International Journal of Bifurcation and Chaos, Vol. 21, No. 6 (2011) 1595–1600

DOI: 10.1142/S021812741102929X

NUMERICAL EVIDENCE OF SOLITON-MEDIATED ELECTRON PAIRING IN HEATED ANHARMONIC CRYSTAL LATTICES*

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Received April 23, 2010; Revised May 28, 2010

Soliton-mediated electron pairing (both in real space and in momentum space) is shown to occur in heated one-dimensional (1D) molecular *anharmonic* systems with Morse interactions.

Keywords: Morse interaction; anharmonicity; solitons; solectron; electron transport; electron pairing.

Solitons in molecular systems are local compressions due to the interaction between the molecules or atoms which typically have a strongly repulsive part and a weakly attractive one. Approximating this interaction by Morse exponential potentials (akin to Lennard–Jones power laws) it has been shown that, in an appropriate temperature range, solitons may be excited (for biomolecules this corresponds to room temperature/physiological region) [Christiansen & Scott, 1990]. Adding an excess electron to the system, it has also been shown that solectrons, i.e. traveling bound states of the electron to solitons, may be formed (by adding the lattice nonlinear elasticity, i.e. the lattice *anharmonicity*, the *solectron* is a generalization of the *polaron* [Velarde, 2010]). It has also been shown that both electron trapping by solitons and a new form of (generally supersonic) electric conduction mediated by solitons are possible in such *anharmonic* one-dimensional (1D) lattice [Velarde *et al.*, 2005, 2008b; Velarde *et al.*, 2006; Velarde *et al.*, 2008a; Velarde *et al.*, 2010; Chetverikov *et al.*, 2006a, 2006b, 2009, 2010; Ebeling *et al.*, 2009a; Hennig *et al.*, 2006; Hennig *et al.*, 2007; Makarov *et al.*, 2006].

As solectrons are a new kind of single-charge *quasi-particle* in the anharmonic system, the question arises of whether such quasi-particle may form bound states with spin-up + spin-down electron pairs. In earlier work, the existence of such quasi-particle was shown based on simulations using the corresponding Schroedinger equation [Velarde & Neissner, 2008]. Several estimates of the binding energy of solectron pairs have been given in [Ebeling *et al.*, 2009b]. Indeed the potential well created by a soliton may in principle be occupied by pairs of electrons with opposite spins satisfying Pauli's exclusion principle. At first sight, these electron pairs, which are bosons, appear like "bipolarons" [Alexandrov, 2007]. Yet the solectron pair is something new as it implies the lattice anharmonicity not considered with polarons.

*Dedicated to founding Editor-in-Chief Leon O. Chua on the occasion of his retirement from solo editorship of the *Int. J. Bifurcation and Chaos.*

The problem of pairs or clusters of quantum electrons in a parabolic trap is not new and plays a significant role in modern microelectronics [Bonitz *et al.*, 2002]. In the case of solectrons, the width of the potential well is of the order of a few equilibrium inter-atomic lattice distances. Assuming that the depth of a well is U_0 and the frequency of oscillations around the minimum is $\omega_{\min}$, an estimate for the energy of a pair located at the minimum is

$$\epsilon_{p0} = 2U_0 + 3\hbar\omega_{\min} + \Delta\epsilon_{qm}, \tag{1}$$

corresponding to twice the ground state energy of a solectron plus the energy of the repulsion between the electrons. An estimate for the mean energy of repulsion is [Ebeling *et al.*, 2009b]

$$\Delta\epsilon_{qm} = \left\langle \frac{e^2}{\epsilon_0 r} \right\rangle \approx \frac{e^2}{3\epsilon_0 r_0}, \tag{2}$$

