

Electronic dynamics under effect of a nonlinear Morse interaction and a static electric field

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Abstract. In this work we study the one-electron dynamics in a one-dimension alloy in which atoms are coupled by a Morse potential. In our model, we consider the presence of a static electric field parallel to chain. Our formalism consists of a quantum mechanics treatment for the electron transport and a classical Hamiltonian model of lattice vibrations. We also introduce an electron-lattice interaction by considering electron hop between neighboring atoms as a function of its effective distance. We solve numerically the dynamic equations for the electron and lattice performing calculations for the spreading of an initially localized electronic wave-packet. We report numerical evidences of the existence of a pair soliton-electron even at the presence of electric field. We offer a detailed analysis of the dependence of this electron-soliton pair according to the magnitude of the electric field and the electron-phonon interaction.

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1. Introduction

The problem concerning the time-dependent behavior of an initially localized electronic wave-packet has a direct connection with the electrical properties of materials [1, 2, 3, 4, 5, 6]. The seminal works of Anderson and several co-workers have shown that the presence of disorder is a key factor governing the extension of the wave function [7]. It was demonstrated that in a disordered system with dimensions below two, all eigenstates are localized in a finite fraction of the system, even in the case of weak disorder degree. The Anderson localization has been developed in the electronic context, however such prediction is still valid for every field described by a wave equation. In fact, the Anderson localization of electromagnetic fields [8], water waves [9] and Bose-Einstein Condensates (BEC) [10] has been reported in the literature. Within the context of BEC, we emphasize that its dynamics is well described by the Gross-Pitaevskii equation [11] and the nonlinearity present in this equation reveals exciting new physical properties [12, 13, 14]. It is instructive to point out that, even within the electronic context, nonlinearity

can also be present. It was shown that the interaction between electrons and optical phonons is well described by a nonlinear Schrödinger equation [14, 15]. One of the most interesting phenomenon associated to nonlinearity is the self trapping (ST), which occurs when the nonlinearity strength exceeds a critical value of order of the bandwidth [15, 16, 17, 18, 19, 20, 21]. When ST takes place, an initially localized wave-packet does not spread over the system, remaining localized around its initial position. In a wider sense, transport properties in nonlinear lattices acquired a expressive interest by the solid state community as well as within the nonlinear science field [22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61]. Davydov [41, 42, 43, 44, 45] came up with the idea that the electron-lattice nonlinear term can promote charge transport. The Davidov mechanism is a consequence of nonlinear interaction between a linear electronic model and a linear lattice dynamically described by a soliton-bearing equation. Moreover, in refs. [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57] M.G. Velarde and co-workers demonstrated the existence of a *polaron-soliton* "quasi-particle" in nonlinear lattices and also have emphasized its importance to the carry charge. The coupling of self-trapped states (polaron states) with the lattice solitons has been generally termed as a *solectron* [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57]. We emphasize that the *solectron* theory represents a interesting generalization of the original polaron concept that can mediate non-Ohmic supersonic electric conduction [54]. The electronic transport mediated by nonlinear effects was investigated in several two-dimensional anharmonic lattices, particularly in a square lattice similar to the cuprate lattice [57]. It was found numerical evidence of the electron-soliton transfer along crystallographic axes.

From an experimental point of view, a very interesting advance within the context of electron transport mediated by lattice effect was achieved by R.McNeil and co-workers in ref. [62]. Roughly, the researchers have moved a single electron along a wire, batting it back and forth, rather like the ball in a game of ping-pong [62]. The authors pointed out the possibility of use this "controlled motion" within the framework of quantum computing, for example, moving a quantum 'bit' between two far from places [62]. The above experiment consisted in trapping a single electron in a quantum dot and move this electron around a channel using a surface acoustic wave (SAW). The authors obtained up to 60 shots with a good quality. The possibility of use SAW to move electrons and construct quantum bits has attracted a intense interest [63, 64, 65, 66].

Besides of the fundamental framework about the electronic transport under effect of nonlinearity, the interaction with a static electric field has also attracted the interest of scientific community. It is well known that, at the absence of nonlinearity, a static electric field applied parallel to a periodic lattice promotes the dynamic localization of a given initial wave-packet. Furthermore, the presence of static electric field gives rise to an oscillatory behavior of the electron wave packet (also called " Bloch oscillations") [67]. The size of the region over which the electron oscillates and the period of these oscillations are inversely proportional to the magnitude of the static electric field.

