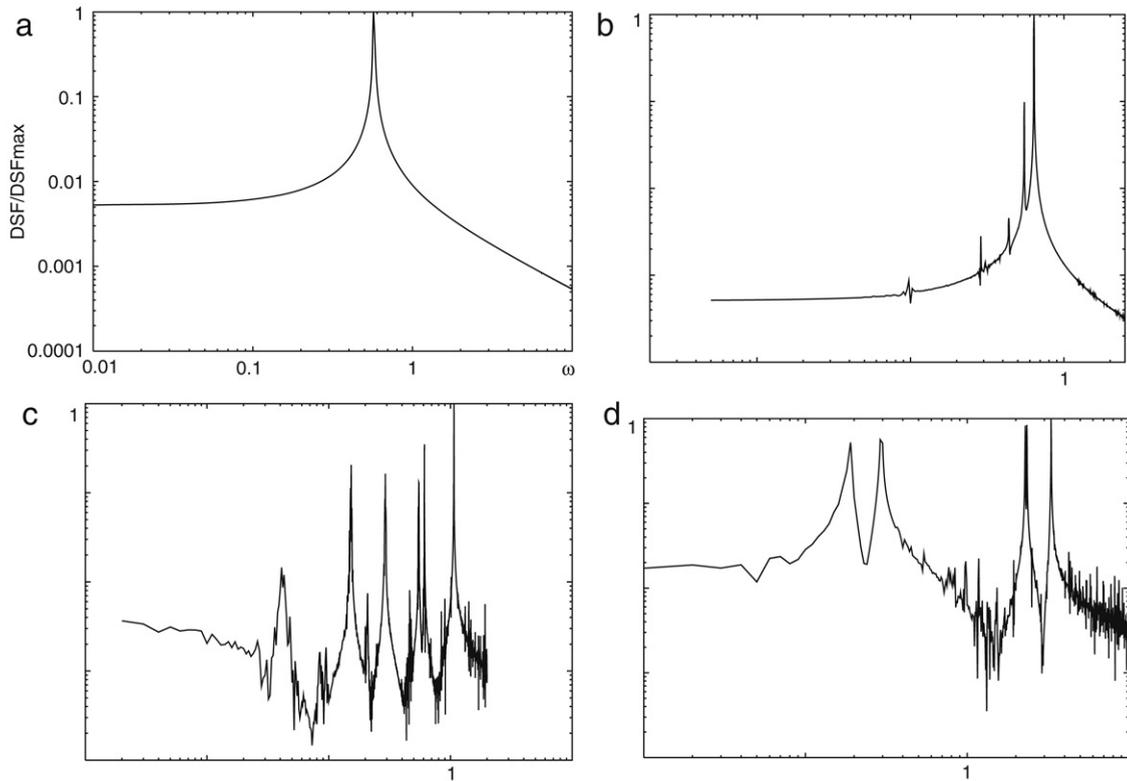


Fig. 5. Typical plot of the dynamic structure factor (DSF) versus frequency for a Toda lattice. In view of Fig. 4 (specific heat) the sequence is as follows: (a) a single phonon peak appears with (practically) linear sound velocity $(ab/m)^{1/2}$; (b) at $T = 10^{-1}T_{transition}$ the spectrum starts being complicated; (c) at $T = T_{transition}$ among the many peaks emerges the (supersonic) soliton as the highest of them all; and (d) at $T = 10T_{transition}$ phonons and solitons provide a “highly deformed phonon spectrum”.

of correlations between density fluctuations. It is the double Fourier transform of the density–density correlation [40, 41]. When T is well below $T = T_{transition}$ one observes a single phonon peak that provides the linear sound velocity, $v_{sound} = (ab/m)^{1/2} = \omega_0$, as earlier indicated. As the transition temperature is approached from below the phonon spectrum gets multi-peaked with many phonons or highly deformed phonons showing up (multiphonon range), until a much higher peak clearly emerges above the messy background. It corresponds to the soliton with supersonic velocity (11). Both the specific heat (Fig. 4) and DSF (Fig. 5) point to the significant role played by strong lattice compressions in the form of solitons. Exaggerating a bit one can say that such role tends to come sharper the nearer the “material” is to the “edge of melting”.

When solitons get excited, at high enough temperature in the lattice, we expect a significant heat transfer enhancement relative to the usual Fourier’s linear law. This prediction agrees beautifully with long ago reported data of Uranium [42]. Fig. 6 shows around 200 °C, or less, a significant change attributed to the onset of the earlier defined *intrinsic localized modes* (ILM) when anharmonicity enters the dynamics [43,44] (locally as a kind of lattice “defect” or all along the lattice; recall that ILM also refers to discrete *breathers*). It is the only experimental data known to this author.