where r_0 is the Bohr radius or "size" of the wave function width,

$$r_0^2 = \left(\frac{\hbar}{m\omega_0}\right). \tag{3}$$

The above given estimate was done by assuming hydrogen ground state wave functions for both electrons. The Coulomb repulsion is weakened by the quantum effects, with the spreading of electron density, thus leading to the mean distance between the electrons in a solectron pair around three times the Bohr radius. In order to find solectron pairs we need conditions where the Coulomb shift is much smaller than the gap to the next level which is $3\hbar\omega_{\min}$ per electron in the pair. Under these conditions, the formation of a solectron pair is favored. In other words, the solectron pairs will be more favorable than clusters of electrons at the minimum. In spite of the fact that these quantum mechanical estimates do not prove the existence of solectron pairs in potential minima formed by strong solitons, this claim is not final and we decide to test it for pair formation in computer simulations. Necessarily such simulations have to include the spin of the electrons and the Coulomb repulsion. Generally, this is a rather difficult task and we better add further simplifications. One is to use the Coulomb repulsion in the Hubbard local form which is a rather crude albeit useful and currently used approximation in condensed matter physics [Montorsi, 1992].

Recently, pairing effects has been analyzed using the Hubbard local Coulomb repulsion [Cruzeiro *et al.*, 2004; Hennig *et al.*, 2008]. Within this model several configurations of soliton-electron pairs have been found. In both cases as here, a mixed classical-quantum problem was considered. Thus we consider a 1D anharmonic lattice with nearest-neighbor (n.n.) dynamics described by the (Morse–Hubbard) Hamiltonian $H = H_{\text{lattice}} + H_{\text{electron}}$, with

$$H_{\text{lattice}} = \sum_n \left\{ \frac{p_n^2}{2M} + D(1 - \exp[-B(q_n - q_{n-1})])^2 \right\}, \tag{4}$$

and

$$H_{e\ell} = -\sum_{n,\sigma} (V_{nn-1} a_{n\sigma}^+ a_{n-1\sigma} + V_{nn+1} a_{n\sigma}^+ a_{n+1\sigma}) + U \sum_n a_{n\uparrow}^+ a_{n\uparrow} a_{n\downarrow}^+ a_{n\downarrow}. \tag{5}$$

The index $n\epsilon\,[1, \ldots, N]$ denotes the site of the nth lattice particle and $\sigma\epsilon[\uparrow, \downarrow]$ determines the spin of an electron which can be up or down. The Fermion operators $a_{n\sigma}^+$, $a_{n\sigma}$ create or annihilate, at site n, an electron with spin $\uparrow$ or $\downarrow$, respectively. The factor V_{nn-1} accounts for the transfer matrix element (its value is determined by an overlap integral) being responsible for the nearest-neighbor hopping of the electron along the lattice in the tight binding approximation (TBA). The second term in Eq. (5) represents the on-site electron-electron interaction due to Hubbard–Coulomb repulsion whose strength is estimated with the positive parameter U. A reasonable and much used choice for V_{nn-1} is

$$V_{nn-1} = V_0 \exp[-\alpha(q_n - q_{n-1})], \tag{6}$$

where the parameter α accounts for the strength of the electron-lattice coupling. We shall measure all energies in units 2D, except for the electron energy levels scaled by $\hbar\omega_0$ which is the quantum of the oscillations around the minimum of the Morse potential. For the sake of universality, it is best to rescale quantities and consider a dimensionless problem. We take as unit of time ω_0^{-1}. For displacements we take B^{-1} as the unit.

Note that the parameter $\tau = V_0/\hbar\omega_0$ gives the ratio of the two time scales involved in the dynamics which, in frequency terms, refer to ultraviolet/electronic *versus* infrared/acoustic processes for electrons and phonons (solitons), respectively. The existence of bound states between electrons

