Eur. Phys. J. B **80**, 545–554 (2011)
DOI: 10.1140/epjb/e2011-10880-0

THE EUROPEAN PHYSICAL JOURNAL B

Regular Article

On the possibility of electric transport mediated by long living intrinsic localized solectron modes

O.G. Cantu Ros[1], L. Cruzeiro[1,2], M.G. Velarde[1,a], and W. Ebeling[1,3]

[1] Instituto Pluridisciplinar, Universidad Complutense de Madrid, Paseo Juan XXIII, No. 1, 28040 Madrid, Spain
[2] CCMAR and FCT, Universidade do Algarve, Campus de Gambelas, 8005-139 Faro, Portugal
[3] Institut für Physik, Humboldt-Universität Berlin, Newtonstrasse 15, 12489 Berlin, Germany

Received 15 November 2010 / Received in final form 25 February 2011
Published online 4 April 2011 –

Abstract. We consider a polaron Hamiltonian in which not only the lattice and the electron-lattice interactions, but also the electron hopping term is affected by anharmonicity. We find that the one-electron ground states of this system are localized in a wide range of the parameter space. Furthermore, low energy excited states, generated either by additional momenta in the lattice sites or by appropriate initial electron conditions, lead to states constituted by a localized electron density and an associated lattice distortion, which move together through the system, at subsonic or supersonic velocities. Thus we investigate here the localized states above the ground state which correspond to moving electrons. We show that besides the stationary localized electron states (proper polaron states) there exist moving localized solectron states which can be easily excited. The evolution of these localized states suggests their potential as new carriers for fast electric charge transport.

1 Introduction

The motion of electrons in polarizable crystals is a long standing and basic topic in solid state physics. Landau was the first to suggest the possibility that an electron may become self-trapped in the distortion it itself induces in the lattice [1], thus leading to the genuine charge carrier known as *polaron* (in present-day terminology it is an electron dressed by a phonon cloud). This idea was further studied by Pekar [2–5]. A microscopic model was proposed first by Fröhlich who considered long-range interactions between the electron and the crystal vibrations [6,7] and, subsequently, by Holstein who considered short-range interactions of an electron in a discrete lattice [8,9]. The analytical wave function obtained by Holstein was formally identical to that later obtained by Davydov [10–22], although to the best of our knowledge Davydov was the first to profit from the nonlinear character of the Hamiltonian and to coin the concept of *electrosoliton* for the newly found charge carrier provided by the nonlinear interaction between a linear electron system and a linear lattice dynamically described by a soliton-bearing equation. Soliton-mediated charge transport was also shown to play a role in the conduction properties of transpolyacetelyne [23–25]. While in the studies mentioned above the nonlinearity comes from the interaction of two systems which, taken separately, are linear, other studies have considered systems in which either the lattice and/or the quantum particle interactions are themselves nonlinear. Indeed, nonlinear discrete lattices are known to possess genuine nonlinear modes called "intrinsic localized modes" or discrete "breathers" [26–73]. We shall be using here the concept of intrinsic localized mode in a general sense embracing, in particular, solitons. Strictly speaking breathers refer to nonlinear localized excitations with internal oscillations or spatially localized time periodic modes. The interaction of a charge with such modes has been investigated by Aubry et al. [59–61] and the concept of *solitobreather* has been coined for the soliton state of an electron interacting with a discrete breather.

While the studies of electron states in polarizable lattices mentioned above follow the initial idea of Landau in that the charge induces lattice distortions which in turn stabilize it, recently a different transport process was proposed in which a moving (non-topological) lattice soliton may not only trap the charge but also drag it along, leading to a new carrier, the *solectron* [74,75]. Several studies have already been done about the stability and transport properties of the solectron which indicate that this compound may play a role in charge conduction [74–83]. We first investigate the characteristics of the ground states of the electron-lattice in tight-binding approximation (solectron) Hamiltonian. Then we estimate the energy difference and hence the temperature needed to obtain traveling excited states (solectrons), and the parameter ranges in which they arise, as well as looking at their time evolution.

The paper is organized as follows. In Section 2 the solectron Hamiltonian is introduced and the approximations included in our approach are described. In Section 3, the influence of parameter values on the ground states is

[a] e-mail: mgvelarde@pluri.ucm.es

presented. Then we provide numerical evidence of the existence of easily excitable states – solectron-like excitations – corresponding to electrons moving with sound or supersonic velocity which are in general energetically in the range of 1–20 meV above the ground state. The paper ends with a discussion (Sect. 4) of results and on the potential applicability of solectron excitations to transport phenomena.

2 Model Hamiltonian

As in the standard polaron studies, the Hamiltonian $\hat{H}$ we consider has three terms:

$$\hat{H} = \hat{H}_{\rm e} + H_{\rm ph} + \hat{H}_{\rm e-ph}, \tag{1}$$

where $\hat{H}_{\rm e}$ describes the hopping of the charged particle from site to site; $H_{\rm ph}$, the lattice Hamiltonian describes the relative motions of the lattice sites and $\hat{H}_{\rm e-ph}$, the interaction Hamiltonian, describes the on-site (diagonal) interaction of the charged particles with the lattice deformations. Although the $\hat{H}_{\rm e}$ Hamiltonian detailed below can be applied both to holes and to electrons, and even to more general quantum excitations, our interest is in electronic conductivity and thus we shall designate it as the *electronic* Hamiltonian.

The *electronic* Hamiltonian we consider here is as follows:

$$\hat{H}_{\rm e} = \sum_{n<m=1}^{N} \left[V_{nm}\ \left(\hat{a}_n^{\dagger}\hat{a}_m + \hat{a}_m^{\dagger}\hat{a}_n\right)\right] + \text{h.c.}, \tag{2}$$

where V_{nm} is the hopping strength between sites n and m; $\hat{a}_n^{\dagger}(\hat{a}_n)$ are the Fermi creation(annihilation) operators (endowed with the standard anticommutation relations) for an electron at site n and N is the total number of lattice sites.

As in most polaron studies, only hopping between nearest neighbors will be considered in this work. However, while in many studies $V_{nm} = V\,\delta_{m,\,n\pm1}$, here we follow Slater [84] and other authors [85–87] considering a nonlinear hopping term with the following form:

$$V_{nn-1} = V_0 \exp\left[-\alpha_0\ (U_n - U_{n-1})\right], \tag{3}$$

where U_n is the displacement from the equilibrium position of the lattice site n. For small lattice distortions, the coupling term becomes:

$$V_{nn-1} = V_0\left[1 - \alpha_0\ (U_n - U_{n-1}) + \cdots\right], \tag{4}$$

in which the dependence on lattice distortions of the hopping terms is as in the Hamiltonian for the charged particle in the Su et al. (SSH) model [23–25]. This term represents the dependence of the electron hopping integral on the relative distance between sites (off-diagonal matrix elements). Besides not having the factor $(-1)^n$ that in the SSH theory leads to the *topological* soliton, which is the electron carrier, arising from the degeneracy of the ground state of the system here we are interested in the *non-topological* lattice soliton originating in the anharmonicity of the $H_{\rm ph}$ Hamiltonian. The expression we use for the hopping term (3) corresponds to an extension of the Peierls-type coupling [88,89] that takes into account the nonlinear nature of electron-lattice interactions. Although we call $\hat{H}_{\rm e}$ the electronic Hamiltonian it clearly appears that this term already includes interactions of the electrons with the lattice vibrations. For small lattice distortions, it reduces to the Davydov-Scott Hamiltonian [17,64,66] with $\alpha_0 = 0$.

