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Wave packet dynamics under effect of a pulsed electric field

A.R.C.B. da Silva, F.A.B.F. de Moura, W.S. Dias

Instituto de Física, Universidade Federal de Alagoas, 57072-970 Maceió, AL, Brazil

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ABSTRACT

We studied the dynamics of an electron in a crystalline one-dimensional model under effect of a time-dependent Gaussian field. The time evolution of an initially Gaussian wave packet it was obtained through the numerical solution of the time-dependent Schrödinger equation. Our analysis consists of computing the electronic centroid as well as the mean square displacement. We observe that the electrical pulse is able to promote a special kind of displacement along the chain. We demonstrated a direct relation between the group velocity of the wave packet and the applied electrical pulses. We compare those numerical calculations with a semi-classical approach.

1. Introduction

The dynamics of a quantum wave-packet on a one-dimensional model under effect of an electric field is a hot topic with several applications in general solid state physics [1–21]. Originally studied by Bloch and Zener about 70 years ago, the most famous phenomenology was obtained by investigating the effect of a constant electric field (DC) under the electronic dynamics in crystalline systems. The main result is the existence of a coherent oscillatory motion with frequency equal to intensity of the static electric field, also called Bloch Oscillations (BO). The experimental observation it was achieved in semiconductor super-lattices only in the nineties [2]. Due to technological advances, BOs have been experimentally studied in other systems, such as Bose–Einstein condensates [3], ultra-cold atoms [4] and optical super-lattices [5]. Within the theoretical point of view , an interesting analysis about the motion of a charged particle on a lattice in the presence of a generic electric field it was done in ref. [8]. The authors demonstrated the presence of a dynamic localization whenever the ratio of the magnitude and the frequency of the electric field is a root of the ordinary Bessel function of order [8]. The effect of scattering caused by imperfections of the lattice it was considered in ref. [9]. In ref. [11] it was shown a detailed analysis of the coherent electronic dynamics under effect of electric static and time-periodic (AC) fields. The authors demonstrated the possibility of to "push" a Gaussian wave-packet by using a oscillating field with frequency tuned at the Bloch frequency [11]. Recently, the properties of Bloch-oscillations in non-Hermitian lattices with a non-vanishing imaginary part of the band dispersion curve it was investigated in ref. [12]. The authors demonstrated by using a generalized acceleration theorem that a wave packet with narrow spectral distribution undergoes a periodic motion, but following a closed orbit in the complex plane. The competition between electron–electron interaction, electric field effect and dissipation terms it was studied in ref. [13]. By using the Keldysh Greens functions in cluster perturbation theory, the steady-state current it was computed. The authors demonstrated that the current properties are controlled by the Wannier-Stark resonances due to anti-ferromagnetic correlations [13].

The effect of the on-site Hubbard interaction U on the Bloch oscillations of two electrons under effect of an external electric field was investigated in refs. [16–18]. By solving the time-dependent Schrödinger equation for an initially localized two-electron state it was proven that the possibility of the wave packet develops Bloch oscillations where the dominant frequency is the twice of the Bloch frequency predicted by semi-classical approach [17]. It was proposed that this effect is strongly related with the set of two-electron bound states that appear for $U > 0$. That hypothesis was investigated in detailed and proven in ref. [18]. Experimental investigations of Bloch oscillations in optical lattice and ring cavity were done in refs. [20,21]. By using interacting atoms in optical lattices, it was observed strongly correlated Bloch oscillations as well as correlations in two-particle quantum movement [21]. In special, the experiment conducted in ref. [21] proved the existence of Bloch oscillations with double frequency, previously obtained in ref. [17] through theoretical experiments.

In ref. [22] it was proposed that a superposition of a static field and a harmonic one can promote electronic dynamics in low-dimensional systems. It was also shown that the electronic velocity depends on the magnitudes of the AC and DC field

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components and the initial phase of the AC field. Transport over macroscopic distances has been recently reported in Bose-Einstein condensates with weak interaction in a tilted lattice under simultaneous influence of a DC and AC fields [23]. In this work we provide further studies about the specificity of the electronic dynamics under effect of time-dependent electric fields. We consider an electron moving in a regular one-dimensional(1D) lattice under effect of an external electric field $F(t)$. The external field consists of a Gaussian-pulse. We emphasize that pulsed external fields (including Gaussian–Pulses) have been used in several contexts of science [24–31]. For example, the effect of ultra short electric pulses on biological cells, tissues, and organs has attracted a great interest [29,30]. In our work, we will follow the time evolution of an initially Gaussian electronic wave packet under effect of an external Gaussian-electric pulse. We will compute typical tools that characterized the wave-packet dynamics along the chain, namely the electron's position and the mean-square displacement. Our calculations demonstrated an unusual electron dynamics quite related with the kind of pulse electric field we have considered. Our analysis suggests that the electrical pulse is able to promote a interesting electronic dynamics along the chain. Results revealed that the velocity of the particle can be controlled through the type electric pulses applied and it is possible to easily speed up or slow down the electron.

