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ELECTRON TRAPPING BY SOLITONS. CLASSICAL VERSUS QUANTUM MECHANICAL APPROACH

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Assuming either classical electrodynamics or the quantum mechanical tight-binding of an electron to a nonlinear lattice with exponentially repulsive potential interactions we show how in both cases electron trapping can be mediated by solitons thus forming similar robust bound states (solectrons).

Keywords: Solitons; solectrons; anharmonicity; lattice dynamics; Morse interactions.

In two previous letters [Velarde *et al.*, 2005, 2006] a new form of electric conduction mediated by solitons was shown to be possible in an anharmonic one-dimensional (1D) lattice. In the first, a strictly classical approach was adopted hence treating the lattice dynamics classically and the electron-(ion) lattice interaction with classical electrodynamics. In the second, the electron-lattice interaction was considered within the tight-binding approximation [Ashcroft & Mermin, 1976] while maintaining the classical approach to the lattice dynamics. The lattice interactions were of Toda or Morse type akin to the Lennard–Jones interaction [Choquard, 1967; Toda, 1989], hence allowing for phonon — and soliton — longitudinal vibrations with compressions governed by the repulsive part of the potential [Chetverikov *et al.*, 2005, 2006a, 2006b]. These compressions were shown to be responsible for electron trapping by the lattice excitations thus leading to the formation of dynamic bound states (solectrons) of the electron with the soliton (the same phenomenon is valid also for the solitonic peaks of a cnoidal wave moving through the lattice).

In the present letter, we proceed deeper in the analysis and further explore the analogies and differences between the classical electrostatic trapping and the quantum mechanical tight-binding approximation using the Morse interaction. Thus, we consider a 1D anharmonic lattice with dynamics dictated by the following Hamiltonian describing nearest-neighbor Morse interactions:

$$H_{\text{lattice}} = \sum_n \left\{ \frac{1}{2}\frac{p_n^2}{M} + D(1-\exp[-B(q_n - q_{n-1})])^2 \right\}. \quad (1)$$

Here M denotes the mass of a lattice particle, $(q_n, p_n; n = 1, \ldots, N)$ describe their respective displacements from equilibrium positions and

momenta, B characterizes the stiffness of the spring-like constant in the Morse potential, and D is the depth of the potential well.

Considering the lattice particles to be positive ions (or screened ion cores in a broad sense) of charge $+e$, we add electrons to the system. In the strictly classical case we describe the electron dynamics (mass, m_e and charge, $-e$; $m_e \ll M$) by the equations

$$m_e \frac{\partial^2}{\partial t^2} y_j + \frac{\partial U_e}{\partial y_j} = -eE + m_e \gamma_e \frac{\partial}{\partial t} y_j + \sqrt{2D_e}\xi_j(t), \qquad (2)$$

where y_j denotes the position of the electron (for simplicity, to have electroneutrality we may consider as many electrons as ions albeit electrons noninteracting among themselves and hence $j = 1, \ldots, N$). To rule out unnecessary geometric difficulties while at the same time making the model more realistic we have assumed that the electrons are in 3D though the (ion)lattice is 1D. Further, we have considered the electrons in a "thermal bath" characterized by a Gaussian white noise, ξ_j, of zero mean and delta correlated. The parameter γ_e denotes electron friction satisfying Einstein's relation with D_e. For the electron-(ion) lattice interaction, we take

$$U_e(y_j) = -\sum_{k=1}^{N} [(y_j - q_k - k\sigma)^2 + h^2]^{1/2}. \qquad (3)$$

The parameter h is a suitable cut-off ($h \approx \sigma/2$) to rule out unnecessary Coulomb potential difficulties; σ defines equilibrium lattice spacing.

