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

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ABSTRACT

Considering non-interacting electrons in a one-dimension alloy in which atoms are coupled by a Morse potential, we study the system dynamics in the presence of a static electric field. Calculations are performed assuming a quantum mechanical treatment for the electronic transport and a classical Hamiltonian model for the lattice vibrations. We report numerical evidence of the existence of a soliton–electron pair, even when the electric field is turned on, and we offer a description of how the existence of such a phase depends on the magnitude of the electric field and the electron–phonon interaction.

1. Introduction

The issue concerning the time-dependent behavior of an initially localized electronic wave-packet has a direct connection with the electrical properties of materials [1–6]. The seminal works of Anderson and other co-workers have shown that the presence of disorder is a key factor governing the extension of the wave function [7–10]. They demonstrated that in a disordered system with dimension $d \leq 2$, all eigenstates become localized in a finite fraction of the system, even in the case of weak disorder. The Anderson localization theory has been developed for electrons. However, such a prediction is valid for any field described by a wave equation. Examples for electromagnetic fields [11], water waves [12] and Bose–Einstein Condensates (BEC) [13] have been reported in the literature. Within the context of BEC, we emphasize that its dynamics is well described by the Gross–Pitaevskii equation [14], and the nonlinearity present in this equation reveals exciting new physical properties [15–17].

Nonlinearity can also be found in electronic systems. Some authors [18] have shown that the interaction between electrons and optical phonons is well described by a nonlinear Schrödinger equation. An interesting nonlinear phenomenon, called self trapping (ST), occurs when the nonlinearity strength exceeds the magnitude of the electronic bandwidth [19–26]. 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 have attracted a great deal of interest among the solid state community, as well as within the nonlinear science field [27–74]. Davydov [55–59] came up with the idea

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that the electron–lattice nonlinear term can promote charge transport. That mechanism is a consequence of the nonlinear interaction between a linear electronic model and a linear lattice, whose dynamics are described by a soliton-bearing equation.

Moreover, in [60–71], Velarde and co-workers have shown the existence of a polaron-soliton "quasi-particle" in nonlinear lattices, and also its importance to the charge carry. The coupling of self-trapped states (polaron states) with the lattice solitons has been generally termed as a solectron [60–71]. We highlight that solectron theory represents a generalization of the original polaron concept that is able to mediate non-Ohmic supersonic electric conduction [68]. The electronic transport mediated by nonlinear effects has been investigated in several two-dimensional anharmonic lattices, particularly in a square lattice similar to the cuprate lattice [71]. They found numerical evidence of electron–soliton transfer along the crystallographic axis.

McNeil and co-workers in ref. [75] provided an interesting experimental advance in electron transport. They were able to move a single electron along a wire, batting it back and forth, like the ball in a ping-pong game. The possibility of using this "controlled motion" within the framework of quantum computing, for example, to move a quantum 'bit' between two far places, was noted. This experiment consisted of trapping a single electron in a quantum dot and moving 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 using SAW to move electrons and to construct quantum bits has attracted the attention of the scientific community [76–82].

It is well known that, in 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 a static electric field gives rise to an oscillatory behavior of the electron wave packet (also called "Bloch oscillations") [83]. 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. It is worth mentioning that the effect of an electric field in linear chains of molecules was also studied in [84]. These workers considered the Holstein Hamiltonian under the effect of an electric field. Within the Holstein formalism, the lattice is harmonic and the charge becomes trapped due to the presence of a diagonal term related to the lattice oscillations. In particular, they studied the Bloch oscillations of the trapped state and their association with the electron–phonon coupling.

In this work, we push forward the understanding of electronic transport in low-dimensional nonlinear systems under the effect of a uniform electric field. We develop a numerical study of the non-interacting electron dynamics in a one-dimension alloy where the nearest neighbor atoms are coupled by a Morse potential. In addition, we assume a static electric field parallel to the chain. In such a model, the electron transport is treated quantum-mechanically over the alloy in the tight-binding approximation, and the longitudinal vibrations of the lattice are described using a classical formalism. The electron–phonon interaction is introduced by considering electron hopping as a function of the effective distance between neighboring atoms. By solving numerically the dynamic equations for both the electron and the lattice vibrations, we compute the spreading of an initially localized electronic wave-packet. We report numerical evidence of the existence of an electron–soliton pair, even for the presence of a static electric field. We offer a detailed analysis of the dependence of this electron–soliton pair on the magnitude of the electric field and the electron–phonon interaction.

2. Model and numerical calculation

In our work, we consider one electron moving in a $1d$ anharmonic lattice of N masses under the influence of a static electric field. Our formalism consists of two parts: a quantum Hamiltonian to treat the electron dynamics, and a classical anharmonic Hamiltonian in order to account for the atomic vibrations. The electronic Hamiltonian H_e is defined as [54]:

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

It is a typical one-electron Hamiltonian under the effect of a static electric field E . Here, $D_n^\dagger$ and D_n are the creation and annihilation operators for the electron at site n. eE represents the electric force on the electron of charge e. $(n - N/2)eE$ is the potential energy due to the coupling between the electron and the static electric field E. In order to avoid dealing with large variations in the magnitude of energy along the chain, we shift to zero the potential energy on the center of the lattice by including the constant $-eEN/2$. This is a simple and useful trick that decreases the absolute values of the potential energy, thus improving the numerical stability of our calculations. V_n is the hopping amplitude.

The atomic lattice in our work is defined by a classical Hamiltonian H_{lattice} that considers the nearest neighbor sites coupled by the Morse Potential [52,54]:

$$H_{\text{lattice}} = \sum_n \frac{p_n^2}{2m_n} + C_1\{1 - \exp[-C_2(q_n - q_{n-1})]\}^2. \tag{2}$$

where p_n and q_n are the momentum and displacement of the mass at site n, respectively. C_1 represents the typical energy of a bond and C_2 is the range parameter of the Morse potential [52,54]. We set $m_n = 1$ and we obtain a dimensionless representation of the quantities q_n, p_n, H by absorbing the constants C_1 and C_2 according to [52,54] : $q_n \to C_2 q_n$; $p_n \to p_n/\sqrt{2C_1}$ and $H_{\text{lattice}} \to H_{\text{lattice}}/(2C_1)$.

Here we follow [52,54] on the interaction between the electron and the vibrational modes. This is considered in our model by relating the electronic parameters $V_{n+1,n}$ to the displacements of the molecular masses from their equilibrium positions. The hopping elements $V_{n+1,n}$ depend on the relative distance between two consecutive molecules of the chain