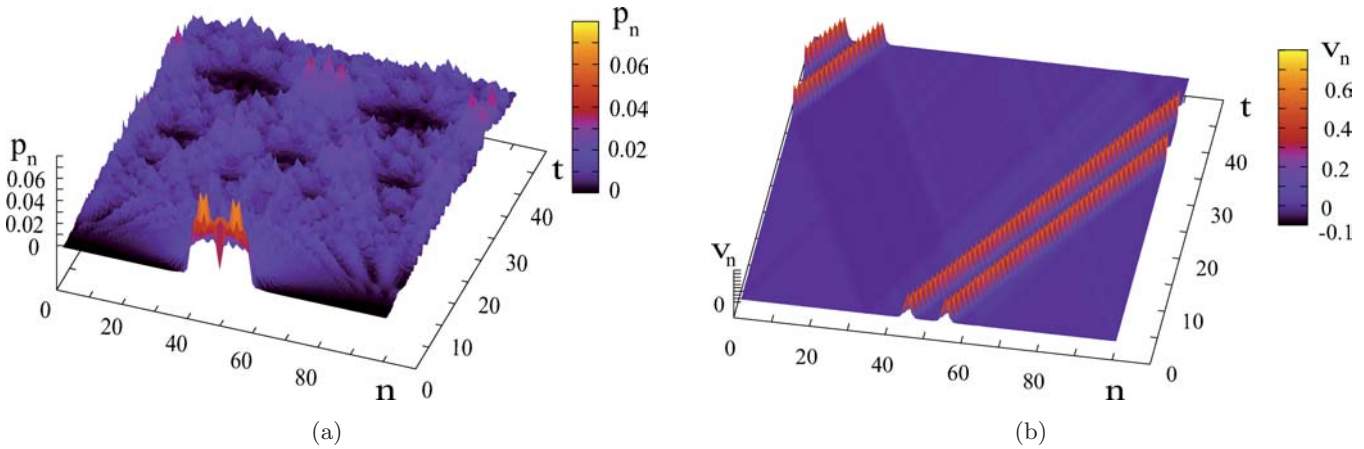
and lattice deformations in 1D lattices was studied in the *continuum* case by Davydov and collaborators [Brizhik & Davydov, 1983; Cruzeiro-Hansson & Takeno, 1997]. Clearly, in our discrete lattice case, we can have a polaron-like effect due to the electron–phonon (or soliton) interaction augmented with the influence of the dynamics of the lattice solitons. This permits soliton rather than phonon-assisted hopping. In the computer simulations, a significant role is played by temperature. Indeed, for solitons to be sustained moving unaltered along the lattice the temperature must be high enough. This follows from inspection of the specific heat characteristics and the dynamic structure factor of the lattice. The solitons are expected beyond the Dulong–Petit *plateau* before the transition to the gas-like regime [Chetverikov *et al.*, 2006a]. All our simulations refer to the same value of repulsion strength, $U = 1$, which is a moderate one, and to the same value of the time scales parameter $\tau = 10$. Our strategy is to vary from simulation to simulation the value of both V and α. The numerical procedure is as follows: first we construct Langevin equations corresponding to the classical Hamiltonian (4) including white noise corresponding to the chosen temperature of the "heat bath". Then we "heat up" the system up to thermal equilibrium. After switching-off the "heat bath" we solve simultaneously the classical mechanical equations of lattice motions and the discrete Schröedinger equations resulting from the quantum Hamiltonian (5) which are coupled to the former.

Figure 1 illustrates the time evolution of the probability distribution for the spin-up electron (↑) and the velocity of particles of the 1D lattice when exciting two solitons but there is no coupling of electrons to the lattice excitations. One may observe the evolution of the initial form of a wave function corresponding to excitations of some eigen functions of the system with periodic boundary conditions considered. On the other hand, two traveling identical solitons are observed as well.

In the case of interaction of electrons with solitons (Fig. 2), with $\alpha = 1$ and a moderate value of V ($V = 0.1$), both electrons are trapped by a pair of solitons. The formed soliton-electron pair moves as a stable nonlinear structure in spite of the high repulsion strength chosen ($U = 1$). A paired-solectron travels with constant velocity just below the velocity of noninteracting solitons because now they carry electrons and hence the mass of the newly formed bound state is larger for the same momentum initially given.

