ON SOLITON-MEDIATED FAST ELECTRIC CONDUCTION IN A NONLINEAR LATTICE WITH MORSE INTERACTIONS

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Assuming the quantum mechanical "tight binding" of an electron to a nonlinear lattice with Morse potential interactions we show how electric conduction can be mediated by solitons. For relatively high values of an applied electric field the current follows Ohm's law. As the field strength is lowered the current takes a finite, constant, field-independent value.

Keywords: Solitons; nonlinearity; lattices; electric conduction; Morse interaction.

In a previous letter [Velarde *et al.*, 2005] a new form of electric conduction mediated by solitons was shown to be possible in an anharmonic Toda lattice. In the presence of an external electric field this current can be much higher than the Drude-Ohm linear current and, as the field is lowered, the current achieves a finite, constant, field-independent value. The model studied therein is strictly classical. The electron-ion (lattice) interaction is Coulombic, albeit with an appropriate pseudopotential. The lattice interactions are of Toda type [Toda, 1989], hence allowing for phonon — and soliton — longitudinal vibrations with compressions governed by the repulsive part of the potential [Chetverikov *et al.*, 2005a, 2005b]. These compressions were shown to be responsible for electron trapping (or electrostatic "localization") by the lattice ions, and the formation of dynamic bound states (solectrons) of the electron with the soliton (the cnoidal wave moving through the lattice). The phenomenon discovered is similar to surfing on a bore as it travels along a river. The surfer ought at an appropriate time to be ready to go on top of the bore and, on the other hand, the bore (call it "topological" soliton) travels rapidly upstream, at a constant speed relative to the downstream flow.

In the present letter we pursue the same idea in view of applying the results to a more realistic situation. We improve upon the previous model by replacing the classical electrostatic trapping with the quantum mechanical "tight binding" approximation, currently in use in solid state physics [Ashcroft & Mermin, 1976; Heeger *et al.*, 1988; Yu, 1988]. Furthermore, we replace the Toda interaction, which has unphysical aspects (particularly its attraction), with the Morse interaction, akin to the Lennard–Jones interaction [Choquard, 1967; Chetverikov *et al.*, 2005c]. Figure 1 compares these two interaction potentials, as well as the Toda potential. Figure 2 shows how the Morse interaction approaches the Toda interaction felt by an ion from its nearest neighbors, when repulsion dominates the dynamics, a feature we shall make use of later on (the harmonic case is also depicted for
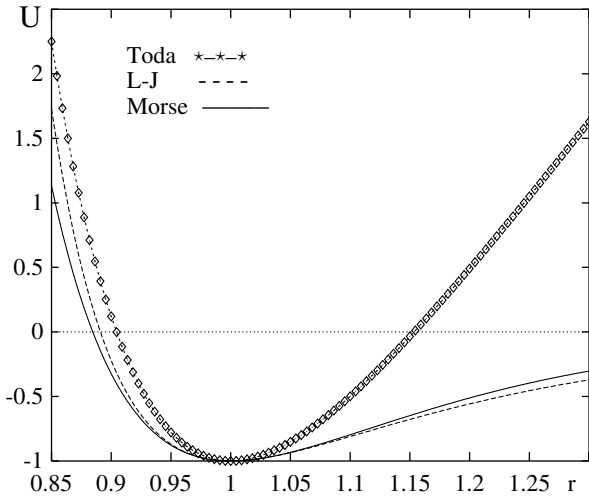
Fig. 1.   Lennard–Jones potential ($U = U^{L-J} = U_0[(1/r^{12}) - (1/r^6) - 1]$), Morse potential ($U = U^M = (a/2b)[(e^{-b\sigma(r-1)} - 1)^2 - 1]$), and Toda potential ($U = U^T = (a/b)[e^{-b\sigma(r-1)} - 1 + b\sigma(r-1)]$). In order to have all the three minima of the potential functions at the same location $(1, -1)$ we have suitably adjusted the free parameters with the basic frequency the same; $r = R/\sigma$. It clearly appears that Toda's interaction captures well the repulsive core whereas its attractive part becomes unphysical for large values of the displacement. Due to the use of exponentials both the Toda and the Morse potentials are easily implemented with present-day electronics.

reference). Finally, in contrast to earlier work [Velarde *et al.*, 2005], we do not make use here of Rayleigh's active (negative) friction to pump energy out of a thermal bath. Noise is introduced merely to test the robustness of the dynamics, and hence the

domain of validity of our results. We do not consider here the role of temperature on the soliton-mediated conduction process.