4. Electron capture and electron transfer

4.1. The sollectron concept

Turning to electric conduction in the (charged) adapted Toda–Morse lattice and in view of the results recalled above one can treat *classically* the lattice dynamics while treating *quantum mechanically* the electron and the electron–lattice interaction. Indeed, this fits well with the fact that solitons appear above the multiphonon range as shown in Figs. 4 and 5. Relative to what has been recalled in Section 1 there is the need of choosing (computing) the transfer matrix elements [13, 14], taken here as

$$V_{n,n-1} = V_0 e^{-\alpha(\xi_n - \xi_{n-1})} \quad (16)$$

and so on. The parameter α is an inverse decaying “length” scale.¹⁰

¹⁰ Note that the choice (16) adds a *second nonlinearity* to the polaron description. Indeed, as for the on-site energy, E_n , here (16) could be taken linearized and then the coupling between c_n and ξ_n would be nonlinear made with linear contributions from each of them, hence $(\xi_n - \xi_{n-1})c_{n-1}$, and so on in the

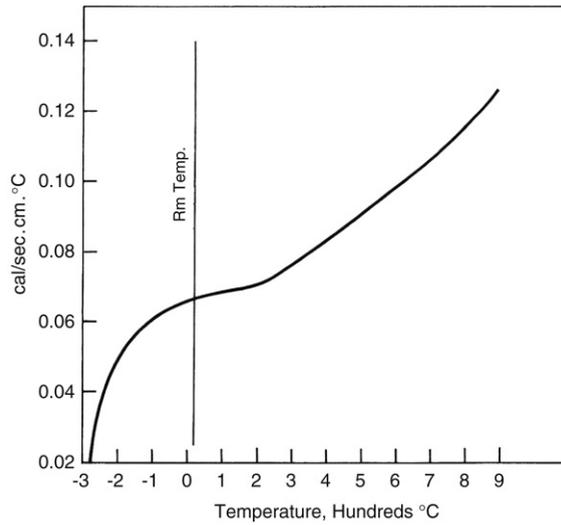


Fig. 6. Thermal conductivity of Uranium [42]. Around 200 °C there appears clear indication of soliton-mediated transport [44].

To have a universal description it suffices to make quantities dimensionless by introducing suitable scales/units: $\tau = V_0/\hbar\omega_M$, $\tilde{\alpha} = \alpha/B$, and $\tilde{V} = V_0/2D$ thus using the depth of the Morse potential as unit/scale; $\omega_M = (DB^2/M)^{1/2}$, M denotes lattice units mass (typical parameter values for some biomolecules are: $B = 4.45 \text{ \AA}^{-1}$, $\alpha = 1.75B$, $D = V_0 = 0.1 \text{ eV}$, $\omega_M = 3 \times 10^{12} \text{ s}^{-1}$, $V_0/\hbar = 0.6 \times 10^{14} \text{ s}^{-1}$, $\tau = 10$). Then disregarding the tilde and also the diagonal terms, Eq. (4) becomes

$$\dot{c}_n = -\tau \left[e^{-\alpha(\xi_n - \xi_{n-1})} c_{n-1} + e^{-\alpha(\xi_{n+1} - \xi_n)} c_{n+1} \right]. \tag{17}$$

The parameter τ shows explicitly the time scale of electron motions while the time t corresponds to the slower time scale of the lattice vibrations. The latter obey the Eq. (8) augmented with the coupling to electron hopping motions or better said, electron probability density,

$$\ddot{\xi}_n = \left[1 - e^{(\xi_{n+1} - \xi_n)} \right] e^{-(\xi_{n+1} - \xi_n)} - \left[1 - e^{-(\xi_n - \xi_{n-1})} \right] e^{-(\xi_n - \xi_{n-1})} - \alpha V \left[(c_{n+1}^* c_n + c_{n+1} c_n^*) e^{-\alpha(\xi_{n+1} - \xi_n)} + (c_n^* c_{n-1} + c_n c_{n-1}^*) e^{-\alpha(\xi_n - \xi_{n-1})} \right]. \tag{18}$$

Accordingly, taking into consideration the large disparity between τ and t (and also between energies involved), quite a strong claim is here made: viewed from Eq. (17), if solitons are excited in the lattice following Eq. (8), then Eq. (18) brings a *dominant* soliton influence upon the electron probability density, hence upon electron hopping motions (and eventually trapping as shown below). In turn, the electron evolution, Eq. (17), affects lattice vibrations. There is feedback or feedforward action of one upon the other, depending on where we start from (18) (the position taken by the present author here) or (17) (the original approach when introducing the *polaron*). Needless to say, when no electron is present, Eq. (18) reduces to Eq. (8). What really matters is that the interplay between electron and lattice vibrations has now, in view of Eqs. (17) and (18), a genuinely new element, the soliton-mediated effect, recalling its “universal” carrier character [30]. This permits one to consider the compound *polaron-soliton* “quasiparticle” as a new physical entity which is the “solelectron”. Thus, the *solelectron* concept appears as a significant generalization of the original *polaron* concept (or in stronger terms a genuinely new concept in electric conduction). Before proceeding to the analysis of solelectron-mediated electric conduction let us add further support to this concept by analyzing some striking results thus permitting one to firmly justify the possible “truth and consequences” of the *new* concept. [N.B. As one might have guessed, unlike in older times, these days when a new idea is put forward, one soon realizes that someone else has already thought about it. Indeed, variants of the *solelectron* concept have been explored by several authors [45–53]. For instance, Zolotaryuk et al. [47,48], in the nearest work to this and related contributions of the present author, alerted about the above discussed two nonlinearities (the polaron coupling and the lattice anharmonicity), a mixture that “gives rise to very complicated dynamics”, with possible consequences like supersonic charge transfer and “the coupling of the self-trapping states (polaron) with the lattice solitons”. Zhou and Xu [51], following that earlier work [47,48], considered a hydrogen-bonded lattice composed of a proton sublattice and a heavy-ion sublattice backbone. Then they added an excess electron to the proton sublattice where vibrations or deformations were treated with a *quartic (anharmonic)* potential (one of the cases treated by FPU and by Visscher and collaborators; it is also the potential used in textbooks [13,14]).

second term of the r.h.s. of Eq. (4). As *supra* noted, one must be aware that linearization may put at stake the significance and self-consistency of nonlinear elasticity in the context of soliton-mediated transport.