An alternative approach to the above given electron-lattice dynamics is to take the tight-binding Hamiltonian [Ashcroft & Mermin, 1976]:

$$H_{el} = -\sum_n V_{nn-1}(c_n^* c_{n-1} + c_n c_{n-1}^*), \qquad (4a)$$

where n denotes here the site where one electron is "placed" on the lattice and $|c_n|^2$ gives the probability of finding the electron residing at the site n. The quantity V_{nn-1} defines the transfer matrix element responsible for the hopping of the electron along the chain (considering only nearest neighbor hopping). This matrix is the key ingredient, allowing for the coupling of the electron to the lattice displacements, and hence the lattice vibrations, phonons or solitons. A reasonable choice for V_{nn-1} is [Hennig *et al.*, 2000, 2006]

$$V_{nn-1} = V_0 \exp[-\alpha(q_n - q_{n-1})], \qquad (4b)$$

where the parameter α accounts for the strength of the coupling.

For the sake of universality, it is best to rescale quantities and consider a dimensionless problem. We take as unit of time $\Omega_{\text{Morse}}^{-1}$, where $\Omega_{\text{Morse}} = (2DB^2/M)^{1/2}$ denotes the frequency of harmonic oscillations (linear, first-order approximation to the Morse exponential). For displacements we take B^{-1} as the unit, for momenta we take $(2MD)^{-1/2}$, hence for the interaction force we have $\alpha V_0/2BD$, and α is measured in (B^{-1}) units. Then, expecting no confusion in the reader, denoting the new dimensionless quantities with the same symbols as the old ones, the dynamics of the Hamiltonian system (1), (4a), (4b) is given by the following equations for the electron, c_n, and lattice vibrations, q_n,

$$i\frac{dc_n}{dt} = -\tau\{\exp[-\alpha(q_{n+1} - q_n)]\, c_{n+1} + \exp[-\alpha(q_n - q_{n-1})]\, c_{n-1}\}, \qquad (5a)$$

$$\begin{aligned}\frac{d^2 q_n}{dt^2} = {} & \{1 - \exp[-(q_{n+1} - q_n)]\}\exp[-(q_{n+1} - q_n)] \\ & - \{1 - \exp[-(q_n - q_{n-1})]\} \\ & \times \exp[-(q_n - q_{n-1})] \\ & - \alpha V\{(c_{n+1}^* c_n + c_{n+1} c_n^*) \\ & \times \exp[-\alpha(q_{n+1} - q_n)] \\ & + (c_n^* c_{n-1} + c_n c_{n-1}^*) \\ & \times \exp[-\alpha(q_n - q_{n-1})]\},\end{aligned} \qquad (5b)$$

where $\tau = V_0/\Omega_{\text{Morse}}\hbar$ and $V = V_0/2D$. Needless to say, in general the two time scales in (5a) and (5b) are not the same (which in frequency terms refer to ultraviolet/electronic versus infrared/acoustic), for most cases with electrons and phonons. For purposes of illustration we shall use the following parameter values: $B = 4.45\,\text{Å}^{-1}$, $\alpha = 1.75B$, $D = V_0 = 0.1\,\text{eV}$, $\Omega_{\text{Morse}} = 3.04 \cdot 10^{12}\,\text{s}^{-1}$, $\Omega_{\text{electron}} = V_0/\hbar = 0.608{\cdot}10^{14}\,\text{s}^{-1}$, and $\tau = 20.00$. These numerical values are relevant, e.g. for electron transport along hydrogen bonded polypeptide chains such as α-helices [Davydov, 1991; Christiansen & Scott, 1983; Scott, 1992].

Now, we take advantage of the similarity between the Morse and the Toda interactions in the repulsive range where phonons as well as solitons can be excited in the lattice [Toda, 1989; Chetverikov *et al.*, 2006a, 2006b]. Accordingly, for the lattice vibrations we make the ansatz

$$\exp[-3(q_n - q_{n-1})] = 1 + \beta \cosh^{-2}(\kappa n - \beta t), \qquad (6)$$