The *lattice* Hamiltonian $H_{\rm ph}$ we use also goes beyond the standard polaron theories as we include the anharmonic modes described by the Morse potential:

$$H_{\rm ph} = D\sum_{n=1}^{N}\left\{1 - \exp\left[-B\left(U_n - U_{n-1}\right)\right]\right\}^2 + \frac{1}{2M}\sum_{n=1}^{N} p_n^2, \tag{5}$$

where D is the break-up energy and B is related to the stiffness of the lattice, M is the mass of each lattice unit and p_n is its momentum at site n. Note that the linear expansion of (1)–(5) reduces to the Hamiltonian used by Alder et al. [90] for the 1D case.

Noteworthy is that the Morse potential can be adapted to the Toda potential [91] up to the third derivative [92–95] (hence matching frequency and stiffnes) as shown in Figure 1, where, just for reference, we also display the (12, 6) Lennard-Jones potential. These potentials offer a very similar strong repulsive component. Since the suitably scaled relative lattice displacements of the states dealt with in this work are much smaller than unity, the unphysical region of the Toda potential is not relevant for the conclusions drawn here. One advantage of the Toda potential is that it is integrable and explicit analytical solutions exist.

While equation (3) includes the influence of the relative distance between sites on electron hopping, the following Hamiltonian includes the influence of that distance on on-site electron energy:

$$\hat{H}_{\rm e-ph} = \chi\sum_{n=1}^{N}\left[\left(U_{n+1} - U_{n-1}\right)\hat{a}_n^{\dagger}\hat{a}_n\right], \tag{6}$$

where χ is the strength of the interaction an electron at site n has with the lattice distortions at that site.

To give universality to our argument we shall use dimensionless quantities:

$$\tilde{U}_n = BU_n; \qquad \tilde{p}_n = \frac{p_n}{\sqrt{2MD}}; \qquad \tilde{V} = \frac{V_0}{2D};$$
$$\tilde{\chi} = \frac{\chi}{2DB}; \qquad \tilde{\alpha} = \frac{\alpha_0}{B}; \qquad \tilde{t} = \Omega_{Morse}t, \tag{7}$$

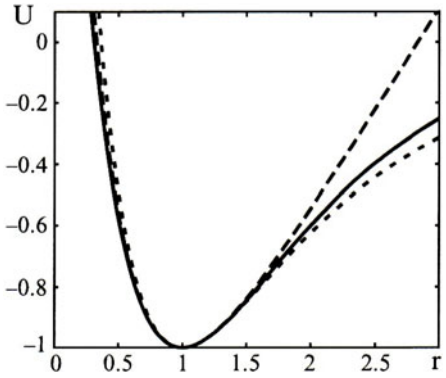

Fig. 1. Toda potential $U(r) = e^{-r}$ (dashed line), Morse potential $U(r) = D\left(1 - e[-Br)\right)^2$ (solid line), and (12, 6) Lennard-Jones potential $U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$ (dotted line), by adjusting the relevant parameters D, B, σ, ϵ, the potentials are rescaled around their minima such that the first three derivatives are the same for all potentials. r denotes the scaled equilibrium distance between lattice units. The fourth-power Hamiltonian with a single well can equally be fitted around the minimum.

with $\Omega_{Morse} = \sqrt{2DB^2/M}$. In dimensionless form the energy is scaled by $2D$ and the Hamiltonian becomes

$$\begin{aligned}\frac{H}{2D} = &-\sum_{n=1}^{N}\left[V_{nn-1}\left(\hat{a}_n^{\dagger}\hat{a}_{n-1} + \hat{a}_{n-1}^{\dagger}\hat{a}_n\right) + \text{h.c}\right] \\ &-\chi\sum_{n=1}^{N}\left[\left(U_{n+1} - U_{n-1}\right)\hat{a}_n^{\dagger}\hat{a}_n\right] \\ &+\sum_{n=1}^{N}p_n^2 + \sum_{n=1}^{N}\frac{1}{2}\left\{1 - \exp\left[-\left(U_n - U_{n-1}\right)\right]\right\}^2 \quad (8)\end{aligned}$$

with $V_{nm} = V\exp\left[-\alpha\left(U_n - U_{n-1}\right)\right]$ and where the tildes have been dropped.

As is done in previous solectron and similar studies [23–25,41–43,49,52,53,63–70,75–83], here the lattice is treated classically while the electron is treated quantum mechanically (a difference that is marked by the hats above the corresponding operators in equations (1)–(6)). In this mixed quantum-classical regime, the *exact* wave function for one-electron is:

$$\Psi = \sum_{n=1}^{N}\Phi_n\left(\{\boldsymbol{U}_n\}, t\right)\hat{a}_n^{\dagger}\left|0\right\rangle, \quad (9)$$

where Φ_n is the probability amplitude for an electron to be in lattice site n, whose explicit dependence on the relative lattice displacements is not specified a priori, contrary to what happens when trial wave functions are used.

The minimum energy one-electron states of the electron-phonon system defined by equations (1)–(6) can be determined by numerical minimization, with respect to the electron variables $\{\Phi_n\}$ and to the lattice variables $\{U_n\}$, of the functional $\mathcal{H} = \langle\Psi|\hat{H}|\Psi\rangle$:

$$\begin{aligned}\mathcal{H} = &\sum_n\left\{\frac{1}{2}(1 - \exp[-(U_n - U_{n-1})])^2 + p_n^2\right\} \\ &-\sum_n\{V\exp[-\alpha(U_n - U_{n-1})](\Phi_n^*\Phi_{n-1} + \Phi_n\Phi_{n-1}^*) + \text{h.c.}\} \\ &-\chi\sum_n(U_{n+1} - U_{n-1})\Phi_n^*\Phi_n, \quad (10)\end{aligned}$$

where the probability amplitudes Φ_n obey the normalization condition:

$$\sum_{n=1}^{N}|\Phi_n|^2 = 1. \quad (11)$$

We have adopted a numerical protocol, already applied successfully [64,66,67], which is to minimize directly with respect to the lattice variables only and for each set of $\{U_n\}$ tried during the minimization procedure, solve the eigenvalue problem for the electron and take the lower energy state every time. Since all eigenstates are normalized, the normalization condition (11) is also obeyed.

We also study the evolution of solectron compounds by integrating the equations of motion, which can be derived by a variational principle, and are:

$$\begin{aligned}i\frac{d\Phi_n}{dt} = &-\tau\{\exp[-\alpha(U_{n+1} - U_n)]\Phi_{n+1} \\ &+\exp[-\alpha(U_n - U_{n-1})]\Phi_{n-1}\} \\ &-\frac{\chi}{\Omega_{Morse}}(U_{n+1} - U_{n-1})\Phi_n \\ \frac{d^2U_n}{dt^2} = &\{1 - \exp[-(U_{n+1} - U_n)]\}\exp[-(U_{n+1} - U_n)] \\ &-\{1 - \exp[-(U_n - U_{n-1})]\}\exp[-(U_n - U_{n-1})] \\ &-\alpha V\{(\Phi_{n+1}^*\Phi_n + \Phi_{n+1}\Phi_n^*)\exp[-\alpha(U_{n+1} - U_n)] \\ &-\text{h.c.}\} - \chi(|\Phi_{n+1}|^2 - |\Phi_{n-1}|^2)\end{aligned} \quad (12)$$

where the adiabaticity parameter $\tau = V/\hbar\Omega_{Morse}$ determines the degree of time scale separation between the electronic and the acoustic phonon and soliton processes.