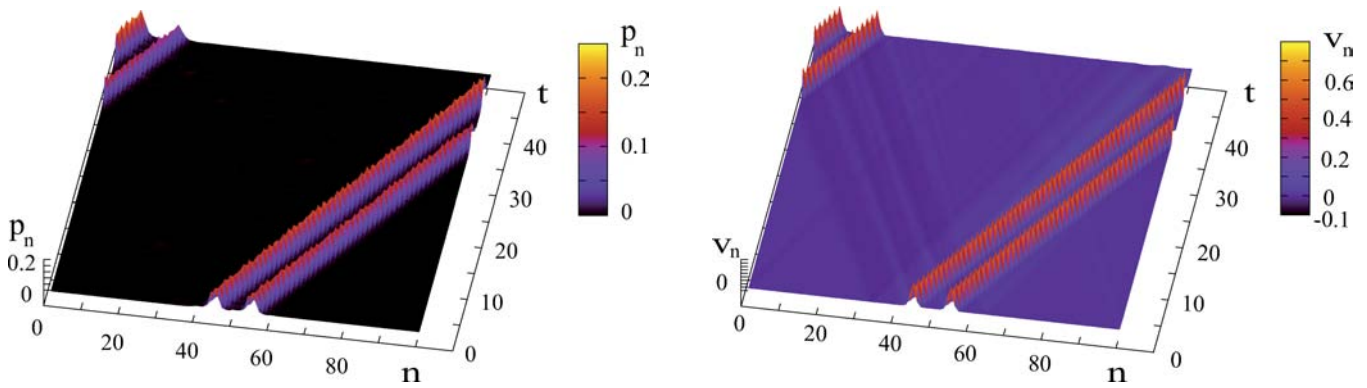
Illustration of the case when both electrons, albeit with opposite spins, occupy the potential well of a single soliton, is provided in Fig. 3. In this case, both electrons (in probability density) are centered at site $n = 50$ where the soliton is placed. One may conclude that this solectron is as stable as that with two solitons and a pair of spatially separated electrons.

Also possible is the case when a pair of *subsonic* solectrons (initially, for time ∼100, the results look like in Fig. 2) is at a high value $V = 0.5$



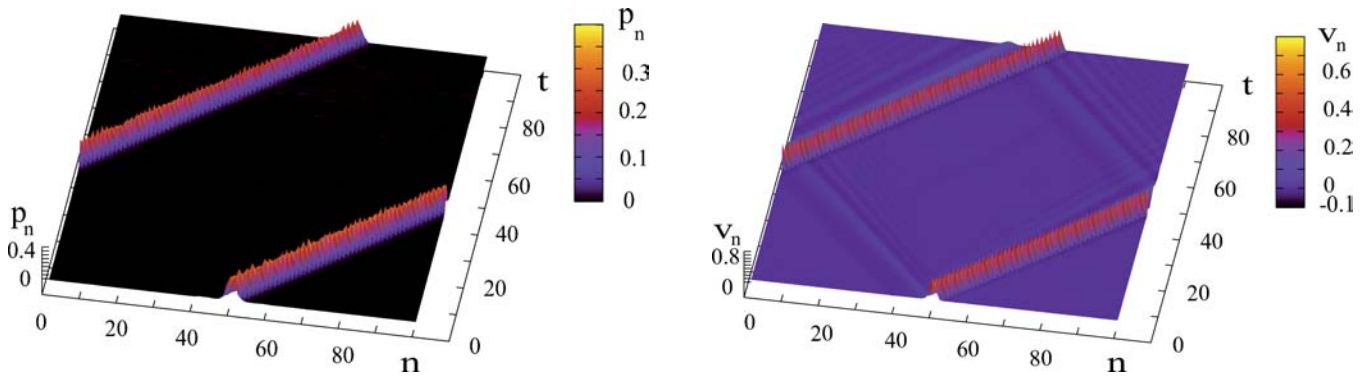
(a) (b)

Fig. 1. Morse–Hubbard 1D lattice of $N = 100$ particles. (a) Evolution of the probability distribution for the spin-up (↑) electron (a distribution for the spin-down (↓) electron looks exactly the same). (b) Velocity $v_n(t)$. Two solitons have been excited in the lattice (centered initially at sites $n = 45$ and $n = 55$, respectively) in the absence of coupling to the electrons ($\alpha = 0$). The two solitons in the lattice are taken identical and both have velocity about 1.25 of the sound velocity hence both are chosen *supersonic*. The initial form of the wave function corresponds to a pair of electrons centered at the same sites where the solitons are. They are described by narrow Gaussian functions. Parameter values: $\tau = 10$ and $U = 1$.