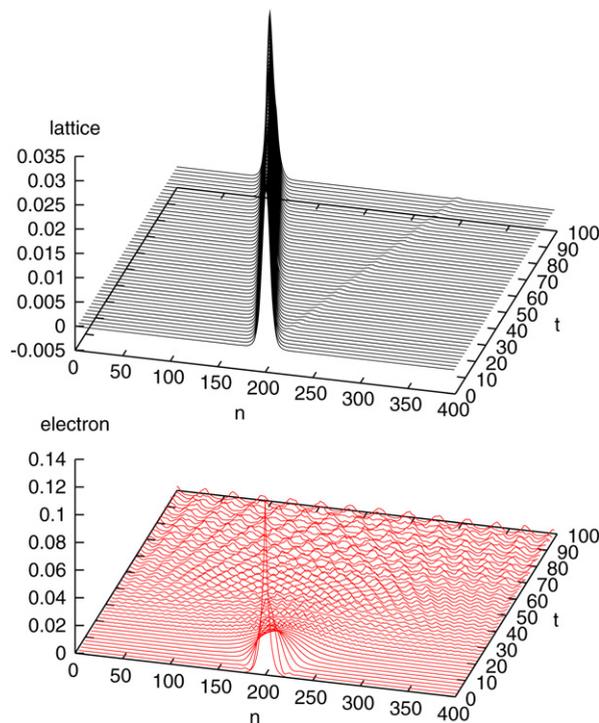


Fig. 7. Soliton and electron taken separately (no interaction). Upper figure: lattice soliton evolution starting at site $n = 200$ following Toda's Hamiltonian equations. Lower figure: electron probability density evolution following Schroedinger equation. From initial "localization" at site $n = 200$ the electron ends up *completely delocalized*, i.e., the probability density is spread "uniformly" everywhere along the lattice [58].

The proton sublattice in turn interacts with the heavy-ion sublattice, the latter considered with just *harmonic* intersite interactions. For the electron–proton sublattice interaction they used the, earlier discussed, lowest order tight binding nonlinearity and no direct electron-heavy-ion lattice interaction was considered. After some approximations made (going to the continuum, etc.) and using a self-consistent method of solution they found that the electron (with a sech^2 probability density) can be trapped in compression areas of the proton sublattice and hence the electron binds to *topological* (tanh-like kink) deformation solitons of the proton sublattice. Thus they concluded that the latter acts as a "ferry boat" for the electron (note that sech^2 is the derivative of \tanh ; the latter refers to unit displacements while the former to its gradient). This is their *electrosoliton* in the sense of Davydov. Unaware of that publication [51] the present author used the "surfing" metaphor for electrons riding on solitons in the Toda lattice [54]. Then as in their solution method the heavy-ion lattice motions are mathematically "slaved" to the proton topological solitons the backbone sublattice exhibits similar soliton deformations (though the intersite potential was harmonic, as earlier noted). They refer to the "electron-soliton"-soliton *pair* as the significant quasiparticle. This *pair* concept is, indeed, embraced by the *solelectron* concept. At variance with the work of Zhou and Xu, let us emphasize that the *solelectron* comes from the definition of the underlying *soliton* as a kind of "universal" carrier whereas for those authors everything is originated by the addition of an excess electron and, in part, like with Davydov's theory, the soliton emerges following mathematical simplifications in the solution methodology.]

4.2. Solitonic electron trapping

Consider an electron placed at site " n " in a lattice (arbitrary for the time being). Then let alone the electron, with no interaction with the lattice units and hence considering the lattice as a discrete space available, its evolution is dictated by the Schroedinger equation (2). Fig. 7 shows how from an initially peaked probability density (the electron is initially "localized" at site " n ") as time proceeds the probability spreads down to a uniform distribution over all lattice sites. This means that the electron ends up by being *completely delocalized* and hence upon adding the ionic character to the lattice no appreciable polaron effect or self-trapped state is to be expected (not to be confused with a largely extended polaron, as the electron is everywhere so weak as not being able to significantly alter the lattice motions).

