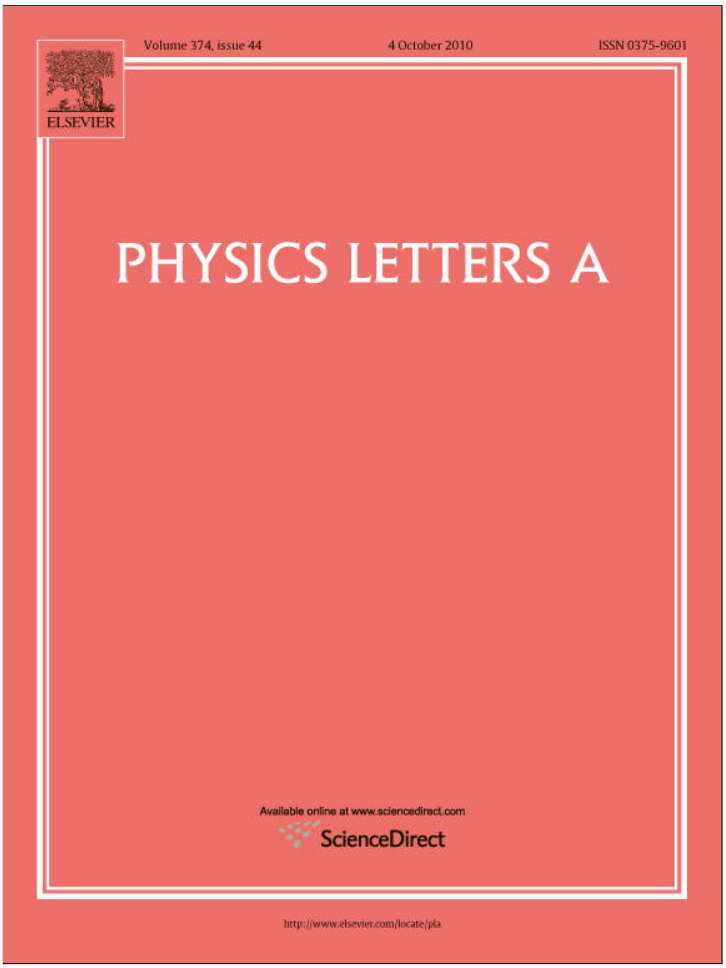

Physics Letters A 374 (2010) 4554–4558

Contents lists available at ScienceDirect

Physics Letters A

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The role of Hubbard-like interaction in the dynamics of two interacting electrons

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ARTICLE INFO

Article history:
Received 26 August 2010
Accepted 1 September 2010
Available online 6 September 2010
Communicated by V.M. Agranovich

Keywords:
Wave-packet dynamics
Bloch oscillation
Hubbard interaction

ABSTRACT

We study the effects of a Hubbard-like interaction on the dynamics of two electrons restricted to move in a linear chain. Our calculations suggest that the presence of bounded two-electron states in the initial Gaussian wave-packet plays significative roles on both unbiased and the electric-field biased wave-packet dynamics.

Advancing the understanding of the transport properties of interacting electrons in low dimensional systems usually consists of a step ahead in condensed matter theory. Usually, the presence of a Coulomb repulsion term ($U \propto e^2/r$) challenges the theoretical treatment of the many body Hamiltonians. However, the competitive electric forces and the presence of mobile charge carriers promote the damping of electric fields, also called screening. The resulting electronic interaction, called screened Coulomb potential, is exponentially damped. Therefore, from the quantum mechanics point of view an extremely short-ranged repulsive Coulomb interaction i.e., an effective on-site Coulomb repulsion U can be used to simulate the electron–electron interaction. The Hubbard model is the most used Hamiltonian model describing systems of itinerant electrons within the on-site electron–electron interaction framework. From the analytical point of view in the absence of on site disorder, the most remarkable development was introduced about 60th years through the exact solution of a one-dimensional (1D) model of interacting spinless bosons by Lieb [1]. By using a Bethe ansatz formalism, a complete solution in the absence of disorder was provided as a function of the interaction strength. For the infinite Coulomb interaction limit, the Lieb–Liniger model [1] showed that strongly interacting bosons effectively behave like noninteracting fermions, i.e. the well-known model of impenetrable bosons discussed by Girardeau [2]. Following the Bethe ansatz framework introduced in [1], the problem of N interacting fermions without disorder moving in 1D was solved by Lieb and other authors [3]. Furthermore, it was shown that Hubbard systems can display a correlation-driven transition, called Mott-transition, from a paramagnetic metal to a paramagnetic insulator [4–13]. Studies of the Hubbard model reveal a wealthy of new phenomena in low dimensional electronic systems. One of the most famous applications, pointed by Anderson, consists of the understanding of the mechanisms underlying the high-T_c superconductivity observed in CuO_2 compounds [11–13]. Even within the on-site Coulomb interaction formalism, the analytical or numerical study of many body systems represents a hard task due to the fact that the number of electronic configurations grows exponentially with the system size.