In view of the above, we consider a one-dimensional (1D) anharmonic lattice with dynamics dictated by the following Hamiltonian describing nearest-neighbor Morse interactions:

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

Here M denotes the mass of a lattice particle, (q_n, p_n) describe their respective displacements from equilibrium positions and momenta, and b characterizes the stiffness of the spring constant in the Morse potential.

Considering the lattice particles to be positive ions (in a broad sense), we add electrons to the system, and take for their dynamics the following "tight binding" Hamiltonian [Ashcroft & Mermin, 1976]:

$$H_{el} = -\sum_n V_{nn-1}(c_n^* c_{n-1} + c_n c_{n-1}^*), \tag{2}$$

where n denotes here the site where an electron is "placed" and $|c_n|^2$ gives the probability of finding the charge residing at that site. The quantity V_{nn-1} defines the transfer matrix element responsible for the transport of the electron along the chain (considering only nearest neighbors). This matrix is the key ingredient, allowing for the coupling of the
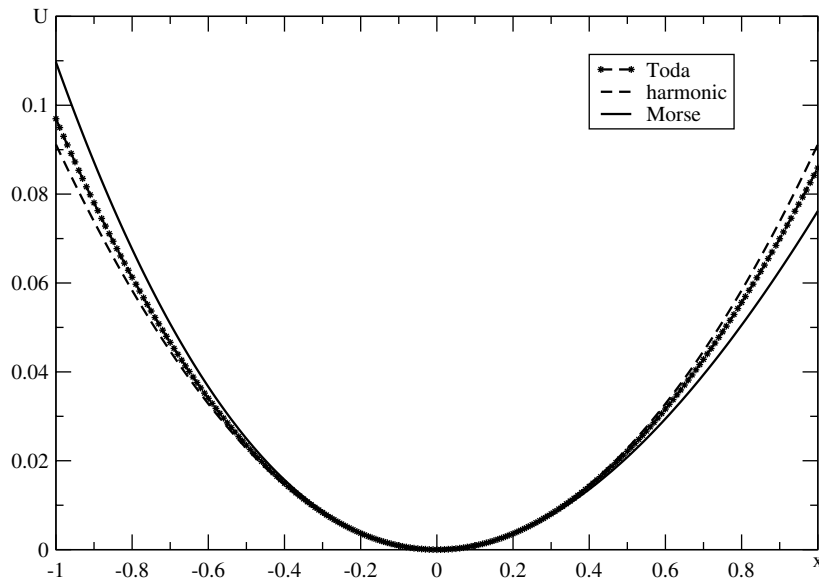

Fig. 2.   Morse, Toda and harmonic (lattice) inter-ionic potentials felt, from its nearest neighbors, by a ion placed at the origin.

electron to the lattice displacements, and hence the lattice vibrations, phonons or solitons. A reasonable choice for V_{nn-1} is

$$V_{nn-1} = V_0 \exp[-\alpha(q_n - q_{n-1})], \qquad (3)$$

where the parameter α accounts for the strength of the coupling. Thus, Eq. (3) describes the *local* impact of the actual charge "trapping" on the longitudinal motions (and hence distortions) of the lattice.