Take now Eq. (8) and launch as an initial condition a soliton at a certain lattice site. The soliton is expected to proceed unaltered as time progresses. Then let us switch-on the electron-lattice interaction hence switch-on Eq. (18) for the case when the electron is *completely delocalized*. The striking result found is illustrated in Fig. 8. Little by little the soliton gathers the electron probability density, packs it reconstructing at its immediate neighborhood the electron original probability density peak. This is quite what a "vacuum cleaner" does with "dust". This result gives a hint on a possible significant consequence. Indeed, once an electron is trapped if a second electron is permitted around (necessarily with opposite spin,

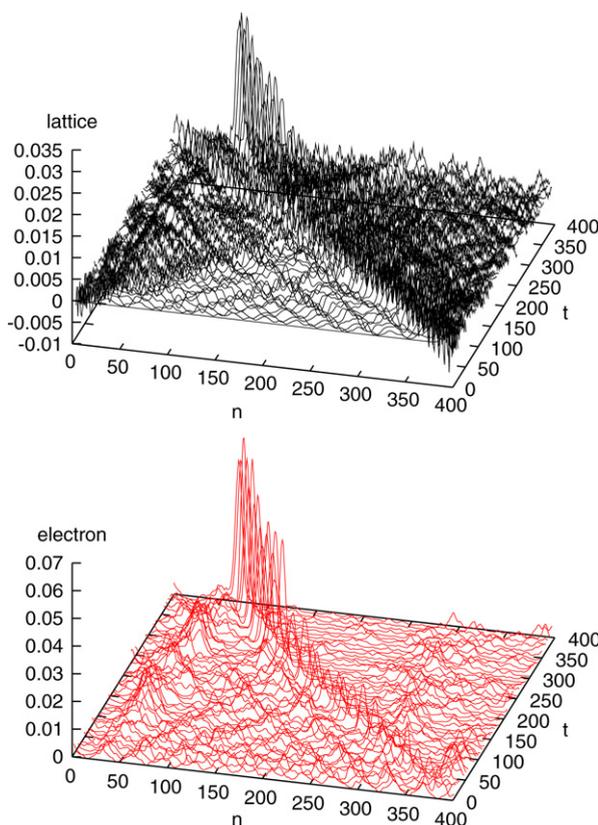


Fig. 8. Interaction of a *soliton* with a *completely delocalized* electron. Lower figure: the electron after following the evolution dictated by Schroedinger equation (see Fig. 7) ends up *completely delocalized* with probability density spread like “dust” over the entire lattice. Then at such time instant the soliton is launched taking as initial condition for the electron the final state of the lower picture in Fig. 7. Upper figure: the soliton after gathering the electron dusty probability density eventually gives rise to the *solectron* current. As the soliton travels there is reconstruction of the electron probability density in a kind of “vacuum cleaner” process done by the soliton, akin to a long range correlation effect or a kind of *global coupling* in the lattice [58].

in accordance with Pauli’s principle) the soliton “attraction” may overcome the repelling Coulomb interaction, thus also trapping the second electron and allowing pairing. Work seems of interest in this direction [55] in view of results obtained by other authors [56,57]. Subsequently, after trapping the electron, the compound or bound state soliton–electron, i.e., the *solectron* proceeds moving unaltered along the lattice. Although as time proceeds, there is indeed action of the electron upon the lattice vibrations, the *polaron* effect, it is clearly a minor element in the early stage of *solectron* formation and time and space evolution and it does depend on the time scales involved in the dynamics. In fact, Fig. 8 shows that the situation is at the opposite extreme of the *polaron* case and also differs from the situation when given an electron *localized* at site “*n*” a soliton is launched at either the same site or at another. Electron trapping ensues irrespective of the possible feedforward or feedback action of the electron upon the soliton (as a *polaron* effect upon *anharmonic* lattice vibrations) enhanced or even dominated by the action of the soliton. Fig. 9 illustrates the *polaron*–soliton case showing trajectories of a more typical trapping process with ensuing *solectron* current.

Let us now launch two solitons which are allowed to collide in their evolution along the lattice. Consider also the added excess electron. Fig. 10 shows a sequence of events numerically observed. The electron starts being trapped and carried by one of the solitons, here by the one moving left-to-right. Then there is collision with the oppositely moving right-to-left soliton. As the collision proceeds and “finishes”, the electron leaves the first soliton and reappears trapped and carried by the second soliton. Accordingly, the electron has changed both partner and direction of motion after the collision. Another striking result also observed numerically is the electron probability density splitting thus illustrating how quantum mechanically the electron moves simultaneously in both directions! A detailed analysis, including numerical evidence of the electron–soliton energy exchanges, with numerous illustrations, of both supersonic and subsonic cases has been given elsewhere [58,59].

5. *Solectron*-mediated electric conduction characteristics

The prediction of *solectron*-mediated electric conduction was first done using the classical Drude–Lorentz approach [54]. It was put forward as a (non-equilibrium) “phase transition” from an Ohmic to a non-Ohmic form of electric conduction in a driven-dissipative system. Subsequent work [60] has added strong support to the original finding delineating a true

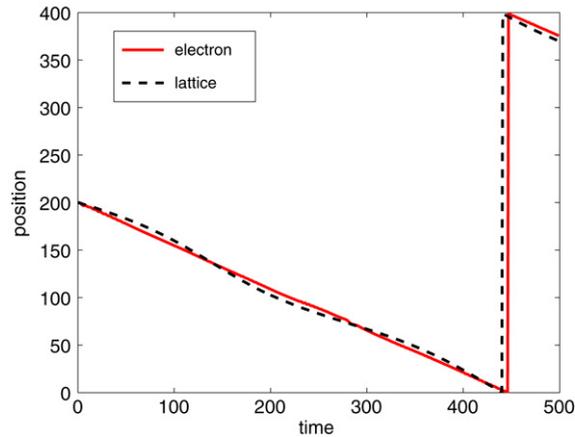


Fig. 9. Soliton and electron interaction leading to a solectronic current from the very beginning. Both are launched and added, respectively, at the same site ($n = 200$). Note the use of (finite) periodic boundary conditions in the computation [58].