where $\beta = \sinh\kappa$, and κ is a parameter with dimensions of inverse length (related to the width of the soliton). The ansatz (6) is the Toda solution with appropriately rescaled stiffness [Chetverikov *et al.*, 2006a, 2006b]. It is a valid approximation leading to localized electronic pulses traveling with the solitons [Hennig, 2000; Hennig *et al.*, 2006]. Using (6), the coupling between Eqs. (5a) and (5b) yields

$$c_n(t) = \beta\cosh^{-1}[\kappa n - \beta t]\exp[-i(\omega t - \delta n + \sigma)], \tag{7}$$

where $\omega \equiv -2\cos\delta\cosh\beta$ and $\delta \in [-\pi, \pi]$. Note that $\sum_n |c_n|^2 = 1$ (conservation of norm, i.e. probability density) holds for $\kappa = 0.465$.

The evolution problem (5) has been solved for one hundred ($N = 100$) particles on a lattice with periodic boundary conditions using a fourth-order Runge–Kutta algorithm. The norm conservation as well as the conservation of the total energy was monitored throughout the integration procedure to ensure consistency. Figure 1 depicts the results found for solitons and for electrons. As initial condition at $t = 0$ we have chosen a cnoidal wave displacement for the lattice particles and a Gaussian distribution located initially at a place 25 lattice units away. At a subsequent time $t = 10$ the electron distribution is completely spread in comparison to the initial distribution which is represented too. At longer times the electron density concentrates around the soliton thus forming a dynamic bound state or solectron (see the snapshot for $t = 300$).