2. Time-dependent Schrödinger equation and formalism

Our model consists of an electron moving in a regular one-dimensional chain with N sites driven by an external field $F(t)$. The internal distance between the nearest neighbors is a. The tight-binding Hamiltonian that describe our model can be written as

$$H = J\sum_{n=1}^{N}(|n\rangle\langle n+1| + |n+1\rangle\langle n|)\sum_{n=1}^{N}(\epsilon_n - eF(t)na)|n\rangle\langle n|, \qquad (1)$$

where $|n\rangle$ is a Wannier state localized at site i with energy ϵ_n, J is the inter-site coupling restricted to nearest-neighbors, e is the particle charge. The temporal evolution of the wave-function components in the Wannier representation ($|\psi(t)\rangle = \sum_n \psi_n |n\rangle$) is governed by the time-dependent Schrödinger equation

$$i\dot{\psi}_n = \psi_{n+1} + \psi_{n-1} - eF(t)n\psi_n. \qquad (2)$$

Here, we will use units such that $\hbar = e = a = J = 1$. The on-site energies ϵ_n were taken as the reference energy ($\epsilon_n = 0$) and time is expressed in units of $\hbar/J$. The external field consists of a Gaussian-pulse [31], which can be expressed as

$$F(t) = B(\rho)\,\exp\left[-\frac{(t-\tau)^2}{4\rho^2}\right], \qquad (3)$$

where ρ controls the duration of each pulse and τ is the time of reference. We can observe that for a finite and small ρ and a single value of τ, $F(t)$ represent a single pulse around $t \approx \tau$. We are interested in consider a collections of pulses, i.e., we will consider some distinct values of τ. The above set of equations were solved numerically by using fourth order Runge–Kutta method with step-size about 10^{-4} in order to to keep the wave-function norm conservation ($1 - \sum_n |\psi_n(t)|^2 \le 10^{-13}$) along the entire time interval considered. The initial wave-packet will be consider a Gaussian wave packet with width σ defined as

$$\psi_n(t=0) = \frac{1}{A(\sigma)}\exp\left[-\frac{(n-n_0)^2}{4\sigma^2}\right], \qquad (4)$$

where the initial position of the particle (n_0) is the center of chain (i.e $n_0 = N/2$). After solving the set of equations we will compute the centroid $\overline{x}(t)$ and the mean-square displacement $\xi(t)$ i.e., typical quantities that can bring information about the eigenstates and wave-packet time-evolution. These tools are defined as:

$$\overline{x}(t) = \sum_n n|\psi_n(t)|^2, \qquad (5)$$

and

$$\xi(t) = \sqrt{\sum_n [n - \overline{x}(t)]^2 |\psi_n(t)|^2} \qquad (6)$$

The centroid $\overline{x}(t)$ represent the electronic position and $\xi(t)$ is a measurement of the spread of the wave-function. We will also analyzing the wave-function profile $|\psi_n(t)|^2$ versus t and n in order to understand better the effect of Gaussian-pulse electric field under the electronic dynamics.

3. Results

We will show initially our results for the temporal wave packet profile $|\psi_n(t)|^2$ versus t and n (see Fig. 1) . Calculations were done for N=400. The initial wave packet it was a Gaussian with $\sigma = 1.0$. In our first numerical experiment we have considered four electric pulses with $\rho = 1$, and $\tau = 10, 25, 45, 55$ time units. We adjusted the value of $B(\rho = 1)$ in order to impose that the impulse I of each pulse is given by: $I = \int_{-\infty}^{\infty} \mathbf{F}(t)\,dt = \pi/2$. In fig. 1 we observe the behavior of the electronic function in time and space. We note that in the early stages of temporal evolution ($t < 10$) the wave packet widens on the lattice. For short times, the electric field is absent and therefore the wave-function moves without any interaction. However, after the first pulse be applied, the wave packet seems to be "pushed " for one of the chain edges. We observe that this driven motion is stopped after the application of the second pulse (t=25). After the second pulse, the wave packet seems to develops movement with small (almost null) group velocity. We also observe a kind of ondulatory behavior. After the third pulse at t=45 a counter-intuitive behavior is observed. The particle restarts its movement however, in the opposite orientation. For t=55 time units, the wave packet is subjected to a new electric field pulse and an interruption of the particle movement can be observed again. This behavior can be understood following semi-classical

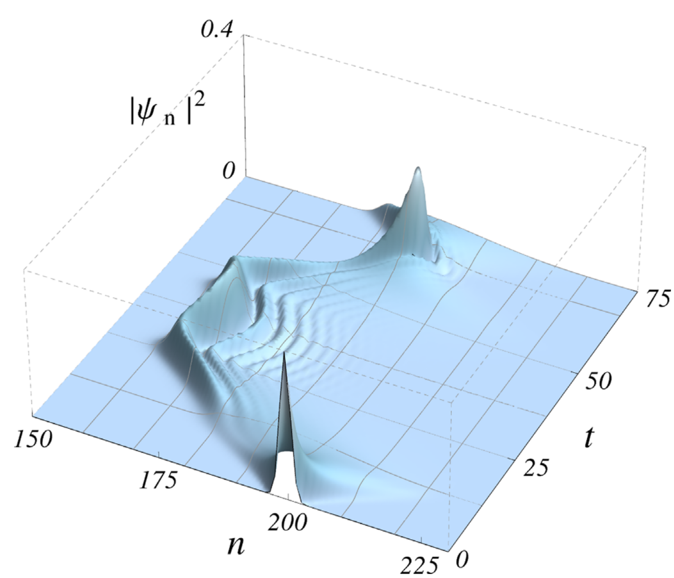

Fig. 1. (Color online) Time evolution of the wave packet with N=400 sites. The initial condition was a gaussian wave packet width $\sigma = 1.0$. We have used four pulses each one with impulses $I = \pi/2$. The pulses were applied at times $\tau = 10, 25, 45, 55$ time units.