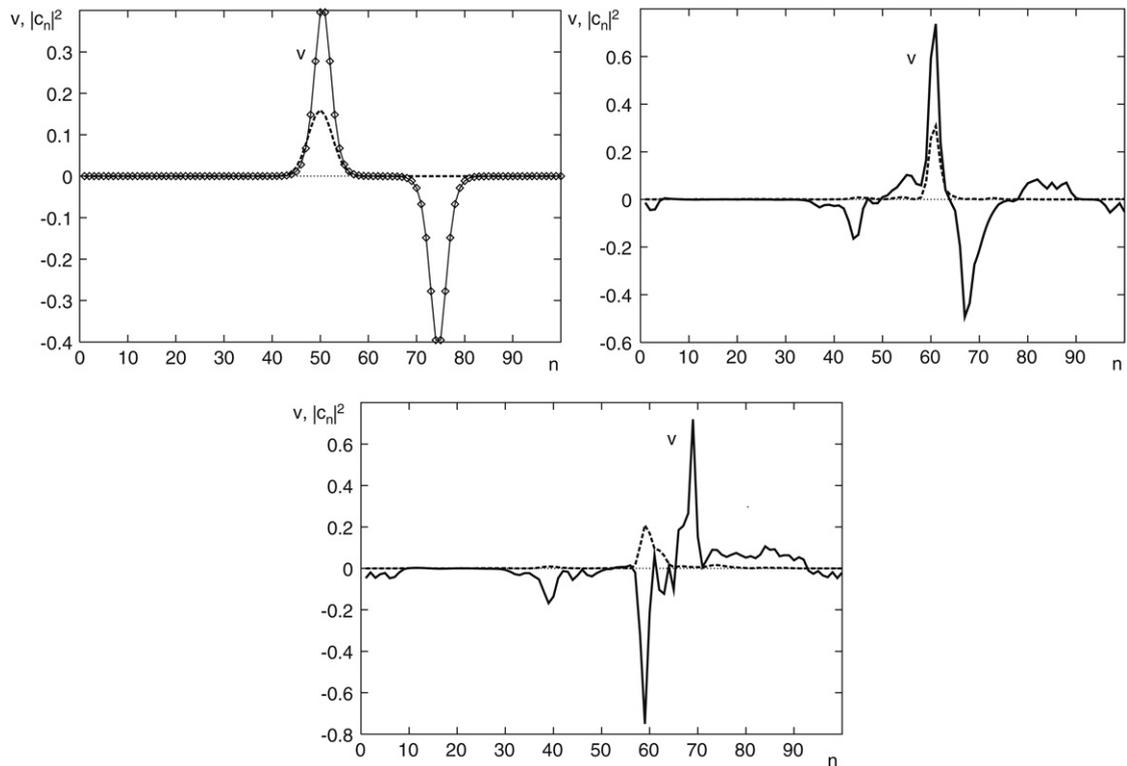


Fig. 10. Head-on collision of a *solectron* (elevation, solid line) moving left-to-right with a *soliton* (depression, solid line) moving right-to-left. v refers to the soliton and $|c_n|^2$ to the electron. Following the collision, the electron (dotted line) decided to change partner. Accordingly, a *solectron* emerges moving right-to-left and the abandoned, lonely *soliton* continues motion left-to-right [59].

(non-equilibrium) phase diagram. Thus the electron-(ion)lattice interaction as well the lattice dynamics were considered in a purely classical description. Later on, the study was extended to the quantum treatment of the electron and the electron-lattice interaction, while maintaining the classical description of the solitonic lattice dynamics [58,59,61,62]. As earlier noted this is acceptable provided one targets phenomena at relative “high” temperatures and might it be better the nearer one is to the “edge of melting” in the system. Recall the experimental evidence of soliton-mediated heat transport enhancement (Fig. 6) in Uranium at about 200 °C (thermal conductivity was measured up to 900 °C). Manley et al. [44] have recently reported the onset of ILM- or lattice solitons at 450 K ($\lesssim 200$ °C). However, electric conductivity in the same material has been measured only up to about 600 °C with no significantly appreciable change or “anomaly” in its increasing trend [42]. Around 600 °C there is a transition from the α -phase to the β -phase and to the γ -phase and no further data exists that