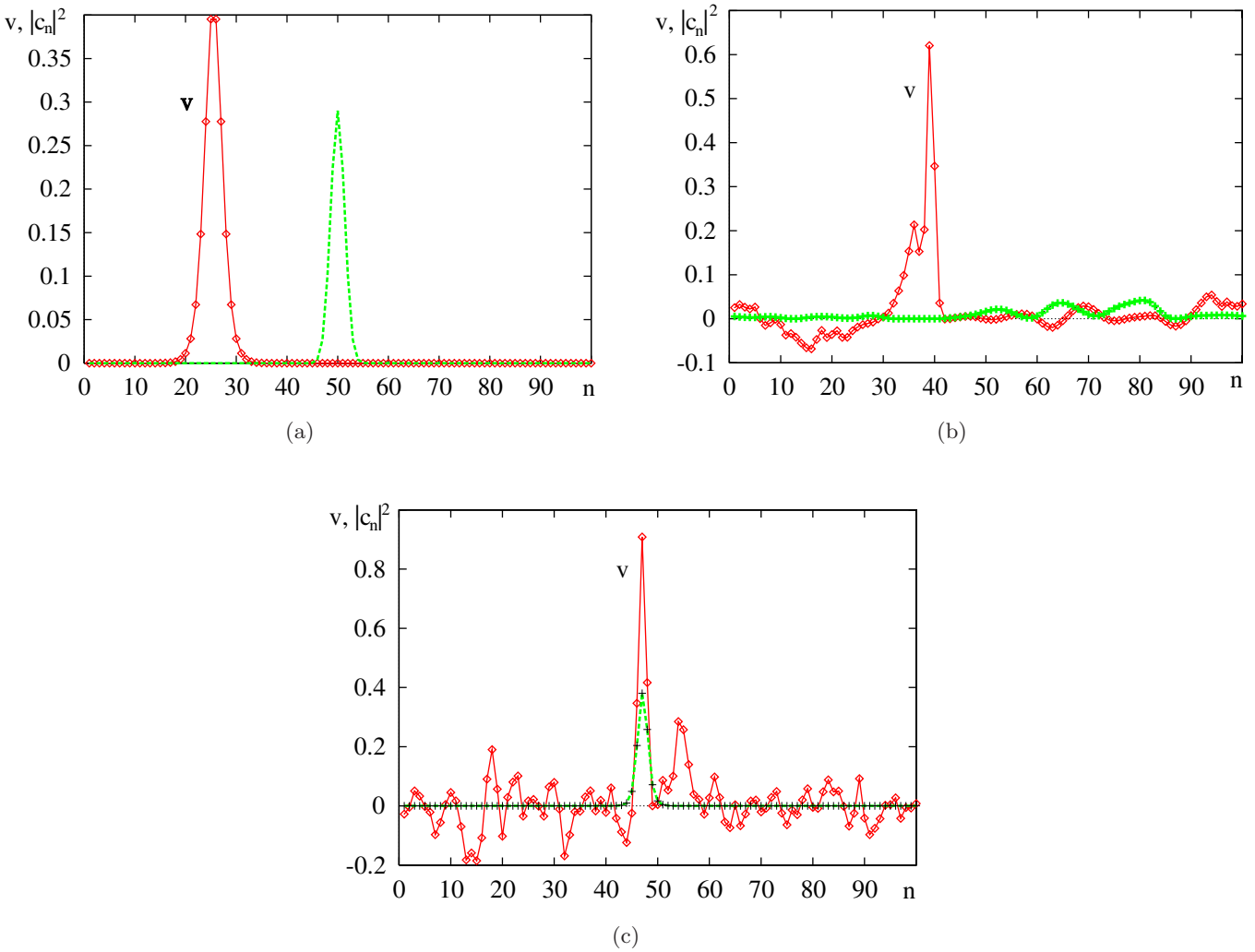

Fig. 1. Simulation according to Eqs. (5a) and (5b). Initially at $t = 0$ [Fig. 1(a)] the electron is represented by a (narrow peaked) Gaussian (dashed curve) with a maximum at $n = 50$ which is clearly distinct from the soliton-like (cnoidal wave) compression at $n = 25$ ($V = 0.5$). At $t = 10$ [Fig. 1(b)] the electron density is quite different from the Gaussian (dashed curve again) and the soliton peak is shifted to $n = 39$. At $t = 300$ [Fig. 1(c)] the electron probability density is gathered by the soliton and becomes again narrow-peaked. The ordinate **v** denotes dimensionless velocity.

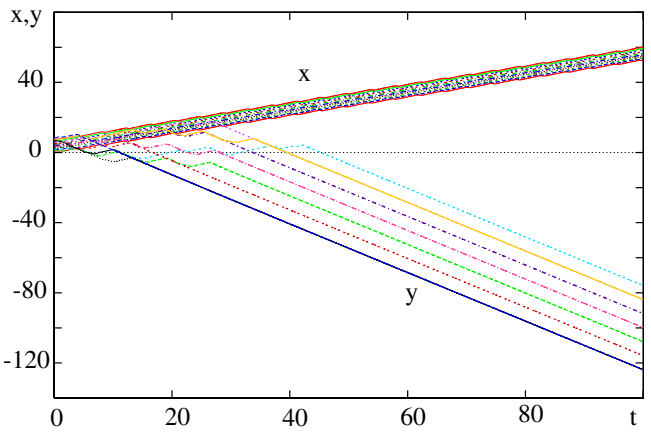

Fig. 2. Trajectories of both "ions" and trapped "electrons" in the classical model of 10 + 10 particles (compare to Fig. 1). We see that in the considered time interval most of the electrons are trapped by a soliton (for related pictures, see also [Chetverikov *et al.*, 2006a, 200b]).

For comparison we have shown in Fig. 2 the dynamics of ten electrons ($N = 10$) found by numerically integrating Eqs. (1) and (2) under the condition that a soliton is running along the lattice. We take this example from an earlier work where the soliton was generated in a chain of ten lattice particles by a suitable input–output energy balance [Chetverikov *et al.*, 2006a; Makarov *et al.*, 2006]. As we see, one after the other all of the electrons are trapped by a soliton (the tangent is parallel to the slope of the solitonic excitation of the lattice). In this way we observe a complete analogy between the classical and the quantum description with respect to the trapping phenomenon. We may state that the trapping of electrons by solitonic compressions is a physical phenomenon and not just an artifact induced by the specificity of either the classical or the quantum-mechanical approach.