Finally, in order to characterize the degree of localization of the electron-lattice states, we use the participation ratio, P, defined as:

$$P = 1/\sum_n|\Phi_n|^4. \quad (13)$$

When the electron is localized in one site the participation ratio is equal to unity and, when the electron is completely delocalized, the participation ratio is equal to the number sites N, the number of lattice sites. All the other electron-lattice states have values of the participation ratio between those two extremes.

3 Results

Our interest is to determine the range of parameter values in which localized electron states are stationary. In contrast to other studies [96], in our finite lattice with N sites,

both localized and delocalized states are normalizable and a completely delocalized state is characterized by a wave function in which the probability for the electron to be in each site is equal for all sites, that is, for a delocalized state $|\Phi_n|^2 = 1/N$. First we investigate the properties of the ground states and the range of parameter values for which they are localized and next we shall study localized states of similarly low energies which correspond to moving electrons and compare it to the known results on solectron states [75–83].

3.1 One-electron ground states

Inspection of the functional $\mathcal{H}$ shows that, when $\chi = 0$, the states of the system can be parameterized by two quantities, namely, V and α. As pointed out before, V affects both the hopping of the electron between neighboring sites and the electron-lattice interaction, while α affects solely the electron-lattice coupling. When $\alpha = 0$, the electron state is not influenced by the lattice and the minimum energy state is delocalized; above a threshold value of α, the minimum energy one-electron state becomes localized. Figure 2 shows this transition from a delocalized state to a localized state characterized by pulse-shaped electron distribution that gets progressively thinner, coupled to the lattice displacement, illustrated here with the site variable U_n, that gets progressively more pronounced as α increases. The dependence of $\alpha_{\rm cr}$, the threshold value of α above which the electron states are localized, as a function of the number of sites, N, for $\chi = 0$, is plotted in Figure 3. It shows that there is a threshold for $\alpha_{\rm cr}$ above which the ground state is localized which decreases as the number of sites, N, increases. This is what is found for the variation with χ of the one-electron ground states of the linear polaron models ($\alpha = 0$) [64], where $N \to \infty$ leads to the nonlinear Schrödinger equation which is known to have localized solutions for any finite value of χ.

In Figure 4 is displayed the dependence of $\alpha_{\rm cr}$ on the hopping amplitude V, for a fixed number of sites. It shows that $\alpha_{\rm cr}$ *decreases* as the hopping parameter increases. In fact, the variation of $\alpha_{\rm cr}$ with V for $N = 100$ is approximately given by the following expression:

$$\alpha_{cr} \approx \frac{1}{4\sqrt{V}} \tag{14}$$

that is, above $\alpha_{\rm cr}$ the one-electron ground states of the solectron Hamiltonian, in a lattice with 100 sites, are localized. Since we are working with the dimensionless variables $\alpha = \alpha_0/B$ and $V = V_0/2D$, translating equation (14) to the real physical variables α_0 and V_0, we obtain a relation that connects the stiffness of the Morse potential, B, its break-up energy, D, and the electron lattice interaction strength, α_0:

$$\alpha_0 > \frac{B}{2}\sqrt{\frac{D}{8V_0}}. \tag{15}$$

For values of the real physical electron-lattice coupling constant α_0 above the physical threshold (15), the electron states become more and more localized, i.e., for a given

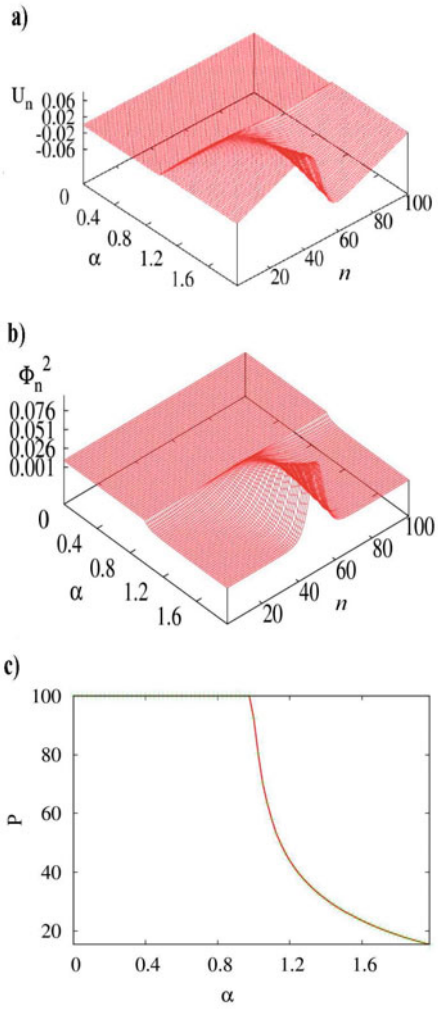

Fig. 2. (Color online) Variation with α of (a)the associated lattice displacements, U_n, (b) the probability for an electron to be at site n, $|\Phi_n|^2$, and (c) the participation ratio (13), for a lattice with $N = 100$ sites, when $\chi = 0$.

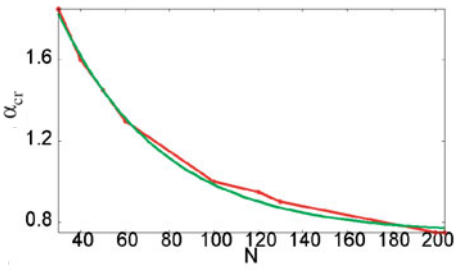

Fig. 3. (Color online) Plot of $\alpha_{\rm cr}$ (see text) as a function of the system size N, when $V = 0.05$ and $\chi = 0$. The red dotted line corresponds to the numerical results and the green solid line is drawn from the expression $\alpha = 0.74 + 0.06\exp(-0.0215N)$, obtained by a fit of the numerical results. It seems that α_{cr} diverges as N decreases. However for small values of N, α_{cr} is bound to be smaller than 2 in order to have physical solutions. Thus for small system sizes a value of $\chi \neq 0$ is needed to have localized states and the value of α_{cr} becomes irrelevant i.e. we are in the Davydov case.

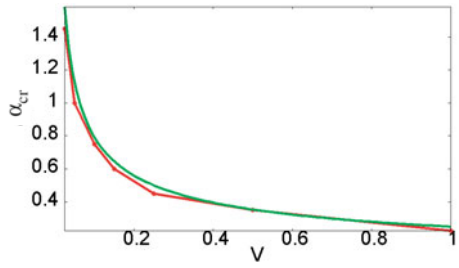

Fig. 4. (Color online) Dependence of $\alpha_{\rm cr}$ on the hopping amplitude V for a lattice with $N = 100$ sites. The red line with dots corresponds to the numerical results and the solid green line is drawn from the expression $1/(4\sqrt{V})$ obtained from a fitting to the numerical results. Since at $\chi = 0$ the electron-lattice interaction depends on the value of αV and not only on α for small values of V then α_{cr} must be large in order to compensate. This is not the case when $\chi \neq 0$ as shown in Figure 5.