In this work we will make a contribution by going forward on the understanding of electronic transport in low-dimensional nonlinear systems under effect of uniform electric field. We study numerically the one-electron dynamics in a one-dimension alloy in which that the atoms are coupled by a Morse potential. In addition, we consider a static electric field parallel to chain. Within our model, the electron transport is treated quantum-mechanically over the alloy in tight-binding approximation and the longitudinal vibrations of the lattice are described by using classical formalism. The electron-phonon interaction was introduced by considering the electron hopping as a function of the effective distance between neighboring atoms. By solving numerically dynamic equations for electron and lattice we can compute the spreading of an initially localized electronic wave-packet. We report numerical evidences of the existence of an electron-soliton pair even at the presence of electric field. We offer a detailed analysis of the dependence of this electron-soliton pair with the magnitude of the electric field and the electron-phonon interaction.

2. Model and Numerical Calculation

In our work, we consider a one-electron moving in a $1d$ anharmonic lattice of N masses under effect of a static electric field. The complete Hamiltonian for the electron and lattice can be written as $H = H_{\text{lattice}} + H_e$ where H_e is the one electron Hamiltonian defined as [46, 47, 48, 49, 50, 51, 52, 53, 54]:

$$H_e = \sum_n [eE(n - N/2)(D_n^\dagger D_n)] + \sum_n V_{n+1,n}(D_{n+1}^\dagger D_n). \quad (1)$$

and H_{lattice} represent the classical Hamiltonian considering the nearest neighbor sites coupled by the Morse Potential:

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

Here, D_n^\dagger and D_n are the creation and annihilation operators for the electron at site n . eE represent the electric force. V_n is the hopping amplitude. p_n and q_n define the momentum and displacement of the mass at site (n). In our work we will consider all masses identical with $m_n = 1$. Here we will follow refs. [46, 47, 48, 49, 50, 51, 52, 53, 54] on the interaction between the electron and the vibrational modes. It will be considered in our model by relating the electronic parameters $V_{n+1,n}$ with displacements of molecular masses from their equilibrium positions. The hopping elements $V_{n+1,n}$ will depend on the relative distance between two consecutive molecules on the chain as : $V_{n+1,n} = -V \exp[-\alpha(q_{n+1} - q_n)]$. The quantity α will represent the degree of relationship of relative displacement of lattice units on the hopping term $V_{n+1,n}$, or in other words, it determines the electron-lattice coupling strength. For small relative displacement we recover the Su, Schrieffer, Heeger approximation $V_{n+1,n} \approx -V[1 - \alpha(q_{n+1} - q_n)]$. The time-dependent wave-function $|\Phi(t)\rangle = \sum_n f_n(t)|n\rangle$ is obtained by numerical solution of the time-dependent Schrödinger equation. We

consider the electron initially localized at site $N/2$, i.e. $|\Phi(t=0)\rangle = \sum_n f_n(t=0)|n\rangle$, where $f_n(t=0) = \delta_{n,N/2}$. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$)

$$i\frac{df_n(t)}{dt} = [F(n - N/2)]f_n(t) - \tau \exp[-\alpha(q_{n+1} - q_n)]f_{n+1}(t) - \tau \exp[-\alpha(q_n - q_{n-1})]f_{n-1}(t) \quad (3)$$

Lattice equation can be written as

$$\begin{aligned} \frac{d^2q_n(t)}{dt^2} = & \{1 - \exp[-(q_{n+1} - q_n)]\}\exp[-(q_{n+1} - q_n)] \\ & - \{1 - \exp[-(q_n - q_{n-1})]\}\exp[-(q_n - q_{n-1})] \\ & - \alpha V \{(f_{n+1}^* f_n + f_{n+1} f_n^*)\exp[-(q_{n+1} - q_n)] \\ & - (f_n^* f_{n-1} + f_n f_{n-1}^*)\exp[-(q_n - q_{n-1})]\} \end{aligned} \quad (4)$$