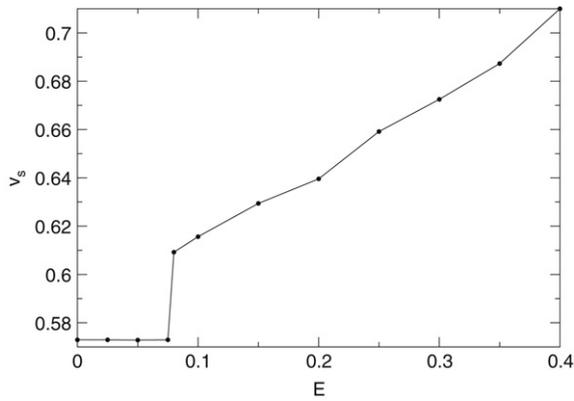


Fig. 11. Typical current-field characteristics of the *solectron* motion (see Fig. 9). The solectron velocity, v_s , is plotted versus suitably normalized electric field intensity. As the field strength is lowered there is a transition from Ohmic to non-Ohmic conduction. As one can expect this transition is affected by temperature [62].

could indicate the role played by solitons already excited in the crystal. Noteworthy is that Uranium melts at 1100 °C. The temperature 600 °C is 40% below the melting point. Clearly, 600 °C is far from the “edge of melting”. Note that the existence of the soliton is a *necessary albeit not sufficient* condition for electric trapping.

Let us comment now on the role played by an externally applied electric field. In order to do this suffices to augment the tight-binding electron evolution equation with a contribution proportional to the field strength. Then Eq. (17) becomes

$$i\dot{c}_n = -\tau \left[e^{-\alpha(\xi_n - \xi_{n-1})} c_{n-1} + e^{-\alpha(\xi_{n+1} - \xi_n)} c_{n+1} \right] - n\tilde{E}c_n, \tag{19}$$

where $\tilde{E} = (e/\hbar\Omega_{Morse}) E$ accounts for the dimensionless applied field strength. Then from the solution of this equation the current is given by

$$j = i \sum_n (c_{n+1}^* c_n - c_n^* c_{n-1}). \tag{20}$$

Using, however, the solectron velocity, v_s , as the computational “measure” to account for the electric current, Fig. 11 shows the theoretical prediction. First, the current is proportional to the field strength following Ohm’s linear law. When the field strength is lowered the electron does not follow the field as the solectron overcomes the action of the field and then the current takes a constant, field-independent value down to zero field strength. Accordingly, there is a *plateau* where the differential conductivity vanishes while demanding a huge value near zero field strength. This prediction was first made in Ref. [54] using purely classical dynamics and electrodynamics. Further details about this characteristics have been given elsewhere for both the *classical* and the *quantum* approaches to the electron-lattice dynamics [39,54,58–62]. Noteworthy is that the solectron-charge transport in the Toda–Morse lattice appears stable up to “room temperature” (about 300 K) [62].

Another interesting characteristics is the relationship between electric current and temperature. To obtain the latter, due consideration ought to be taken of temperature in the compound system, including ion lattice temperature and electron temperature. This study has only been done for the purely *classical* description treating the problem with an appropriate Langevin stochastic dynamics [39,54]. It appears that as the temperature is relatively high but, needless to say, below the melting temperature of the system, the current is practically independent of temperature. Upon lowering it towards the earlier mentioned $T_{transition}$ (Fig. 4) a significant increase occurs thus showing the role played by the *solectron*. This trend is expected to hold in the quantum case.

Clearly, for high field strengths as well as for (relatively) high temperatures the electron rather follows either the field or the disorder induced by $k_B T$. It is for *moderate* values, of both “parameters” that the solectron fully controls the current. This is a clear manifestation of the significant role played by the *nonlinear elasticity* when added to the quantum dynamics (or even to the classical dynamics) evolution of the lattice model system treated here.

6. Concluding remarks

The origin of the *polaron* concept (an electron with an associated phonon cloud composed of a few, finite number of phonons), long ago introduced by Landau and Pekar, has been recalled in order to set the stage and to have solid ground for a significant generalization by introducing the *solectron* concept (by analogy, an electron with a soliton cloud which can be considered with an *infinite* number of phonons; note, however, that the soliton exists even if there is no electron).¹¹ This was done by giving preeminence to *anharmonic* backbone lattice vibrations (and hence nonlinear elasticity) not considered by the

¹¹ A smooth curve is easily reconstructed or analyzed with a few, finite number of Fourier modes while a peaked one like a cornered graph or a *cnoidal* peak demands using an *infinite* number of modes (for a jump recall the Gibbs phenomenon).

earlier authors, limited to *harmonic* lattice vibrations (acoustic phonons). This preeminence offers the possibility of *soliton* excitations (and related deformations) in the lattice. However, at variance with the *polaron*, these excitations, by their very nature, are *mobile*, even if very few (two or three lattice units) are involved. They appear as long lasting, “universal” carriers of matter, energy or electric charge. The addition of an excess electron leads to a polaron–soliton interacting compound. But there is more than that. Indeed, the soliton has been shown to be able to trap an electron even when the latter is *completely delocalized* along the lattice and no significant feedforward *polaron* effect on the lattice motions exists. Numerical evidence has been provided about the onset of such solitons by presenting specific heat (at constant length/volume) and dynamic structure factor results. It has also been shown how the soliton mediates in establishing a non-Ohmic form of electric conduction (generally supersonic; subsonic values are also possible depending on parameter values). A salient feature of such new form of electric conduction is that for a certain range of relatively moderate electric field strengths the current becomes constant, field-independent down to vanishing field values. The soliton formation is not an automatic event for, as already emphasized, the soliton excitation is a *necessary albeit not sufficient* condition for it. The soliton formation demands also the adequacy of conditions (parameter values in the dynamics of both electron and lattice, and their coupling, temperature, etc) for electron trapping to be possible by the soliton. Generally, this latter event is expected to occur at higher temperatures than the temperature at which solitons are excited. In fact, exaggerating somewhat, soliton currents are expected at the “edge of melting” or disaggregation of a material.