(a) (b)

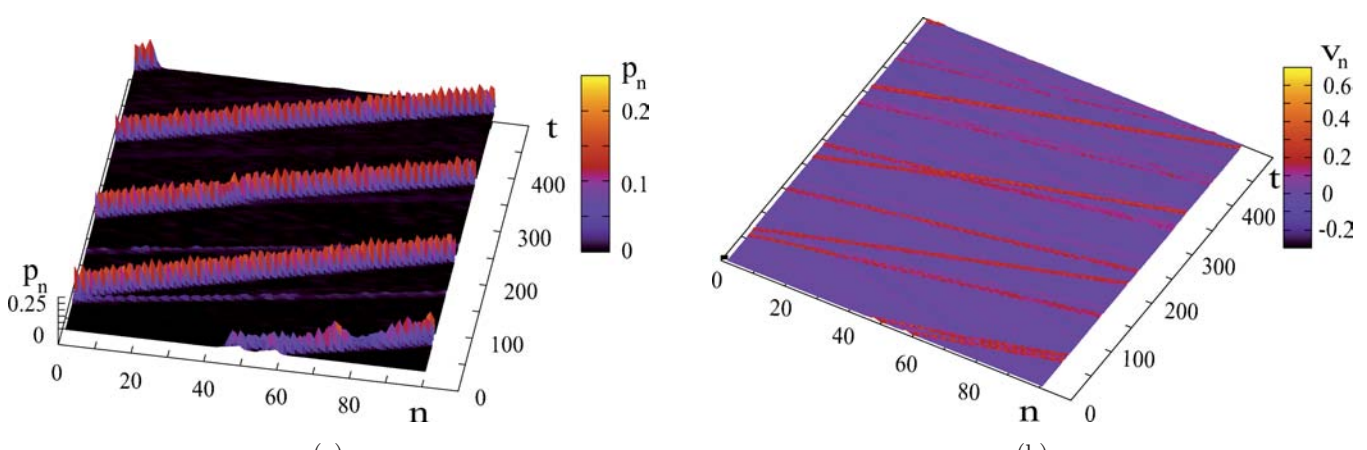
Fig. 2. Morse–Hubbard 1D lattice. The same as in Fig. 1 but electrons are coupled to the lattice solitons. Parameter values: $\alpha = 1$, $V = 0.1$, $\tau = 10$ and $U = 1$.



(a) (b)

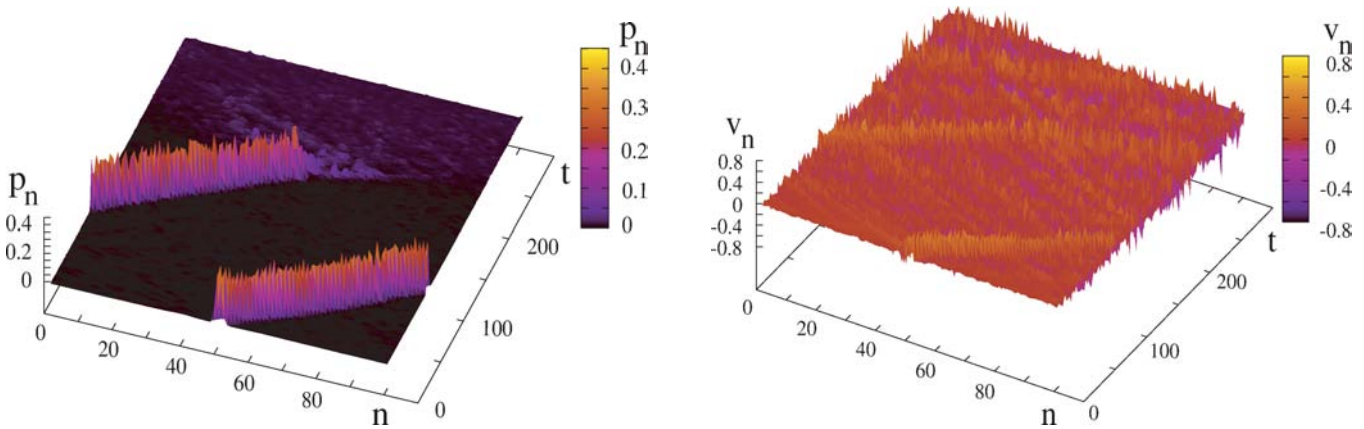
Fig. 3. Morse–Hubbard 1D lattice. The same as in Fig. 2 but both electrons "sit" on a single soliton from the beginning. Parameter values: $\alpha = 1$, $V = 0.1$, $\tau = 10$ and $U = 1$.

though seem to be unstable (Fig. 4). The energy of one of the electrons transfers to the other via electron interactions and a bisolectron (one soliton with two electrons of opposite spins as shown in Fig. 3) is formed. One soliton starts at site $n = 50$ and the other at site $n = 60$. The latter after losing an electron is transformed in a "soliton wave-train".