We have used the formalism defined in ref. [46]. Here $\tau = V/(\hbar\Omega)$, where Ω is the frequency of harmonic oscillations around the minimum of the Morse potential. The generalized hopping τ determines the time scale difference between the fast electronic dynamics and the slow lattice vibrations. F is a generalized electric field in dimensionless scale (electric charge, lattice parameter and \hbar all quantities equal to one). Our calculations are made by using precise numerical solution of the previous eqs. 3 and 4. The equations of electron motion (eq. 3) will be solved numerically employing a high-order method based on the Taylor expansion of time evolution operator $U(\delta t)$ [60, 68]:

$$U(\delta t) = \exp(-i\tilde{H}_e\delta t) = 1 + \sum_{l=1}^{n_o} \frac{(-i\tilde{H}_e\delta t)^l}{l!} \quad (5)$$

where \tilde{H}_e is exactly the same one electron Hamiltonian (eq. 1) with normalized hopping $\tilde{V}_{n+1,n} = -\tau \exp[-\alpha(q_{n+1} - q_n)]$. The wave-function at time δt is given by $|\Phi(\delta t)\rangle = U(\delta t)|\Phi(t=0)\rangle$. The method can be used recursively to get the wave-function at time t . To obtain $\tilde{H}_e^l|\Phi(t=0)\rangle$, we used a recursive formula derived as follows. Let $\tilde{H}_e^l|\Phi(t=0)\rangle = \sum_n D_n^l|n\rangle$. Using the Hamiltonian formula (eq. 1) we compute $\tilde{H}_e^1|\Phi(t=0)\rangle$ and we have D_n^1 as

$$\begin{aligned} D_n^1 = & [F(n - N/2)]f_n(t=0) \\ & - \{\tau \exp[-\alpha(q_{n+1} - q_n)]\}f_{n+1}(t=0) \\ & - \{\tau \exp[-\alpha(q_n - q_{n-1})]\}f_{n-1}(t=0) \end{aligned} \quad (6)$$

Therefore, using $\tilde{H}_e^l|\Phi(t=0)\rangle = \tilde{H}_e \sum_n D_n^{l-1}|n\rangle$, D_n^l can be obtained recursively as

$$\begin{aligned} D_n^l = & [F(n - N/2)]D_n^{l-1}(t=0) \\ & - \{\tau \exp[-\alpha(q_{n+1} - q_n)]\}D_{n+1}^{l-1}(t=0) \\ & - \{\tau \exp[-\alpha(q_n - q_{n-1})]\}D_{n-1}^{l-1}(t=0), \end{aligned} \quad (7)$$

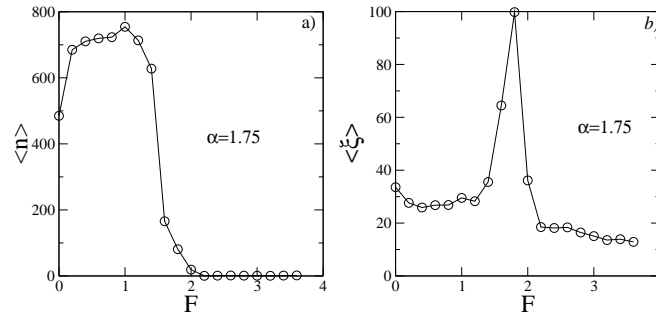


Figure 1. a) Electron mean position (centroid) (a) and participation number (b) for long time versus electric field magnitude F .

The classical equations (eq. 4) will be solved by using a second order Euler method [69]: The procedure starts by using a standard Euler method in order to find a prediction $q_n(\delta t)^*$ at the time δt :

$$q_n(\delta t)^* \approx q_n(t=0) + \delta t \left. \frac{dq_n}{dt} \right|_{t=0} \quad (8)$$

The next step consists of applying a correction formula to find a better approximation to $q_n(t + \delta t)$

$$q_n(\delta t) \approx q_n(t=0) + \frac{\delta t}{2} \left[\left. \frac{dq_n}{dt} \right|_{t=0} + \left. \frac{dq_n^*}{dt} \right|_{\delta t} \right] \quad (9)$$

The above method (eq.8 and 9) can be used recursively to reach $q_n(t)$. The following results were taken by using $\delta t = 10^{-3}$ and the sum of eq. 5 was truncated about $n_o = 15$. We could keep the wave-function norm within the following numerical tolerance: $|1 - \sum_n |f_n(t)|^2| < 10^{-7}$ along the entire time interval. Also, we computed some typical quantities which describes electronic transport on this nonlinear model, namely, mean position (centroid) and participation function. Centroid and participation function are defined as [60, 70]

$$\langle n(t) \rangle = \sum_n (n - N/2) |f_n(t)|^2 \quad (10)$$

and

$$\xi(t) = 1 / \sum_n |f_n(t)|^4. \quad (11)$$

respectively.