In conclusion, quite a strong claim is here made (though theory without experiment is fruitless): nonlinear elasticity (for the time being this claim refers only to a Toda-like lattice model) may decide electric conduction characteristics, like a non-Ohmic form of a relatively fast, constant, field-independent current. There remains the question (not addressed here) of existence and stability of *thermal* solitons (and solitons) up to relatively high temperatures, e.g. room or physiological temperatures. There is only a partial answer to this question in Ref. [62] and in a more recent work [63], where we also have started considering Eq. (7) augmented with a non-uniform diagonal part. Although some numerical evidence shows that the soliton-charge transport in the Toda–Morse lattice appears stable up to room temperature (about 300 K), further work is needed along this line of enquiry before a firmly established conclusion can be drawn.

Before closing let us mention that an approach to the problem discussed here using Kubo-like (Kubo–Greenwood–Green linear response) transport theory valid, in principle, for arbitrary dimension has recently been given elsewhere [64].

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References

- [1] L.D. Landau, Phys. Z. Sowjetunion 3 (1933) 664.
- [2] S.I. Pekar, Sov. Phys. JETP 16 (1946) 335; 341, 993, 17 (1947) 868; 18 (1948) 105.
- [3] S.I. Pekar, Untersuchungen über die Elektronentheorie, Akademie Verlag, Berlin, 1954.
- [4] L.D. Landau, S.I. Pekar, Sov. Phys. JETP 18 (1948) 419.
- [5] H. Fröhlich, Proc. Roy. Soc. London A 215 (1952) 291; Adv. Phys. 3 (1954) 325.
- [6] See e.g. J.T.L. Devreese (Ed.), Polarons in Ionic Crystals and Polar Semiconductors, North-Holland, Amsterdam, 1972.
- [7] R.P. Feynman, Phys. Rev. 97 (1955) 660.
- [8] M.V. Volkenstein, J. Theoret. Biol. 34 (1972) 193, for further details and possible applications of the conform concept see also: Biophysics, Mir, Moscow, 1983.
- [9] A.S. Davydov, Solid State Physics, Nauka, Moscow, 1976.
- [10] A.S. Davydov, J. Theoret. Biol. 38 (1973) 559.
- [11] A.S. Davydov, Solitons in Molecular Systems, 2nd ed., Reidel, Dordrecht, 1991, and references therein.
- [12] P.L. Christiansen, A.C. Scott (Eds.), Davydov’s Solitons Revisited, Plenum Press, New York, 1991; See also A.C. Scott, Davydov’s soliton, Phys. Rep. 217 (1992) 1 and references therein.
- [13] N.W. Ashcroft, N.D. Mermin, Solid State Physics, Thomson Learning, New York, 1976.
- [14] C. Kittel, Introduction to Solid State Physics, 8th ed., Wiley, New York, 2005.
- [15] M. Toda, Phys. Scripta 20 (1979) 424.
- [16] G.D. Mahan, Many-Particle Physics, 3rd ed., Plenum/Kluwer, New York, 2007.
- [17] A.J. Heeger, S. Kivelson, J.R. Schrieffer, W.P. Su, Rev. Modern Phys. 60 (1988) 781.
- [18] L. Yu (Ed.), Solitons and Polarons in Conducting Polymers, World Scientific, Singapore, 1988, and reprints therein.
- [19] J. Hubbard, Proc. Roy. Soc. London A 276 (1963) 238; A 277 (1964) 237; A 281 (1964) 401.
- [20] A. Montorsi (Ed.), The Hubbard Model. A Reprint Volume, World Scientific, Singapore, 1992.
- [21] E. Fermi, J.R. Pasta, S. Ulam, Los Alamos Nat. Lab. Report LA-1940, 1955; in: Collected Papers of Enrico Fermi, University of Chicago Press, Chicago, 1965, pp. 978–988.
- [22] G.P. Berman, F.M. Izrailev, Chaos 15 (2005) 015104.
- [23] D.N. Payton III, M. Rich, W.M. Visscher, Phys. Rev. 160 (1967) 706. See also Procs. Int’l Conf. Localized Excitations in Solids, Plenum Press, New York, 1968, pp. 657–664.
- [24] N. Zabusky, M.D. Kruskal, Phys. Rev. Lett. 15 (1965) 57.
- [25] N. Zabusky, Chaos 15 (2005) 015102.
- [26] M. Toda, J. Phys. Soc. Japan 22 (1967) 432; 23 (1967) 501.
- [27] M. Toda, Theory of Nonlinear Lattices, 2nd ed., Springer, Berlin, 1989.