(a) (b)

Fig. 4. Morse–Hubbard 1D lattice. The same as in Figs. 2 and 3 but here an initially excited paired-solectron as in Fig. 2 transforms to the configuration as in Fig. 3. Parameter values: $\alpha = 1$, $V = 0.5$, $\tau = 10$ and $U = 1$.



(a) (b)

Fig. 5. Morse–Hubbard 1D lattice. The same as in Fig. 3 but the lattice is *adiabatically* "heated" to a temperature that at $t = 200$ is about $T = 0.04$ in our dimensionless units. The initial mean value of energy per particle due to a soliton excited is about 0.01. Parameter values: $\alpha = 1.5$, $V = 0.3$, $\tau = 10$ and $U = 1$.

It is interesting to study the stability of the paired-solectron to thermal heating. The computer simulation has been performed for the case when a lattice with a solectron like that shown in Fig. 3 is *adiabatically* heated via a Langevin equation for the lattice particle [Ebeling *et al.*, 2009]. Earlier computer simulations [Hennig *et al.*, 2006; Chetverikov *et al.*, 2009, 2010] have shown that the solectron is destroyed when the temperature exceeds a certain value $T_{\rm destr} \sim 0.1D$. New computer simulations for the present work in the case illustrated in Fig. 3 but with $\alpha = 1.5$ and $V = 0.3$ confirm the earling findings. One may observe (Fig. 5) that the solectron is destroyed when the temperature exceeds $T_{\rm destr} \sim 0.1D$ and hence the electron probability density either starts spreading over the lattice at small V [Fig. 5(a)] or goes to form a polaron at large V. For $D = 0.1\,{\rm eV}$, $T_{\rm destr} \sim 100\,{\rm K}$ when also other isolated freely moving thermally excited solitons are clearly seen in the lattice [Fig. 5(b)]. Such a value may be inferred from the curve of the adiabatic temperature increasing in time not shown here. Another possible configuration of the electron pair at high values of the Hubbard–Coulomb local repulsion strength looks like a pair of two solitons sharing the probability density of the two-electron state, one with spin-up and the other with spin-down.

In conclusion, the solectron quasiparticle is a new charge carrier that generalizes the polaron due to the added lattice anharmonicity. Pairs of solectrons form a boson. We have considered here only individual solectron pairs embedded in a 1D lattice. The question of whether high density of (boson) solectron pairs may be created and may lead to a boson conduction phase requires further research work. In fact, as the n.n. lattice dynamics used precludes long range order in 1D (at nonzero absolute temperature) we must consider 2D lattices. According to our preliminary numerical findings we foresee that such a new conduction phase is stable only in a bracketted finite range of temperatures, certainly limited from above due to possible lattice melting and metastable at low temperatures, when not enough number of thermal solitons and solectron pairs are excited.

Acknowledgments

The authors wish to express their gratitude to A. S. Alexandrov, E. Brandas, L. Cruzeiro-Hansson, S. Larsson and G. Vinogradov, for enlightening suggestions and to a referee for useful remarks that helped improve the presentation of results. This research has been sponsored by the European Union under Grant SPARK-II-FP7-ICT-216227 and by the Spanish Ministry of Innovation and Research under Grant EXPLORA-FIS2009-06585-E. The authors also acknowledge the hospitality of the International Center for Nonlinear Dynamics and Complex Systems in Pescara (Italy) where part of this research was carried out.

References

Alexandrov, A. S. (ed.) [2007] *Polarons in Advanced Materials* (Springer, Dordrecht).

Bonitz, M., Golubichnyi, V., Filinov, A. V. & Lozovik, Yu. F. [2002] "Single-electron control of Wigner crystallization," *Microelectr. Eng.* **62**, 141–145.