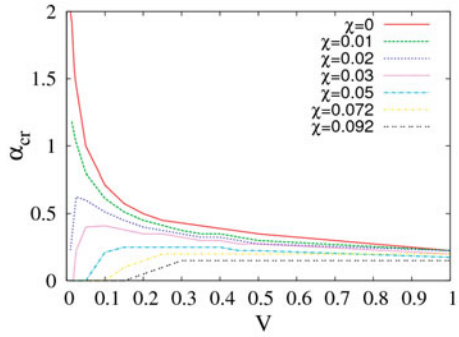

Fig. 5. (Color online) Plot of $\alpha_{\rm cr}$ illustrating where above it *localized* states can be found as a function V for a given value of χ, here taken as a parameter.

value of V_0, the width of the localized state decreases with increasing α, as is shown in Figure 2. Save the restriction to one-dimensional geometry, the parameter space considered here is close to values for biomolecules [11,13,15–17,87,97–105] and for high-$T_{\rm c}$ cuprates [90,106–114]. In either case the results are qualitatively the same. This dependence of the width of the localized state on the strength of the electron-lattice constant agrees with what was observed in the Davydov-Scott model [64]. However, the relation between V and α is opposite to what is found in the Davydov-Scott model and in some of its extensions [64,66]. The reason is that, in the Davydov-Scott model, the electron lattice interaction appears only in the diagonal terms, and does not influence the strength of the electron hopping, resulting in an electron-lattice interaction clearly favoring localization. On the other hand, in the solectron Hamiltonian (1)–(6) with $\chi = 0$, the electron-lattice interaction is off-diagonal and influences the strength of the electron hopping as well. Indeed, in the linear approximation (4), valid for small lattice displacements, the electron hopping depends on the product of $V_0\alpha_0$, so that when the electron-lattice interaction α_0 increases, the hopping strength $V_0\alpha_0$ also increases. The general rule is that the higher the hopping strengths the more delocalized the electron states and thus the net result for the solectron Hamiltonian is that, when V_0 increases, α_0 cannot always increase in order that the effective electron hopping strength $V_0\alpha_0$ remains bounded.

In order to investigate separately the effects of diagonal and off-diagonal electron-lattice interactions, and also to interpolate between these two regimes, we have determined one-electron ground states for different values of χ, V and α. The dependence on the electron hopping strength, V, and on the diagonal electron-lattice interaction, χ, of the critical values of α, $\alpha_{\rm cr}$, above which the ground states are localized, is displayed in Figure 5. This figure depicts the way $\alpha_{\rm cr}$ depends on V parameterized by χ thus separating the *localized* ground states found above it from the *delocalized* ground states below. Notice that all variables only have values equal or greater than zero. We find that, when $\chi = 0$, $\alpha_{\rm cr}$ is always finite and *decreases* as V increases until it reaches an asymptotic value. This is the pure solectron regime, in which localized states can only arise for non-zero values of α, as already explained above. On the other hand, when $\chi \neq 0$ and V is small, the influence of α on the ground states is negligible. Although this is a mixed solectron-Davydov regime, the localizing effect of diagonal electron-lattice interaction dominates over the off-diagonal part of the electron Hamiltonian and $\alpha_{\rm cr}$ is zero for low values of V, and then *increases* until it reaches the same saturation value. For higher values of the hopping strength, V, the diagonal electron-lattice interaction is not strong enough to generate localization and a finite contribution of the off-diagonal electron-lattice interaction is needed. Thus, in this case, $\alpha_{\rm cr}$ *increases* with increasing V until it saturates.

To make a direct evaluation of the influence of the diagonal and of the off-diagonal electron-lattice interactions on the localization, we can compare the one-electron ground states for the pure Davydov-Scott model ($\alpha = 0$) with the ground states obtained in the linear approximation of the pure solectron Hamiltonian ($\chi = 0$ and considering only the linear term in U_n equation (4), that is, the SSH Hamiltonian), when αV in the latter is equal to χ in the former. Figure 6 (top plot) shows how the energy of the ground states of the pure Davydov-Scott model (green line) compares with the energy of the pure solectron model (red line), for the same values of χ and αV, respectively. In the bottom plot the ratio, $R = \frac{E_{\rm DS}}{E_{\rm solectron}}$ between the energies displayed in the top graph is displayed showing that, for localized ground states generated by a diagonal electron-lattice interaction are only marginally more stable than those generated by an off-diagonal electron-lattice interaction. Finally, Figure 7 shows that the lower energy states generated by the diagonal electron-lattice interaction are more localized than the SSH states, for the same values of the electron-lattice interaction.

3.2 Dynamical stability of localized states

In the previous section we investigated the parameter regimes in which one-electron ground states are localized. These minimum energy states are stationary states, that

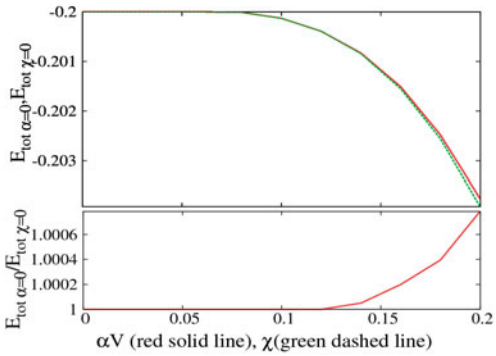

Fig. 6. (Color online) Top plot: total energy of the ground states of the pure Davydov-Scott model (green line) and of the SSH model (red line) as a function of χ and αV, respectively (see text). Bottom plot: ratio, R of the two total energies in the top plot (see text).

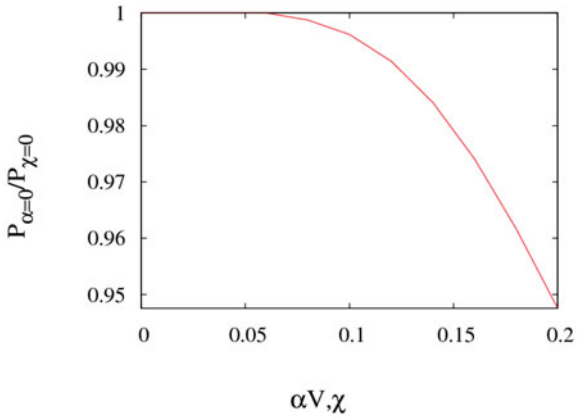

Fig. 7. (Color online) Scaled participation ratio, $P_{\rm DS}$ of the ground states of the Davydov-Scott Hamiltonian with respect to participation ration, $P_{\rm SSH}$, as a function of the corresponding electron-lattice interactions (see text).

is, they have zero momentum and their time evolution is trivial, since they keep their position and shape for ever. Previous studies of the time evolution of the pure solectron model have already demonstrated the existence of long lasting localized states characterized by pulse-shaped electron distributions coupled to lattice solitons that move together with the electron (the solectron state) [75–83]. In this section we study the time evolution of the moving localized excited states that are obtained by perturbations of the ground states. In our calculation we will use the parameter values $\alpha = 1.75$, $V = 0.1$, $D = 0.1$ eV, and $B = 4.45$ Å^{-1}, which yields to an adiabaticity parameter $\tau = 28.47$ unless stated differently.