- [28] M. Toda, *Nonlinear Waves and Solitons*, KTK Scientific Publishers, Tokyo, 1989.
- [29] See e.g. M. Remoissenet, *Waves Called Solitons*, 3rd ed., Springer, Berlin, 1999, and references therein.
- [30] E. del Rio, M.G. Velarde, W. Ebeling, *Physica A* 377 (2007) 435.
- [31] P. Morse, *Phys. Rev.* 34 (1929) 57.
- [32] See, e.g. Ph. Choquard, *The Anharmonic Crystal*, Benjamin, New York, 1967.
- [33] See e.g. V.I. Nekorkin, M.G. Velarde, *Synergetic Phenomena in Active Lattices. Patterns, Waves, Solitons, Chaos*, Springer, Berlin, 2002.
- [34] M. Abramowitz, I.A. Stegun (Eds.), *Handbook of Mathematical Functions, with Formulas, Graphs, and Mathematical Tables*, Dover, New York, 1965.
- [35] T. Schneider, E. Stoll, *Phys. Rev. Lett.* 45 (1980) 997.
- [36] F.G. Mertens, H. Büttner, *J. Phys. A* 15 (1982) 1831.
- [37] M. Toda, N. Saitoh, *J. Phys. Soc. Japan* 52 (1983) 3703.
- [38] A.P. Chetverikov, W. Ebeling, M.G. Velarde, *Eur. Phys. J. B* 44 (2005) 509; 57 (2006) 87.
- [39] A.P. Chetverikov, W. Ebeling, M.G. Velarde, *Internat. J. Bifur. Chaos* 16 (2006) 1613.
- [40] P.A. Egelstaff, *An Introduction to the Liquid State*, Academic Press, London, 1967.
- [41] N.H. March, M.P. Tosi, *Atomic Dynamics in Liquids*, Mcmillan, London, 1976.
- [42] A.N. Holden, *Physical Metallurgy of Uranium*, Addison-Wesley, Reading, Massachusetts, 1958.
- [43] A.J. Sievers, S. Takeno, *Phys. Rev. Lett.* 61 (1988) 970.
- [44] M.E. Manley, M. Yethiraj, H. Sinn, H.M. Voltz, A. Alatas, J.C. Lashley, W.L. Hulst, G.H. Lander, J.L. Smith, *Phys. Rev. Lett.* 96 (2006) 125501, and references therein.
- [45] S. Yomosa, *Phys. Rev. A* 32 (1985) 1752.
- [46] B.G. Vekhtler, M.A. Ratner, *J. Chem. Phys.* 101 (1994) 9710; *Phys. Rev. B* 51 (1995) 3469.
- [47] A.V. Zolotaryuk, K.H. Spatschek, A.V. Savin, *Phys. Rev. B* 54 (1996) 266.
- [48] A.V. Zolotaryuk, St. Pnevmatikos, A.V. Savin, *Phys. Rev. Lett.* 67 (1991) 707.
- [49] S. Flach, K. Kladko, *Phys. Rev. B* 53 (1996) 11531.
- [50] A.V. Zolotaryuk, J.C. Eilbeck, *J. Phys.: Condens. Matter* 10 (1998) 4553.
- [51] B. Zhou, J.-Z. Xu, *J. Phys.: Condens. Matter* 10 (1998) 7929.
- [52] N.K. Voulgarakis, G.P. Tsironis, *Phys. Rev. B* 63 (2000) 014301.
- [53] D. Hennig, *Phys. Rev. E* 62 (2000) 2846.
- [54] M.G. Velarde, W. Ebeling, A.P. Chetverikov, *Internat. J. Bifur. Chaos* 15 (2005) 245.
- [55] M.G. Velarde, C. Neissner, *Internat. J. Bifur. Chaos* 18 (2008) 885. See also D. Hennig, M.G. Velarde, W. Ebeling, A.P. Chetverikov, *Phys. Rev. E* 78 (2008) 066606-1.
- [56] J.K. Freericks, M. Jarrell, G.D. Mahan, *Phys. Rev. Lett.* 77 (1996) 4588.
- [57] B.J. Alder, K.J. Runge, R.T. Scalettar, *Phys. Rev. Lett.* 79 (1997) 3022.
- [58] D. Hennig, A.P. Chetverikov, M.G. Velarde, W. Ebeling, *Phys. Rev. E* 76 (2007) 046602.
- [59] M.G. Velarde, W. Ebeling, A.P. Chetverikov, D. Hennig, *Internat. J. Bifur. Chaos* 18 (2008) 521.
- [60] V.A. Makarov, M.G. Velarde, A.P. Chetverikov, W. Ebeling, *Phys. Rev. E* 73 (2006) 066626.
- [61] M.G. Velarde, W. Ebeling, D. Hennig, C. Neissner, *Internat. J. Bifur. Chaos* 16 (2006) 1035.
- [62] D. Hennig, C. Neissner, M.G. Velarde, W. Ebeling, *Phys. Rev. B* 73 (2006) 024306.
- [63] M.G. Velarde, W. Ebeling, A.P. Chetverikov, *Internat. J. Bifur. Chaos* 18 (2008) 3815.
- [64] A.P. Chetverikov, W. Ebeling, G. Röpke, M.G. Velarde, *Contrib. Plasma Phys.* 47 (2007) 465.