Brizhik, L. S. & Davydov, A. S. [1983] "Soliton excitations in one-dimensional molecular systems," *Phys. Status Sol.* **115**, 615–630.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2006a] "Dissipative solitons and complex currents in active lattices," *Int. J. Bifurcation and Chaos* **16**, 1613–1632.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2006b] "Nonlinear excitations and electric transport in dissipative Morse–Toda lattices," *Eur. Phys. J. B* **51**, 87–99.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2009] "Local electron distributions and diffusion in anharmonic lattices mediated by thermally excited solitons," *Eur. Phys. J. B* **70**, 217–227.

Chetverikov, A. P., Ebeling, W. & Velarde, M. G. [2010] "Thermal solitons and solectrons in nonlinear conducting chains," *Int. J. Quant. Chem.* **110**, 46–61.

Christiansen, P. L. & Scott, A. C. (eds.) [1990] *Davydov's Soliton Revisited. Self-Trapping of Vibrational Energy in Proteins* (Plenum Press, NY).

Cruzeiro-Hansson, L. & Takeno, S. [1997] "Davydov model: The quantum, mixed quantum-classical and full classical systems," *Phys. Rev. E* **56**, 894–906.

Cruzeiro, L., Eilbeck, J. C., Marin, J. L. & Rusell, F. M. [2004] "Dynamical two electron states in a Hubbard–Davydov model," *Eur. Phys. J. B* **42**, 95–102.

Ebeling, W., Velarde, M. G. & Chetverikov, A. P. [2009a] "Bound states of electrons with soliton-like excitations in thermal systems — adiabatic approximations," *Cond. Matt. Phys.* **12**, 633–645.

Ebeling, W., Velarde, M. G., Chetverikov, A. P. & Hennig, D. [2009b] "Anharmonicity and soliton-mediated transport: Thermal solitons, solectrons and electric transport in nonlinear conducting lattices," in *Self-Organization of Molecular Systems. From Molecules and Clusters to Nanotubes and Proteins*, eds. Russo N., Antonchenko, V. Ya. & Kryachko, E. (Springer-Verlag, Berlin), pp. 171–198.

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.

Hennig, D., Chetverikov, A. P., Velarde, M. G. & Ebeling, W. [2007] "Electron capture and transport mediated by lattice solitons," *Phys. Rev. E* **76**, 046602-1-9.

Hennig, D., Velarde, M. G., Ebeling, W. & Chetverikov, A. P. [2008] "Compounds of paired electrons and lattice solitons moving with supersonic velocity," *Phys. Rev. E* **78**, 066606-1-9.

Makarov, V. A., Velarde, M. G., Chetverikov, A. P. & Ebeling, W. [2006] "Anharmonicity and its significance to non-Ohmic electric conduction," *Phys. Rev. E* **73**, 066626-1-12.

Montorsi, A. (ed.) [1992] *The Hubbard Model. A Collection of Reprints* (World Scientific, Singapore).

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.

Velarde, M. G., Ebeling, W., Hennig, D. & Neissner, C. [2006] "On soliton-mediated fast electric conduction in a nonlinear lattice with Morse interactions," *Int. J. Bifurcation and Chaos* **16**, 1035–1039.

Velarde, M. G. & Neissner, C. [2008] "Soliton-mediated electron pairing," *Int. J. Bifurcation and Chaos* **18**, 885–890.

Velarde, M. G., Ebeling, W., Chetverikov, A. P. & Hennig, D. [2008a] "Electron trapping by solitons. Classical *versus* quantum mechanical approach," *Int. J. Bifurcation and Chaos* **18**, 521–526.

Velarde, M. G., Ebeling, W. & Chetverikov, A. P. [2008b] "Thermal solitons and solectrons in 1D anharmonic lattices up to physiological temperatures," *Int. J. Bifurcation and Chaos* **18**, 3815–3823.

Velarde, M. G. [2010] "From *polaron* to *solectron*: The addition of nonlinear elasticity to quantum mechanics and its possible effect upon electric transport," *J. Comput. Appl. Maths.* **233**, 1432–1445.

Velarde, M. G., Chetverikov, A. P. & Ebeling, W. [2010] "On the mathematical modeling of soliton-mediated long-range electron transfer," *Int. J. Bifurcation and Chaos* **20**, 185–194.