The centroid for a given time t represents the mean position of the electron using the center of a self-expanded chain as the origin. The participation function gives an estimate of the number of sites under which the wave packet is spread at time t .

3. Results and Discussions

We initially emphasize that in our calculations the time evolution of a initially localized wave-packet was obtained by using numerical solution of quantum and classical

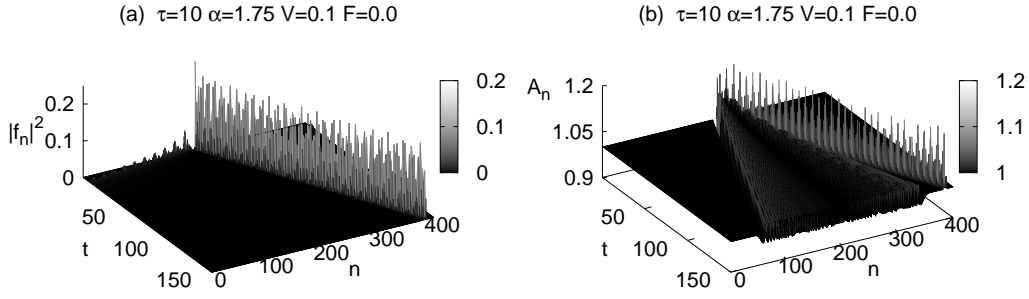


Figure 2. (a) Square wave-function component $|f_n|^2$ versus t and n for $\alpha = 1.75, \tau = 10, V = 0.1$ and $F = 0$. (b) Lattice deformation A_n for the same case in (a).

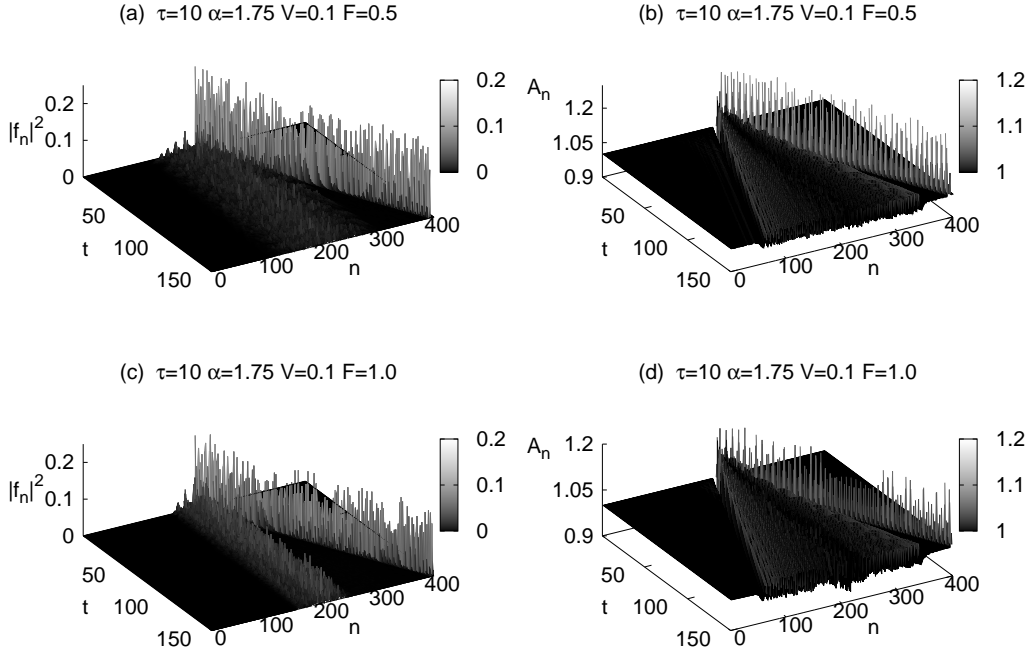


Figure 3. (a,c) Square wave-function component $|f_n|^2$ versus t and n for $\alpha = 1.75, \tau = 10, V = 0.1$ and $F = 0.5, 1$. (b,d) Lattice deformation A_n for the same cases respectively in (a,c).