First we generate moving excited states by adding momentum to the corresponding ground states. Figure 8 shows that, when a localized ground state obtained with a low value of the electron hopping strength V is perturbed by adding a momentum, $p_n = U_n - U_{n-1}$, to each lattice n, a moving localized state arises, that remains stable for at least 300 lattice cycles. Moreover, Figure 9 shows that when a higher momentum is added (in this

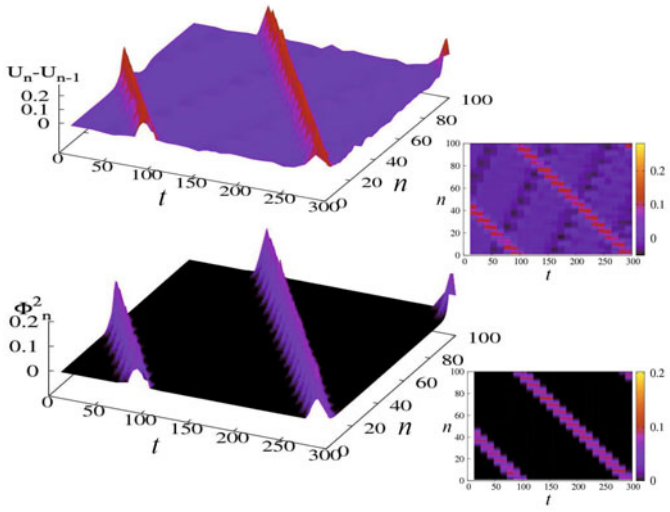

Fig. 8. (Color online) Time evolution of the relative lattice displacements, $U_n - U_{n-1}$ (top plot) and of the electron density, $|\Phi_n|^2$ (bottom plot) of the ground state for $V = 0.1$, $\alpha = 1.75$ and $\chi = 0$, perturbed by an initial momentum $p_n(t = 0) = U_n - U_{n-1}$. Notice that both relative lattice displacement and electron density follow the same trajectory and the former appears as bell-shaped, non-topological soliton.

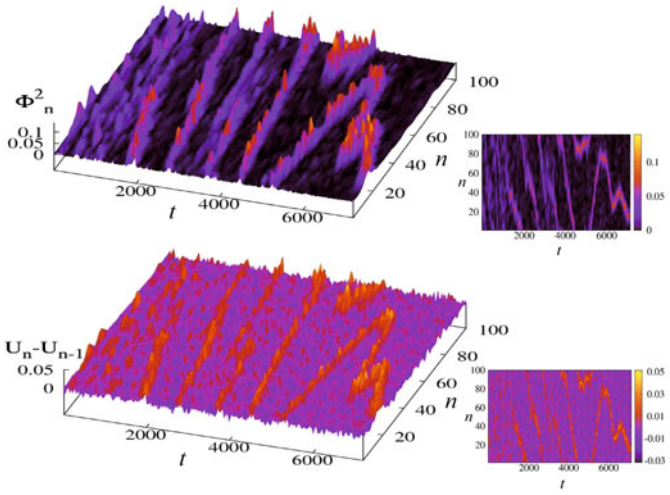

Fig. 9. (Color online) Time evolution of the lattice deformation, $U_n - U_{n-1}$ (top plot) and of the electron density, $|\Phi_n|^2$ (bottom plot), of the ground state for $V = 0.1$, $\alpha = 1.75$ and $\chi = 0$, perturbed by an initial momentum $p_n(t = 0) = 8(U_n - U_{n-1})$.

case $p_n = 8(U_n - U_{n-1})$), a similarly stable localized dynamical state arises that travels with a speed that is approximately five times higher. It should also be pointed out that in our dimensionless variables (7), the velocity of sound is $v_{sound} = 1$, which means that the localized states in Figure 9 move with supersonic velocity, as solectron states described in earlier studies [75–83].

Another way to generate excited states is to inject an excess electron at one lattice site and follow the perturbation that it induces in the lattice. This situation was simulated by an initial condition in which the electron

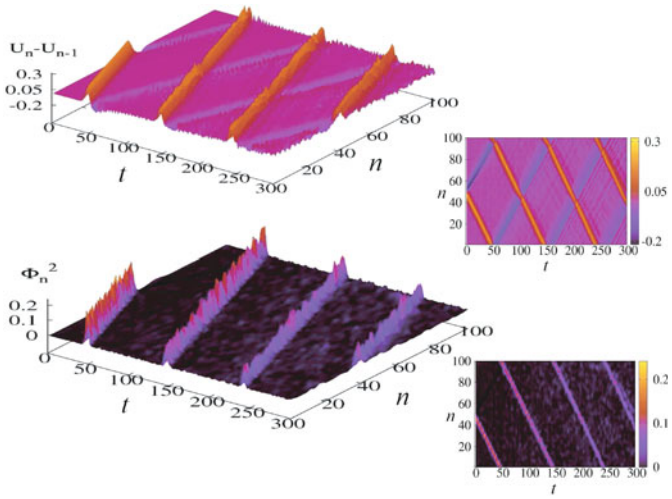

Fig. 10. (Color online) Time evolution of the electron density, $|\Phi_n|^2$ (top plot) and of the relative lattice distortion, $U_n - U_{n-1}$ (bottom plot) when the initial electron density is equal to that of the ground state for $V = 0.1$, $\alpha = 1.75$ and $\chi = 0$, and when the initial lattice deformations and momenta are zero. Notice that purposely here and in subsequent figures we have inverted the order in the plots relative to Figures 8 and 9 as here the electron is leading the dynamics of the process as in the original Landau polaron case.

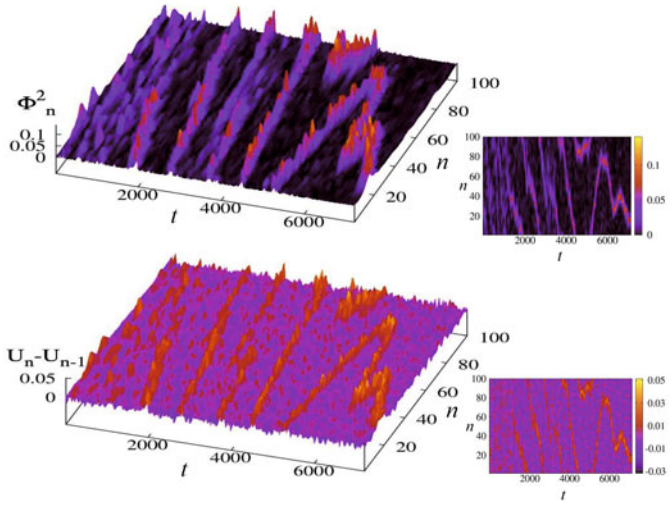

Fig. 11. (Color online) Time evolution of the electron density, $|\Phi_n|^2$ (top plot) and of the relative lattice distortion, $U_n - U_{n-1}$ (bottom plot) when the initial electron density is equal to that of the ground state for $V = 0.1$, $\alpha = 1.75$ and $\chi = 0$, and when the initial lattice deformations are zero and the initial lattice momenta are $p_n(t = 0) = 0.8(U_n - U_{n-1})$, where the U_n are the lattice deformations of the ground state.

distribution is the same as the ground state, while the lattice is undistorted. Figures 10 and 11 illustrate the Landau process [1], i.e., as time evolves the electron distribution induces a deformation in the lattice and that this deformation traps the electron. Furthermore, although for the results displayed in Figure 10 the initial momentum of each lattice site was zero, both the electron and the lattice deformation move. Initially, the radiation created by the trapping process leads to a few scattering processes but, after some time, the movement of the electron and its associated lattice distortion through the system tends to a steady state with an almost constant velocity, as can be observed in Figure 10 where time-position curve tends to a straight line beyond $T = 1000$, just like the solectron. Inspection of Figures 8 and 10 shows that the velocity of the solectron that arises from the Landau process is five times smaller than that induced by the addition of momenta. Additional momenta, together with the Landau process, leads to more energy in the form of radiation which leads to a delay in the formation of the solectron but which also leads to faster moving electrons, as can be seen in Figure 11. Noteworthy, is that clearly the polaron effect is capable of exciting finite amplitude lattice excitations, thus leading to the solectron.