More recently, the competitive role between dynamical localization and electron–electron interaction was reported [14–18]. It was shown that the N-particle problem is identical to that of a single particle moving in an N-dimensional lattice, with defect surfaces dividing the space in symmetric domains. It has been shown that in the limit of weak hopping integral, the electron–electron interaction induces an additional oscillation of the eigenstates drift velocity. The period of this oscillation was found to be determined solely by the range and strength of the electron–electron interaction [14]. Furthermore, the two-electron problem on a one-dimensional lattice subject to a static electric field was revisited in Ref. [17]. It was numerically demonstrated the existence of a frequency doubling of the Bloch oscillations as a function of the two-electrons interaction. As the interaction is turned on, the emergence of bounded states correlates the two electrons dynamics. In a intermediate range of interaction strengths, the initial state is mostly superposed to bound states and, therefore, the double occupancy remains close to unity. This means that the electrons behave as a single particle executing coherent hoppings. The coupled electrons effectively behave as a single particle with charge $2e$, thus explaining the frequency doubling of the Bloch oscillations. The frequency doubling phenomenon for intermediate electron–electron couplings was also obtained in 1D chains with a long-range correlated on-site disorder distribution [18].

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2010.09.005

In this work, we report further progress along the above lines. Our main aim is to focus on the influence of the on-site Coulomb interaction and of a static electric field in the dynamics of two-electrons restricted to move in a low dimensional lattice. The frequency doubling phenomenon previously reported in Refs. [17,18] as a consequence of bounded states present in the two-electron spectrum will be discussed in detail, pointing out the role of those states plays in the electronic biased transport. To this end, we use numerical methods to solve the Schrödinger equation and follow the wave-packet dynamics of two electrons in a 1D pure chain. Starting from an initial Gaussian wave-packet in the absence of an electric field, we show a non-usual dynamics associated with the two-electrons wave packet. The wave-packet width grows ballistically even in the regime of strong Coulomb interaction. However, for $U > 0$, the participation number shows a slower spread. Our calculations suggest that this unusual behavior is related to the presence of bound states in the initial Gaussian wave-packet. In addition, the electric-field biased wave-packet dynamics was revisited. We numerically show that the spatial extension of the Bloch oscillations depends non-monotonically on the electron–electron coupling and that the contribution of bounded states to the wave-packet dynamics is strongly dependent of the overall wave-vector of the initial wave-packet.

1. Model and formalism

The tight-binding Hamiltonian for two interacting electrons in the presence of a static uniform electric field F is given by [14–21]

$$H = \sum_n \sum_s W\left(c^\dagger_{n+1,s}c_{n,s} + c^\dagger_{n,s}c_{n+1,s}\right) + \sum_n \sum_s [\epsilon_n + eFa\mathbf{n}]c^\dagger_{n,s}c_{n,s} + \sum_n U c^\dagger_{n,\uparrow}c_{n,\uparrow}c^\dagger_{n,\downarrow}c_{n,\downarrow} \qquad (1)$$