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). As unit of energy we take $(2D)$, 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)–(3) is given by the following equations for the electron, c_n, and lattice vibrations, q_n,

$$i\frac{dc_n}{dt} = -\tau(\exp[-\alpha(q_{n+1} - q_n)]c_{n+1}$$
$$+ \exp[-\alpha(q_n - q_{n-1})]c_{n-1}) \qquad (4\text{a})$$

$$\frac{d^2q_n}{dt^2} = [1 - \exp\{-(q_{n+1} - q_n)\}]\exp[-(q_{n+1} - q_n)]$$
$$- [1 - \exp\{-(q_n - q_{n-1})\}]$$
$$\times \exp[-(q_n - q_{n-1})]$$
$$- \alpha V((c_{n+1}^* c_n + c_{n+1} c_n^*)$$
$$\times \exp[-\alpha(q_{n+1} - q_n)]$$
$$- (c_n^* c_{n-1} + c_n c_{n-1}^*)\exp[-\alpha(q_n - q_{n-1})]),$$
$$(4\text{b})$$

where $\tau = V/\Omega_{\text{Morse}}\hbar$. Needless to say, in general the two time scales in (4a) and (4b) 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: $b = 4.45\,\text{Å}^{-1}$, $\alpha = 1.75\,b$, $D = V_0 = 0.1\,\text{eV}$, $\Omega_{\text{Morse}} = 3.04 \cdot 10^{12}\,\text{s}^{-1}$, $\Omega_{\text{electron}} = V_0/\hbar = 0.608 \cdot 10^{14}\,\text{s}^{-1}$, and $\tau = 20.00$. These numerical values are relevant, e.g. for electron transport along hydrogen bonded polypeptide chains such as α-helices [Davydov, 1973, 1991; Davydov & Kislukha, 1977; Christiansen & Scott, 1983; Scott, 1992].

Now, we take advantage of the similarity between the Morse and the Toda interactions in the repulsive range (see Fig. 2) where phonons as well as solitons can be excited in the lattice [Toda & Saitoh, 1983; Ebeling *et al.*, 2000; Chetverikov *et al.*, 2005a]. Accordingly, for the lattice vibrations we make the ansatz [Toda, 1989]

$$\exp[-(q_n - q_{n-1})] = 1 + \beta \cosh^{-2}(\kappa n - \beta t), \quad (5)$$

where $\beta = \sinh \kappa$, and κ is a parameter with dimensions of inverse length (related to the width of the soliton). The ansatz (5) is a valid approximation leading to localized solectronic pulses traveling with Toda solitons [Hennig, 2000]. Using (5), the coupling between Eqs. (4a) and (4b) yields

$$c_n(t) = \beta \cosh^{-1}[\kappa n - \beta t]\exp[-i(\omega t - \delta n + \sigma)], \qquad (6)$$

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) for $\kappa = 0.465$, which is therefore what we use.

The evolution problem (4) has been solved for 99 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 3 depicts the results found for solitons and Fig. 4 for electrons. The soliton binding energy here is $0.0281\,\text{eV}$. Both the electron and lattice excitation (soliton) move along the lattice retaining their respective localized structure save the emission of negligible radiation. The soliton is *supersonic* with velocity $v_{\text{sol}} = 1.036 v_{\text{sound}}$, where v_{sound} is the (linear) sound velocity in the Morse lattice.

To test the robustness of the dynamics and hence the stability of the soliton motion, we considered Eq. (4b) in the presence of noise, leading to the corresponding Langevin equation

$$\frac{d^2q_n}{dt^2} = [1 - \exp\{-(q_{n+1} - q_n)\}]\exp[-(q_{n+1} - q_n)]$$
$$- [1 - \exp\{-(q_n - q_{n-1})\}]$$
$$\times \exp[-(q_n - q_{n-1})]$$
$$- \alpha V((c_{n+1}^* c_n + c_{n+1} c_n^*)$$
$$\times \exp[-\alpha(q_{n+1} - q_n)]$$
$$- (c_n^* c_{n-1} + c_n c_{n-1}^*)$$
$$\times \exp[-\alpha(q_n - q_{n-1})]) - \gamma p_n + \sqrt{2D_b}\xi,$$
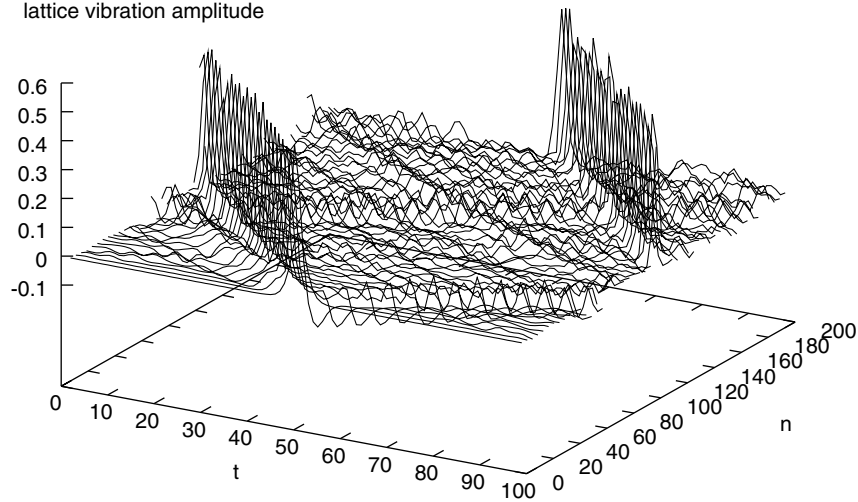$$(7)$$