3.3 Comparison with previous solectron simulations

One advantage of the Toda potential is that we know explicitly analytical travelling soliton wave solutions. One such solution of the Hamiltonian (1)–(6), with $\chi = 0$, has the form [91]:

$$\exp[U_n - U_{n-1}] = 1 + \left(\frac{\sinh(\kappa)}{\cosh(\kappa n)}\right)^2 \tag{16}$$

to which we add, as done in earlier publications [76–79], as *ansatz* for the electron

$$\Phi = \frac{1}{\text{Norm}} \frac{\sinh(\kappa)}{\cosh(\kappa n)} \exp(-i\delta n) \tag{17}$$

where $\text{Norm} = \sum_1^N \left(\frac{\sinh(\kappa)}{\cosh(\kappa n)}\right)^2$ and $0 < \delta < \pi$. This compound state, which corresponds to a lattice soliton deformation travelling together with the electron, is a solectron state and was shown to be a stable solution of (1)–(6). Though solitons alone (16) always travel supersonically, solectrons i.e. compounds of interacting electron and soliton, may travel at sub or supersonic velocities depending on the electron lattice interaction and on the value of κ. By increasing κ, and thus decreasing the soliton width, the velocity and the energy of the solectron state increase. Previous solectron simulations [75–83] show states that travel at much higher velocities than those presented in the previous section. For example, the solution plotted in Figure 12, for a $\kappa = 1.15$ and for $V = 0.1$, $\alpha = 1.75$, $\chi = 0$ and $p(n) = U_n - U_{n-1}$ has a much higher energy E_S than that of the corresponding ground state which is $E_G = -0.2025$. For a break-up energy, $D = 0.1$ eV, the energy difference $E_S - E_G = 0.0948$ requires a temperature in the range of 220 K to be thermally generated. On the other hand, the solectron state that arises by playing with the electron initial conditions (Fig. 10) has a total energy difference with respect to the ground state $E_{inj} - E_G = 5.49 \times 10^{-3}$ which requires a temperature of about 12 K to be thermally generated. For smaller values of κ, i.e., for $\kappa = 0.1$,

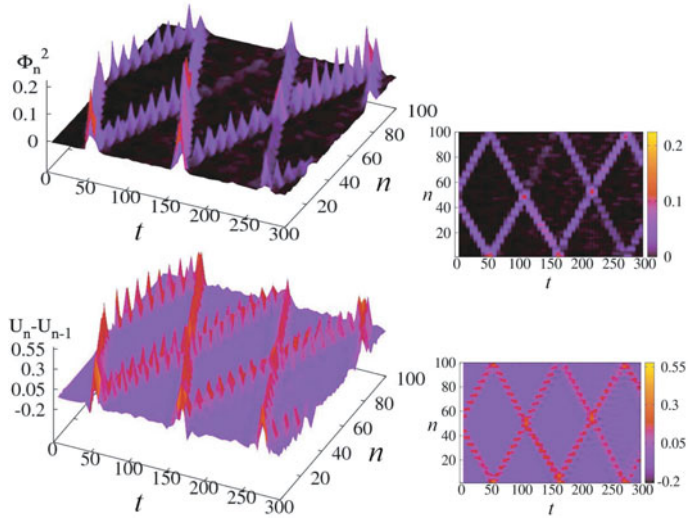

Fig. 12. (Color online) Time evolution of the electron density, $|\Phi_n|^2$ (top plot) and of the relative lattice distortion, $U_n - U_{n-1}$ (bottom plot) for the soliton solution (16) with $V = 0.1$, $\alpha = 1.75$, $\chi = 0$, $\kappa = 1.15$ and $\delta = 3$ with initial lattice momenta $P_n = 0.01(U_n - U_{n-1})$.

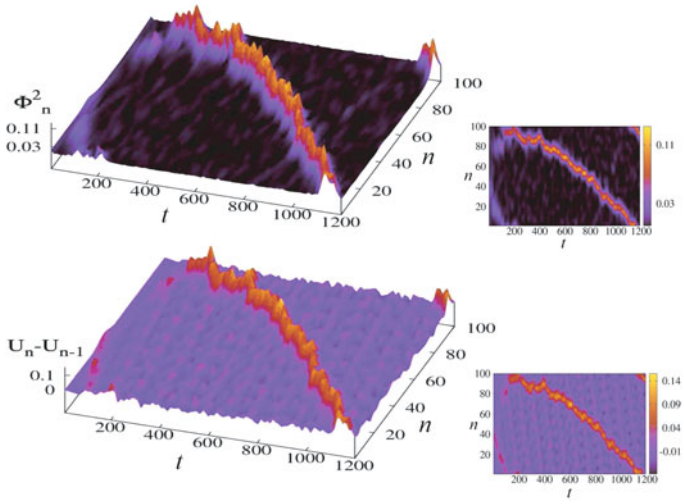

Fig. 13. (Color online) Same as in Figure 12 but with $\kappa = .1$ and zero initial momenta.

the energy difference with respect to that of the solectron in Figure 10 is $E_S - E_{inj} = 1.647 \times 10^{-5}$ which is almost vanishing. Its evolution, which can be seen in Figure 13, is also very similar to that observed in Figure 10. Hence, we can conclude that the intrinsic localized modes observed in Section 3.2 are low energy solectrons induced by the polaron action of the electron upon the lattice. Incidentally for similar parameter values, the Davydov electrosoliton does not survive above 10 K [17,65,69,70].

4 Discussion

All states found for an electron in the presence of a "polarizable" lattice share the same physical origin in that they are the result of a distortion induced by the electron on the lattice, which, in turn, affects the state of the electron, as long ago suggested by Landau [1]. The different designations for these states found in the literature (small polaron, large polaron, electrosoliton, solitobreather, solectron) merely reflect the values of the electron-lattice interactions and the nature (linear or nonlinear) of the lattice and/or electron systems. However, the different designations are useful because the corresponding states do have different properties such as dynamical stability, thermodynamic stability, conductivity, etc. The lattice system we have considered here, is known to be able to exhibit intrinsic localized modes as traveling solitons at sufficiently high energies. The question we addressed here is whether adding an electron the latter is able to induce such distortions and hence via polaron effect being able to yield a solectron. This is the opposite question to that so far proposed in earlier solectron studies [75–83] where the soliton in an anharmonic Hamiltonian was shown to be able to trap and subsequently carry away the added electron.

We have found that, although in the case of purely off-diagonal electron-lattice interactions, the effect of the electron hopping strength V and of the electron-lattice interaction α, must be considered together, for a vast region of the parameter space spanned by V, α and χ, the one-electron ground states are indeed localized states (Fig. 5). This is in contrast to the results so far found for the Davydov-Scott system, which is characterized by a diagonal electron-lattice interaction, and for which the degree of localization of the one-electron ground states depends only on the ratio $V(DB)/\chi^2$, where DB is the linear elastic constant [64]. Also, while in the Davydov-Scott system an increase in the electron-lattice coupling constant χ *always* leads to more localized ground states, in the solectron case (1)–(6), with $\chi = 0$, an increase in the corresponding electron-lattice coupling constant, α, can result in a more *delocalized* ground state. This is because, in the solectron Hamiltonian, α affects both the electron-lattice interaction and the electron hopping, with the effective hopping strength being dependent on the product αV.