equations. We considered the electron fully localized at the center of a self-expanding chain (i.e. $\{f_n(t=0) = \delta_{n,N/2}\}$). The self-expanding chain was used to minimize border effects; whenever the probability of finding the electron or the atomic vibration at the ends of the chain exceeded 10^{-30} , ten new sites were added to each edge. The lattice was initialized by using the following initial excitation : $p_n = \delta_{n,N/2}, a_n = 0$. The numerical convergence of our calculations was ensured by checking the conservation of the norm of the wave-packet at every time step; our results provide $|1 - \sum_n |f_n(t)|^2| < 10^{-7}$ for

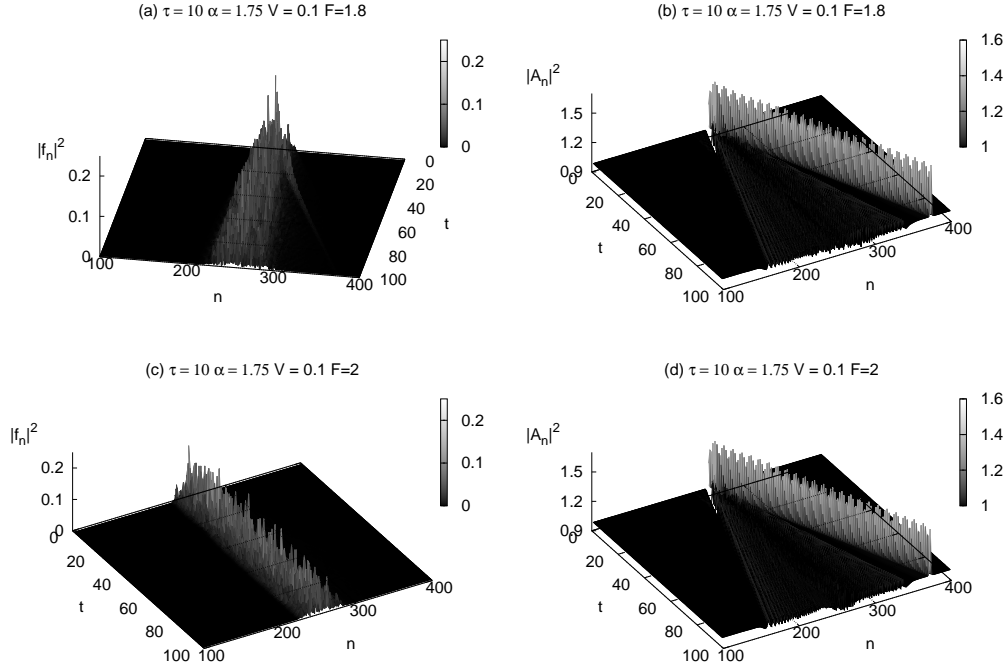


Figure 4. (a,c) Square wave-function component $|f_n|^2$ versus t and n for $\alpha = 1.75, \tau = 10, V = 0.1$ and $F = 1.8, 2$. (b,d) Lattice deformation A_n for the same cases respectively in (a,c).

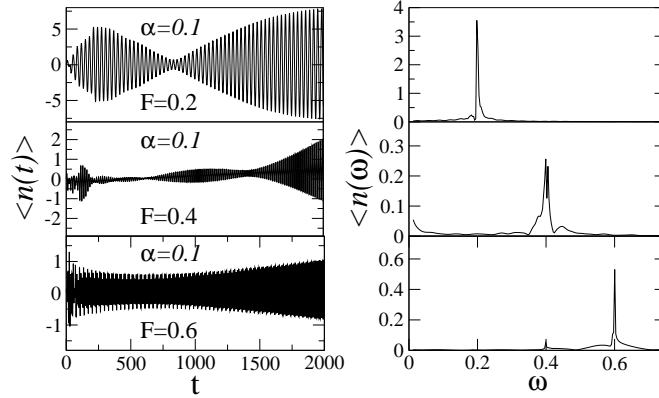


Figure 5. Left panel: the electron centroid for $\alpha = 0.1$ and $F = 0.2, 0.4, 0.6$. Right panel: The Fourier transform $\langle n(\omega) \rangle$ of the centroid for the same cases showed in left panel. We observe that for all electric field considered, the electron position exhibits a Bloch-like oscillatory behavior with frequency ($\omega \approx F$).