where $c_{n,s}$ and $c^\dagger_{n,s}$ are the annihilation and creation operators for the electron at site n with spin s, $\mathbf{n}$ is the position operator, W is the hopping amplitude, U is the on-site Hubbard electron–electron interaction and e is the electron charge. Here we are considering the external electric field applied parallel to the chain length. In order to follow the time evolution of wave-packets, we solve the time dependent Schrödinger equation by expanding the wave-function in the Wannier representation $|\Phi(t)\rangle = \sum_{n,m} f_{n,m}(t)|ns_1, ms_2\rangle$ where the ket $|ns_1, ms_2\rangle$ represents a state with one electron with spin s_1 at site n and the other electron with spin s_2 at site m. In order to allow for double occupancy of the on-site orbital, we will consider in the following that the electrons are in distinct spin states (singlet state). Once the initial state is prepared as a direct product of states, the electrons will always be distinguishable by their spins since the Hamiltonian does not involve spin exchange interactions. The time evolution of the wave-function in the Wannier representation becomes

$$i\frac{df_{n,m}(t)}{dt} = f_{n+1,m}(t) + f_{n-1,m}(t) + f_{n,m+1}(t) + f_{n,m-1}(t) + \left[F(n+m) + \delta_{n,m}U\right]f_{n,m}(t), \qquad (2)$$

where we used units of $\hbar = W = e = a = 1$. The on-site energies ϵ_n were taken as the reference energy ($\epsilon_n = 0$) without any loss of generality. The above set of equations were solved numerically by using a recursive high-order method based on the Taylor expansion of the evolution operator $[V(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{n_o}(-iH\Delta t)^l/(l!)]$ where H is the Hamiltonian. The wave-function at time Δt is given by $|\Phi(\Delta t)\rangle = V(\Delta t)|\Phi(t=0)\rangle$. The following results were taken by using $\Delta t = 0.05$ and the sum was truncated at $n_o = 20$. This cutoff was sufficient to keep the wave-function norm conservation along the entire time interval considered.

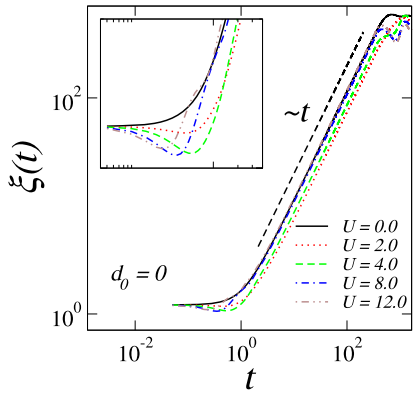

Fig. 1. The time dependent spatial extension ξ versus time t. Calculations were done using $N = 1500$, $U = 0$ up to 12, $\sigma = 1$ and $d_0 = 0$. After an initial transient, ξ diverges linearly $\xi \propto t$ even in the regime of strong interaction. In the transient period (inset), the spatial extension depicts a small decrease due to the electron–electron coupling.

2. Results

2.1. Unbiased dynamics ($F = 0$)

We firstly investigate the two-electrons wave-packet dynamics in the absence of an electric field ($F = 0$). Specifically, we followed the time-evolution of an initially Gaussian wave-packet with width σ:

$$\langle ns_1, ms_2|\Phi(t=0)\rangle = \frac{1}{A(\sigma)}\exp\left[-\left(n-n^0\right)^2/4\sigma^2\right] \times \exp\left[-\left(m-m^0\right)^2/4\sigma^2\right] \qquad (3)$$

and computed the participation function $P(t)$ and the spacial extension $\xi(t)$ defined as [17]

$$P(t) = \frac{1}{\sum_{n,m}|f_{n,m}(t)|^4}, \qquad (4)$$

and

$$\xi(t) = \sum_{n,m}\sqrt{\left[\left(n-\langle n\rangle(t)\right)^2 + \left(m-\langle m\rangle(t)\right)^2\right]}\left|f_{n,m}(t)\right|^2, \qquad (5)$$