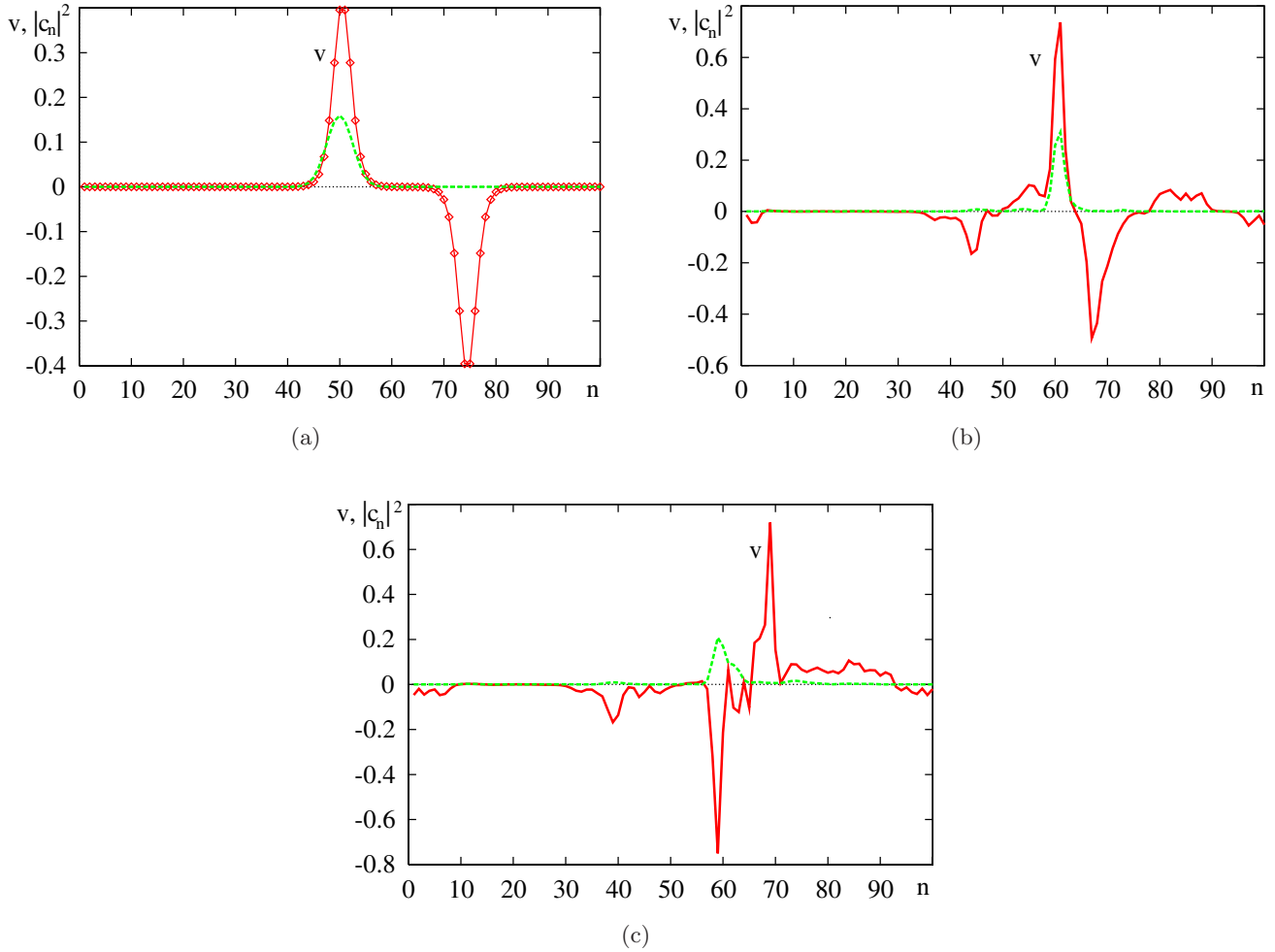

Fig. 3. Dynamics of two solitons and one electron ($V = 0.5$). The initial distribution of the $c(n)$ is Gaussian placing the electron at the soliton-like (cnoidal wave) compression running from left to right. We see that upon collision with the oppositely moving (from right to left) soliton there is an exchange of partner for the electron as its probability density is matched by the second oppositely moving soliton. (a–c) Correspond, respectively, to the situation before, at, and after the collision. The ordinate **v** denotes dimensionless velocity.