all times considered. In our work we will considered exactly the same case which was studied in refs. [46, 47]: $\tau = 10, \alpha = 1.75$ and $V = 0.1$. In figure 1(a) we show the long time behavior of the mean position ($\langle n \rangle$) versus the magnitude of electric field F . We emphasize that $\langle n \rangle$ was computed as the average of $\langle n(t) \rangle$ at long time limit : $\langle n \rangle = (\sum_{t=0.8t_{max}}^{t_{max}} \langle n(t) \rangle) / N_{times}$ (here $t_{max} = 2 \times 10^3$). For the electric field

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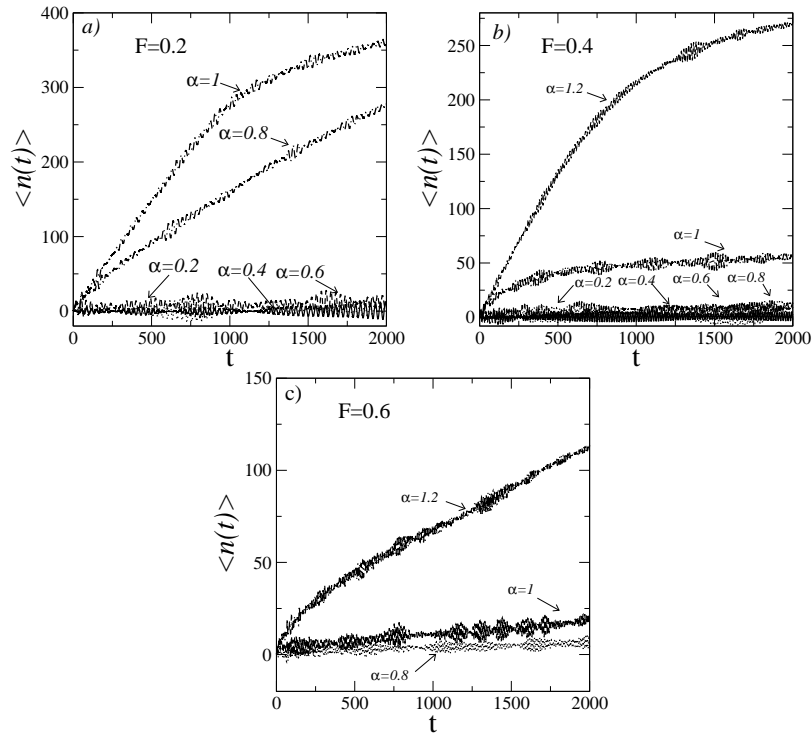


Figure 6. Electronic centroid $\langle n(t) \rangle$ versus time for $F = 0.2, 0.4, 0.6$ and several values of electron-phonon coupling α . We observe that for each electric field considered there is a specific value of α that separates the phase in which that the electron exhibit a Bloch-like oscillation behavior and the phase with the electron-soliton pair formation.

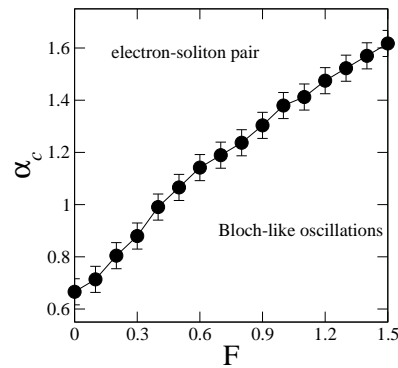


Figure 7. The phase diagram $\alpha_c \times F$ in order to characterize the (Bloch-like oscillation)/(electron-soliton pair) transition.