lattice vibration amplitude

Fig. 3.   Morse lattice. Spatiotemporal evolution of the lattice deformations $\{\exp[-(q_n(t) - q_{n-1}(t))] - 1\}$ illustrating the robustness of (pulse) soliton propagation apart from small-amplitude radiation.
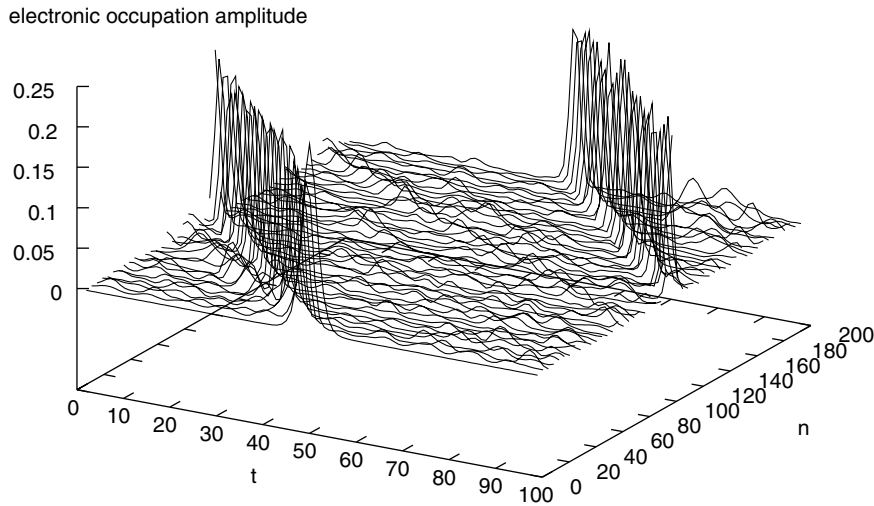
electronic occupation amplitude

Fig. 4.   Morse lattice. Spatiotemporal soliton-driven evolution of the electronic occupation probability distribution $|c_n(t)|^2$ illustrating the maintenance of localization. Electric conduction is a consequence of the companion soliton travel in Fig. 3.

where $\xi(t)$ denotes Gaussian white noise with zero mean, and delta function-correlated. The damping constant obeys Einstein's relation (the fluctuation-dissipation theorem) $D_b = \kappa_B T \gamma / M$, where γ, κ_B and T denote the (passive) friction with the bath, Boltzmann's constant and absolute temperature, respectively. For illustration, we take $\gamma \leq 0.02$ corresponding to "life times" of at least $10\,ps$ characteristic of charge transport in biomolecules. No significant deviations from the deterministic trajectories have been observed, even at temperatures of the order $T = 300\,K$.