We also did a numerical experiment with two solitons moving in opposite directions (Fig. 3). Initially, the electron is trapped and, consequently, moves with the soliton moving to the right (the alternative is also expected due to symmetry). Then following the collision with the soliton moving to the left the electron probability density transfers to the second oppositely moving (to the left) soliton and further travels with it. Hence the electron changes partner in the formation of the bound state (solectron). In another case, we have seen the splitting of the electron probability density when two solitons oppositely moving collide with each other. In such a case the outcome of the collision leads to two solectrons moving away in opposite direction. Finally, there are cases where the electron probability density once captured by a soliton remains with it although that soliton may experience collision with other oppositely moving solitons.

Finally, we have calculated also the (dimensionless) current density, j, in the quantum picture given by

$$j = i \sum_n (c^*_{n+1} c_n - c^*_n c_{n+1}). \tag{8}$$

Under the assumption that a soliton is generated and runs from left to right along the lattice, in average we see a *negative* current, the sign is due to the negative charge of the electrons which moves with the soliton from left to right (Fig. 4, lower part). The larger fluctuations of the current underlies that the trapping is in terms of probability. The electron is making forward–backward oscillations around its mean position. In another with a soliton running from right to left we observed a *positive* current (Fig. 4, upper part).

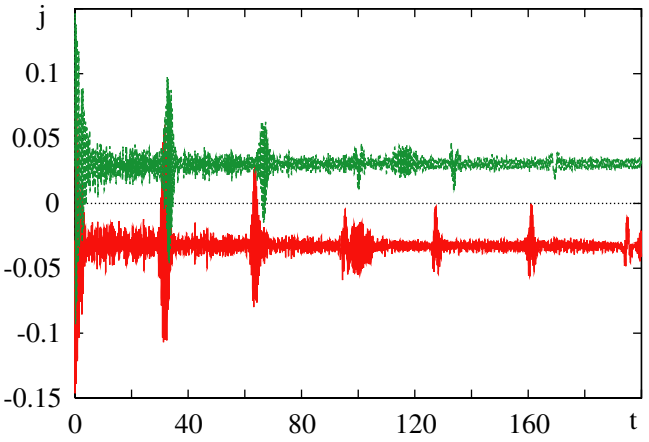

Fig. 4. Electric density current versus time appearing when the electron is quantum mechanically trapped by solitons. For comparison we have plotted in the same figure the outcome of two different events. In both cases the initial probability density, $c(n)$, is Gaussian. The upper (respectively, lower) signal refers to the right-to-left (respectively, left-to-right) moving soliton with $V = 0.4$ ($V = 0.5$). Accordingly the mean current exhibits positive (respectively, negative) value in the absence of an external field.

In conclusion, we have shown that soliton-mediated electron trapping is possible in a nonlinear lattice when the value of the stiffness of the "ion–ion" (Morse) lattice interactions allows strong enough compression. Then the electron-(ion)lattice interaction can be treated in the classical electrostatic approximation or in the quantum mechanical tight-binding approximation. In both cases there is electron "localization" on the lattice while the soliton provides the carrier. Needless to say, the difference between the classical and the quantum approaches is that in the former case, as we follow trajectories, the electron could jump from a right moving soliton to a left moving one [Makarov *et al.*, 2006], while in the other case the probability density associated to an electron could split leading to trapping by two oppositely moving solitons. A discussion of electron trapping, including electron–electron interaction and electron spin (satisfying Pauli's exclusion principle) thus allowing for electron-pair trapping, would be given elsewhere.

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