within the interval ($F < 2.$), we observe that $\langle n \rangle$ is large thus suggesting that the electron still moves along the chain. However, outside this interval, the electron remains trapped around the initial position. Although this result seem simple, there is a more complicated phenomenology behind this calculations. Formally, when a static electric field is applied parallel to chain, the electron should remain trapped around the initial position performing an oscillatory behavior with frequency equal to magnitude of electric

field (Bloch-Oscillation). In our case we observe that the competition between the static electric field and the electron-soliton term seem to break down the phenomenology of the Bloch-Oscillations. For $F > 2$ the electron becomes trapped around the initial position even at the presence of electron-soliton term. The fig. 1(b) shows the long term mean participation number $\langle \xi \rangle = (\sum_{t=0.8t_{max}}^{t_{max}} \langle \xi(t) \rangle) / N_{times}$ versus the electric field F . We observe that for all electric fields values considered the participation number is small, thus signaling the trapped character of the electron wave-packet. We will return to discuss particularly the behavior of the participation number at the end of paper. For now, we are able to comment that for $F \leq 2$ the electron is trapped by the solitonic modes that exists within the chain. For $F > 2$, the electric field effect is dominant and keeps the electron trapped around the initial position. For the electric field within the interval ($1.5 < F < 2$) we found a crossover region in which that a finite fraction of the wave-function remains trapped around the initial position and an another small part participate in the electron-soliton dynamics. This crossover effect increases the participation number (as we can observe for example in figure 1(b) for $F \approx 1.8$). We get a major comprehension of electronic behavior for ($F \leq 2$) by analyzing the wave-packet profile and lattice deformation.

In figure 2(a) we plot the electronic wave-function at the $n \times t \times |f_n|^2$ plane as well as in (b) the lattice deformation in the $n \times t \times A_n$ plane where $A_n = \exp[-q_n - q_{n-1}]$ at the absence of electric field ($F = 0$). We observe that the wave-function remains trapped in a finite fraction of lattice. In addition, we notice that the localized electronic wave-packet is moving along the chain in good agreement with the centroid results showed in Fig. 1(a)). The results for the deformation A_n reveals that the initial energy propagates along the classical chain in a solitonic state. Our calculations for $F = 0$ are in accordance with the previous works of M.G. Velarde [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57] where this kind of electron-soliton pair was reported at the first time. For $F \neq 0$ the results of wave-packet and the lattice deformation can be found in fig. 3 and 4. We observe in fig.3 for $F = 0.5, 1$ that the wave function is divided in two parts: one moves along the chain and the other (the smallest part) remains trapped around initial position. Therefore, for weak electric field, the solitonic mode can still trap a finite fraction of wave-packet and drag it along the chain. We can also observe that the lattice deformation A_n still exhibit a solitonic behavior. However, this soliton also exhibits some losses in its magnitude and we can see a initial spread of the deforming wave along the chain. In fig.4 we plot our results for $F = 1.8$ and 2. For $F = 1.8$, the most part of the wave-function remains trapped around the initial position. However, a small part of the initial wave-packet seems to be still captured by the solitonic modes. The configuration found for $1.5 < F < 2$ is just the opposite of the behavior for $F = 0.5, 1$. (see figure. 3) where the majoritary part of the wave-packet remains trapped by the solitonic mode. This behavior is the key ingredient behind the increasing of the participation number for $F = 1.8$ (see fig. 1(b)). Our results suggests that for $F \lesssim 1.5$, there is the possibility of electron-soliton pair due to the Morse interaction and the electron-phonon coupling. For $F > 2$ the electron become localized around the initial position for this degree

of electron-phonon coupling. We emphasize that the electron-phonon term $\alpha = 1.75$ considered in the previous results is a reasonable amount of electron-lattice interaction as was pointed out in ref. [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57]. Moreover, this value is quite close of the higher values of α we have considered. We will discuss more about the electron-phonon interaction values at the end of this work. The region with $1.5 < F < 2$ represents an anomalous crossover region in which that the electron-phonon term is not sufficient to promotes the capture of the electron by the solitonic mode, remaining a largest fraction of the wave-packet around lattice center.