Finally, we have considered the response of the system to an external electric field, E. Then,

Eq. (4a) becomes

$$i\frac{dc_n}{dt} = -\tau(\exp[-\alpha(q_{n+1} - q_n)]c_{n+1}$$
$$+ \exp[-\alpha(q_n - q_{n-1})]c_{n-1}) - n\tilde{E}c_n, \quad (8)$$

where $\tilde{E} = e/(\hbar\Omega_{\mathrm{Morse}})E$. The results found do not differ qualitatively from the predictions made using the purely classical model [Velarde *et al.*, 2005]. There is a critical field strength, E_c, below which the (supersonic) current, hence the solectron current, is finite, constant and independent of $\tilde{E}$. For the above given parameter values it is $E_c \approx 0.042 \cdot 10^5\,\mathrm{V/cm}$. Upon further increasing

the field strength, the current follows Ohm's law until E reaches a certain value, here $E_{\text{diss}} \approx 0.484 \cdot 10^5$ V/cm, past which dissociation occurs and the electron breaks loose from the lattice vibrations.

In conclusion, we have shown that soliton-mediated electric conduction is possible in a nonlinear lattice when (i) the stiffness constant of the "ion-ion" (Morse) lattice interactions allows strong enough compression, and (ii) the electron-lattice "ion" interaction is treated in the quantum mechanical "tight binding" approximation. The latter leads to the electron "localization" on the lattice while the soliton provides the carrier. A salient feature of soliton-mediated transport is that, over a wide range of electric field values, the current assumes a finite, constant, field-independent value. Upon increasing the field strength further this gives way to a linear response, i.e. to a current following Ohm's law. Further details and alternative approach can be found elsewhere [Hennig *et al.*, 2006].

Acknowledgments

References

Ashcroft, N. W. & Mermin, N. D. [1976] *Solid State Physics* (Holt, Rinehardt & Winston, Philadelphia).

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2005a] "Dissipative solitons and complex currents in active lattices," *Int. J. Bifurcation and Chaos*, to appear.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2005b] "Nonlinear ionic excitations, dynamic bound states, and nonlinear currents in a one-dimensional plasma," *Contrib. Plasma Phys.* **45**, 275–283.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2005c] "Thermodynamics and phase transitions in dissipative and active Morse chains," *Eur. Phys. J. B.* **44**, 509–519.

Choquard, Ph. [1967] *The Anharmonic Crystal* (Benjamin, NY).

Christiansen, P. L. & Scott, A. C. (eds.) [1983] *Davydov's Soliton Revisited. Self-Trapping of Vibrational Energy in Protein* (Plenum Press, NY).

Davydov, A. S. [1973] "The theory of contraction of proteins under their excitation," *J. Theor. Biol.* **38**, 559–569.

Davydov, A. S. & Kislukha, N. I. [1977] "Solitons in one-dimensional molecular chains," *Sov. Phys. JETP* **44**, 571–575.

Davydov, A. S. [1991] *Solitons in Molecular Systems*, 2nd edition (Reidel, Dordrecht).

Ebeling, W., Chetverikov, A. P. & Jenssen, M. [2000] "Statistical thermodynamics and nonlinear excitations of Toda systems," *Ukr. J. Phys.* **45**, 479–487.

Heeger, A. J., Kivelson, S., Schrieffer, J. R. & Su, W. P. [1988] "Solitons in conducting polymers," *Rev. Mod. Phys.* **60**, 781–850.

Hennig, D. [2000] "Solitonic energy transfer in a coupled exciton-vibron system," *Phys. Rev. E* **61**, 4550–4555.

Hennig, D., Neißner, C., Velarde, M. G. & Ebeling, W. [2006] "Effect of anharmonicity on charge transport in hydrogen-bonded systems," *Phys. Rev. B* **73**, 024306-1–10.

Scott, A. [1992] "Davydov's soliton," *Phys. Rep.* **217**, 1–67.

Toda, M. & Saitoh, N. [1983] "The classical specific heat of the exponential lattice," *J. Phys. Soc. Japan* **52**, 3703–3705.

Toda, M. [1989] *Theory of Nonlinear Lattices*, 2nd edition (Springer-Verlag, NY).

Velarde, M. G., Ebeling, W. & Chetverikov, A. P. [2005] "On the possibility of electric conduction mediated by dissipative solitons," *Int. J. Bifurcation and Chaos* **15**, 245–251.

Yu, L. (ed.) [1988] *Solitons & Polarons in Conducting Polymers* (World Scientific, Singapore).