We have also investigated the evolution of the solectron states that are obtained by low energy perturbations of the one-electron ground state and have found that both the excited states that result from an addition of initial momenta to lattice sites and those that arise after playing with electron initial conditioons lead to the formation of solectron states that are long living intrinsic localized modes, and that some of them can even travel at supersonic velocities. The higher the energy of the excited states, the longer it takes for a solectron to form because of the larger amount of energy that goes into radiation and thus, the greater the number of scattering processes undergone by the localizing state.

The results obtained here pertain to the *microcanonical* ensemble since the time evolution of the excited one-electron states conserved the total energy of the system. Comparing the energies of these excited states to the energy of the ground state we find that, while the solectron

states investigated in previous publications [75–83] would require, for about the same parameter values, temperatures of the order of 220 K to be thermally generated, the solectron states investigated here only require a temperature of 12 K to arise. A proper study of the thermal stability of the solectron state must be done within the *canonical* ensemble and will be discussed elsewhere. However, we feel there is already enough evidence to anticipate that the solectron states studied here will be stable at finite temperature, hence showing their potential as charge carriers for fast electric transport at room temperature.

The authors express their gratitude to Professors A.P. Chetverikov, G. Röpke, D. Hennig, E. Brändas, L. Brizhik, S. Larsson, A.S. Alexandrov, F.M. Russell, R. Miranda, G. Tsironis and G. Vinogradov for enlightening discussions and suggestions. They are also grateful to the two anonimous referees for suggestions and criticism that helped improving posing the problem and the presentation of results. This work was sponsored by the Spanish *Ministerio de Ciencia e Innovacion* through grant EXPLORA-FIS2009-06585-E. L. Cruzeiro acknowledges partial support from *Fundação para a Ciência e Tecnologia (FCT)*, Portugal.

References

1. L.D. Landau, Phys. Z. Sowjettunion **3**, 664 (1933)
2. S.I. Pekar, Soviet Phys. JETP **16**, 335 (1946)
3. S.I. Pekar, *Untersuchungen über die Elektronentheorie* (Akademic-Verlag, Berlin, 1954)
4. L.D. Landau, S.I. Pekar, Sov. Phys. JETP **18**, 419 (1948)
5. E.I. Rashba, in *Polaron in Advanced Matherials*, edited by A.S. Alexandrov (Springer, Dordrecht, 2007), pp. XI-XIV
6. H. Fröhlich, H. Pelzer, S. Zienau, Philos. Magn. **41**, 221 (1950)
7. H. Fröhlich, Adv. Phys. **3**, 325 (1954)
8. T. Holstein, Ann. Phys. **8**, 325 (1959)
9. T. Holstein, Ann. Phys. **8**, 343 (1959)
10. A.S. Davydov, Phys. Stat. Sol. **36**, 211 (1969)
11. A.S. Davydov, J. Theoret. Biol. **38**, 559 (1973)
12. A.S. Davydov, *Biology and Quantum Mechanics* (Pergamon, New York, 1982)
13. A.S. Davydov, *Solitons in Molecular Systems*, 2nd edn. (Reidel, Dordrecht, 1991)
14. J.A. Tuszynski, R. Paul, R. Chaterjee, S.R. Sreenivasan, Phys. Rev. A **30**, 2666 (1984)
15. A.C. Scott, Phys. Rev. A **26**, 578 (1982)
16. A.C. Scott, Phys. Rev. A **27**, 2767 (1983)
17. A.C. Scott, Phys. Rep. **217**, 1 (1992)
18. M.A. Collins, Chem. Phys. Lett. **77**, 342 (1981)
19. S. Yomosa, Phys. Rev. A **32**, 1752 (1985)
20. O.H. Olsen, M.R. Samuelsen, S.B. Petersen, L. Nørshov, Phys. Rev. A **38**, 5856 (1988)
21. O.H. Olsen, M.R. Samuelsen, S.B. Petersen, L. Nørshov, Phys. Rev. A **39**, 3130 (1989)
22. P.L. Christiansen, A.V. Zolotaryuk, A.V. Savin, Phys. Rev. E **56**, 877 (1997)
23. W.P. Su, J.R. Schrieffer, A.J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979)
24. W.P. Su, J.R. Schrieffer, A.J. Heeger, Phys. Rev. B **22**, 2099 (1980)
25. A.J. Heeger, S. Kivelson, J.R. Schrieffer, W.P. Su, Rev. Mod. Phys. **60**, 781 (1988)
26. A.A. Ovchinnikov, Sov. Phys. JETP **30**, 147 (1970)
27. A.M. Kosevich, A.S. Kovalev, Soviet Phys. JETP **67**, 1793 (1973)
28. A.S. Dolgov, Sov. Phys. Solid State **28**, 907 (1986)
29. A.J. Sievers, S. Takeno, Phys. Rev. Lett. **61**, 970 (1988)
30. S. Takeno, A.J. Sievers, Solid State Commun. **67**, 1023 (1988)
31. J.B. Page, Phys. Rev. B **41**, 7835 (1990)
32. S.R. Bickham, A.J. Sievers, Phys. Rev. B **43**, 2339 (1991)
33. W.Z. Wang, J.T. Gammel, A.R. Bishop, M.I. Salkola, Phys. Rev. Lett. **76**, 3598 (1996)
34. A.N. Holden, *Physical Metallurgy of Uranium* (Addison-Wesley, Reading Massachusetts, 1958)
35. M.E. Manley, M. Yethiraj, H. Sinn, H.M. Volz, A. Alatas, J.C. Lashley, W.L Hults, G.H. Lander, J.L. Smith, Phys. Rev. Lett. **96**, 125501 (2006)
36. M.E. Manley, A. Alatas, F. Trouw, B.M. Leu, J.W. Lynn, Y. Chen, W.L. Hults, Phys. Rev. B **77**, 214305 (2008)
37. M.E. Manley, A.J. Sievers, J.W. Lynn, S.A. Kiselev, N.I. Agladze, Y. Chen, A. Llobet, A. Alatas, Phys. Rev. B **79**, 134304 (2009)
38. B.G. Vekhter, M.A. Ratner, J. Chem. Phys. **101**, 9710 (1994)
39. B.G. Vekhter, M.A. Ratner, Phys. Rev. B **51**, 3469 (1995)
40. B.I. Swanson, J.A. Brozik, S.P. Love, G.F. Strouse, A.P. Shreve, A.R. Bishop, W.Z. Wang, M.I. Salkola, Phys. Rev. Lett. **82**, 3288 (1999)
41. A.V. Zolotaryuk, St. Pnevmatikos, A.V. Savin, Phys. Rev. Lett. **67**, 707 (1991)
42. A.V. Zolotaryuk, K.H. Spatschek, A.V. Savin, Phys. Rev. B **54**, 266 (1996)
43. J.C. Eilbeck, P.S. Lomdahl, A.C. Scott, Physica D **16**, 318 (1985)
44. S. De Filippo, M.F. Girards, M. Salerno, Nonlinearity **2**, 477 (1989)
45. H. Feddersen, Phys. Lett. A **154**, 391 (1991)
46. M. Salerno, Phys. Lett. A **162**, 381 (1992)
47. V.M. Burlakov, S.A. Kiselev, V.N. Pyrkov, Phys. Rev. B **42**, 4921 (1990)
48. K.W. Sandusky, J.B. Page, K.E. Schmidt, Phys. Rev. B **46**, 6161 (1992)
49. S. Flach, K. Kladko, Phys. Rev. B **53**, 11531 (1996)
50. S. Flach, K. Kladko, R.S. MacKay, Phys. Rev. Lett. **78**, 1207 (1997)
51. D. Chen, S. Aubry, G.P. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996)
52. A.V. Zolotaryuk, J.C. Eilbeck, J. Phys.: Condens. Matter **10**, 4553 (1998)
53. B. Zhou, J.Z. Xu, J. Phys.: Condens. Matter **10**, 4553 (1998)
54. R.S. MacKay, S. Aubry, Nonlinearity **7**, 1623 (1994)
55. J.L. Marin, S. Aubry, Nonlinearity **9**, 1501 (1996)
56. F.M. Russell, Y. Zolotaryuk, J.C. Eilbeck, T. Dauxois, Phys. Rev. B **55**, 6304 (1997)
57. N.K. Voulgarakis, G.P. Tsironis, Phys. Rev. B **63**, 014302 (2000)
58. S. Aubry, Physica D **103**, 201 (1997)
59. G. Kalosakas, S. Aubry, Physica D **113**, 228 (1998)
60. S. Aubry, Physica D **216**, 1 (2006)
61. S. Aubry, in *Polarons in Advanced Materials*, edited by A.S. Alexandrov (Springer, Dordrecht, The Netherlands, 2007), pp. 311–371