The main conclusion of the previous figures is that, within the framework of a one-electron subjected to a static electric field and the electron-phonon coupling, the interaction with the nonlinear lattice vibrations plays the dominant rules. We will analyze in more detail this competition between the electric field and the electron-phonon coupling following a systematic procedure. We will analyze critical value of electron-phonon interaction (α_c) necessary to promote the electron-soliton pair formation under the effect of a static electric field. In fig. 5 (left panel) we plot the electron position for $\alpha = 0.1$ and $F = 0.2, 0.4, 0.6$. We can observe that for all electric field considered, the electron exhibits a oscillatory behavior quite compatible with the well know Bloch oscillations phenomenon. In fig. 5 (right panel), we plot the Fourier transform $\langle n(\omega) \rangle$ of the mean centroid. In good agreement with the semi-classical approach, the main frequency value is around the generalized electric field magnitude ($\omega \approx F$). It is a clear signature that for a weak electron-phonon interaction, the electric field can trap the electron wave-function and promotes a coherent (or quasi-coherent) Bloch-like oscillatory mainframe. We emphasize that, in our model, the electronic hopping, even for weak electron-phonon coupling, changes slightly along the chain thus promoting a weak absence of periodicity that can "destroy" the Bloch oscillations for sufficient long-times. We will analyze now the electron-phonon threshold necessary to promotes the electron-soliton pair formation. In figures 6(a-c) we plot the electronic centroid $\langle n(t) \rangle$ versus times for $F = 0.2, 0.4, 0.6$ and several values of electron-phonon coupling α . We observe that for each electric field value there is a specific values of α that separates the Bloch-like oscillation phase and the electron-soliton pair phase. Therefore, we will provide in figure 7 a phase diagram $\alpha_c \times F$ in order to characterize the (Bloch-like oscillation)/(electron-solliton pair) transition. Our calculations suggest that, even for a zero electric field there is a minimum value of the nonlinearity ($\alpha_c \approx 0.65$) necessary to bind the electron to the solitonic modes of the chain. We also observe that, as the electric field value F is increased, the critical electron-phonon value α_c also increases. In spite of we do not have any formal demonstration for this phase diagram, it is quite intuitive. At the absence of electric field, the electron becomes free to move in a crystalline chain, thus, we did not expect that values of α slightly larger than zero would be enough to promote pair formation. For $F \neq 0$ the dynamics localization in general takes place. The interaction of the electron with the static electric field promotes the appearance of linear potential energy that trap the electron around the initial position and induce the Bloch-oscillations. As the electric field increases, it becomes more difficult to the

electron-phonon term capture a large fraction of electron wave, thus α_c should increase also (as we can observe in fig. 7). For $F > 2$ the electron becomes roughly trapped and the electron-phonon coupling, within our numerical accuracy, can not promotes the pair formation. For the electric field within the interval ($1.5 < F < 2$), as it was described previously, we found a crossover region in which a larger fraction of the wave-function remains trapped around the initial position and a small part join the electron-soliton dynamics. In our calculations we have found good accuracy until $\alpha \approx 2$. Maybe, it is possible that, for the electron-phonon couplings larger than $\alpha = 2$, electron-soliton pair formation could happen also for $F > 1.5$. However, it is complicated to solve with good accuracy the set of quantum/classical equations for large electric field and electron-phonon interaction.

4. Conclusions

In this work we studied the one-electron dynamics in a one-dimension Morse model considering a static electric field applied parallel to chain. Besides, we have considered electron dynamics by using a quantum-mechanical formalism and longitudinal vibrations of the lattice were described by using standard classical theory. The electron-phonon interaction was introduced by considering the hopping between neighboring sites dependent on their effective distance. By solving numerically the equations for electron and lattice we compute the dynamics of an initially localized electronic wave-packet. Our results can be summarized as follows: For weak electric field our calculations reveals evidence of existence of a electron-soliton pair . We also found, for numerical means, that the electron-phonon coupling dominates the dynamics, thus destroying the Bloch-Oscillation phenomenon. For strong electric field, the wave-packet remains trapped around the initial position. The solitonic lattice deformations exhibits small losses and remains trapped due to the electric field competitive effect. We also have analyzed in more detail the competition between the electric field and the electron-phonon coupling by examining the critical value of electron-phonon interaction necessary to promote the electron-soliton pair formation under the effect of a static electric field. By following a systematic and accuracy procedure we provide a phase diagram in order to characterize the dependence of the critical electron-phonon interaction values with the electric field intensity. We hope our work stimulates further investigations along these lines.

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