62. G.P. Tsironis, Chaos **13**, 657 (2003)
63. J.C. Eilbeck, H. Gilhoj, A.C. Scott, Phys. Lett. A **172**, 229 (1993)
64. L. Cruzeiro-Hansson, V.M. Kenkre, Phys. Lett. A **190**, 59 (1994)
65. L. Cruzeiro-Hansson, S. Takeno, Phys. Rev. E **56**, 894 (1997)
66. L. Cruzeiro-Hansson, Phys. Lett. A **249**, 465 (1998)
67. L. Cruzeiro-Hansson, J.C. Eilbeck, J.L. Marin, F.M. Russell, Physica D **142**, 101 (2000)
68. L. Cruzeiro-Hansson, J.C. Eilbeck, J.L. Marin, F.M. Russell, Eur. Phys. J. B **42**, 95 (2004)
69. P.S. Lomdahl, W.C. Kerr, Phys. Rev. Lett. **55**, 1235 (1985)
70. *Davydov's Soliton Revisited, Self-Trapping of Vibrational Energy in Protein*, edited by P.L. Christiansen, A.C. Scott (Plenum Press, New York, 1990), and references therein
71. *Proton Transfer in Hydrogen-Bonded Systems*, edited by T. Bountis (Plenum Press, New York, 1992), and references therein.
72. S. Flach, C.R. Willis, Phys. Rep. **295**, 181 (1998), and references therein.
73. S. Flach, A.V. Gorbach, Phys. Rep. **467**, 1 (2008), and references therein.
74. M.G. Velarde, W. Ebeling, A.P. Chetverikov, Int. J. Bifurc. Chaos **15**, 245 (2005)
75. M.G. Velarde, J. Comput. Appl. Math. **233**, 1432 (2010)
76. M.G. Velarde, W. Ebeling, D. Hennig, C. Neissner, Int. J. Bifurc. Chaos **16**, 1035 (2006)
77. D. Hennig, C. Neissner, M.G. Velarde, W. Ebeling, Phys. Rev. B **73**, 024306 (2006)
78. A.P. Chetverikov, W. Ebeling, M.G. Velarde, Eur. Phys. J. B **51**, 87 (2006)
79. D. Hennig, A.P. Chetverikov, M.G. Velarde, W. Ebeling, Phys. Rev. E **76**, 046602 (2007)
80. M.G. Velarde, W. Ebeling, A.P. Chetverikov, Int. J. Bifurc. Chaos **18**, 3815 (2008)
81. A.P. Chetverikov, W. Ebeling, M.G. Velarde, Eur. Phys. J. B **70**, 217 (2009)
82. A.P. Chetverikov, W. Ebeling, M.G. Velarde, Int. J. Quantum Chem. **110**, 46 (2010)
83. M.G. Velarde, A.P. Chetverikov, D. Hennig, J.J. Kozak, Int. J. Bifurc. Chaos **20**, 185 (2010)
84. J.C. Slater, *Quantum Theory of Molecular and Solids, The Self-Consistent Field for Molecules and Solids* (McGraw-Hill, New York, 1974), Vol. 4
85. L.A. Curtiss, J.R. Miller, J. Phys. Chem. A **102**, 160 (1998)
86. D. Hennig, Phys. Rev. E **61**, 4550 (2000)
87. D. Hennig, Physica A **309**, 243 (2002)
88. J. Zaanen, P.B. Littlewood, Phys. Rev. B **50**, 7222 (1994)
89. K. Yonemitsu, N. Maeshima, Phys. Rev. B **76**, 075105 (2007)
90. B.J. Alder, K.J. Runge, R.T. Scalettar, Phys. Rev. Lett. **79**, 3022 (1997)
91. M. Toda, *Theory of Nonlinear Lattices*, 2nd edn. (Springer, Berlin, 1989)
92. T.J. Rolfe, S.A. Rice, J. Dancz, J. Chem. Phys. **70**, 26 (1979)
93. J. Danz, S.A. Rice, J. Chem. Phys. **67**, 1418 (1977)
94. M. Toda, *Nonlinear Waves and Solitons* (KTK Scientific Publishers, Tokyo, 1989)
95. T. Dauxois, M. Peyrard, *Physics of Solitons* (Cambridge University Press, Cambridge, 2006)
96. B. Gerlach, H. Löwen, Rev. Mod. Phys. **63**, 63 (1991)
97. C. Branden, J. Tooze, *Introduction to Protein Structure* (Garland, New York, 1991)
98. J.A. McCammon, S.C. Harvey, *Dynamics of Proteins and Nuclei Acids* (Cambridge University Press, Cambridge, 1987)
99. D. Hennig, Phys. Rev. B **65**, 174302 (2002)
100. D. Hennig, Eur. Phys. J. B **30**, 211 (2002)
101. M. Barbi, S. Cocco, M. Peyrard, Phys. Lett. A **253**, 358 (1999)
102. L. Stryer, *Biochemistry* (Freeman, New York, 1995)
103. J. Agarwal, D. Hennig, Physica A **323**, 519 (2003)
104. D. Hennig, J.F.R. Archilla, J. Agarwall, Physica D **180**, 256 (2003)
105. D. Hennig, E.B. Starikov, J.F.R. Archilla, F. Palmero, J. Biol. Phys. **30**, 227 (2004)
106. J. Zhong, H.B. Schüttler, Phys. Rev. Lett. **69**, 1600 (1992)
107. H.B. Schuttler, C.H. Pao, Phys. Rev. Lett. **75**, 4504 (1995)
108. F.C. Zhang, T.M. Rice, Phys. Rev. B **37**, 3759 (1988)
109. M. Schluter, M.S. Hybertsen, Physica (Amsterdam) **162C–164C**, 583 (1989)
110. M.S. Hybertsen, E.B. Stechel, M. Schluter, D.R. Jennison, Phys. Rev. B **41**, 11068 (1990)
111. R.E. Cohen, W.E. Pickett, L.L. Boyer, H. Krakahuer, Phys. Rev. Lett. **60**, 817 (1988)
112. R.E. Cohen, W.E. Pickett, H. Krakahuer, Phys. Rev. Lett. **62**, 831 (1989)
113. R.E. Cohen, W.E. Pickett, H. Krakahuer, Phys. Rev. Lett. **64**, 2575 (1990)
114. W.E. Pickett, R.E. Cohen, H. Krakauer, Phys. Rev. Lett. **67**, 228 (1991)