where $\langle n\rangle(t)$ and $\langle m\rangle(t)$ are the average position of each electron at time t. The initial position of the electrons (n^0, m^0) will be considered to be $(N/2 - d_0, N/2 + d_0)$. The participation function $P(t)$ varies from 1, corresponding to states with each electron fully localized in a given pair of sites (n, m), to N^2 when both electrons are uniformly distributed along the chain [17]. This function gives information about the product of the number of sites that are visited by each electron during the time evolution of the wave-packet over the underlying lattice. The spacial extension $\xi(t)$ measures the wave-function width on the $n \times m$ plane. In Fig. 1, we show results for the spatial extension ξ versus time t using a chain with $N = 1500$ sites, $U = 0$ up to 12 and $d_0 = 0$. After the initial transient, ξ diverges linearly $\xi \propto t$ even for strongly interacting electrons, thus indicating a ballistic spread of the two-electrons wave-packet. One also notices a dip in the spatial extension in the short time region for the case of interacting electrons. Such decreasing induced by the electron–electron interaction is related to the presence of bounded eigenstates in the initial wave-packet. Fig. 2(a) shows the participation number $P(t)$ versus time t computed using the same parameters as in Fig. 1. In the absence of electron–electron interaction ($U = 0$), the participation number grows as $P(t) \propto t^2$, signaling that the electrons spread uniformly and independently over the chain, in agreement with the time dependent behavior of the electronic participation number in 1D crystal lattices. However, when

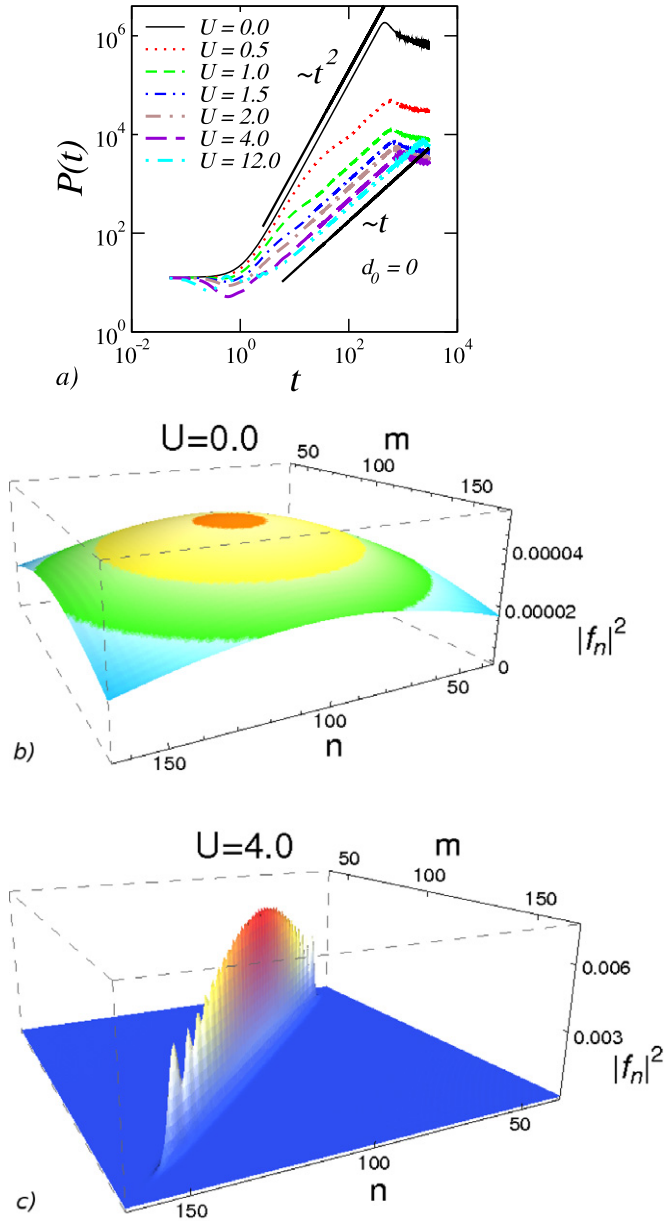

Fig. 2. (a) Participation number $P(t)$ versus time t computed using $N = 1500$, $U = 0$ up to 12 and $d_0 = 0$. In the absence of interaction ($U = 0$) the participation number displays a ballistic growth ($P(t) \propto t^2$). With the electron–electron coupling turned on, a crossover to an unusual dynamical behavior is observed ($P(t) \propto t$). (b–c) The two-electron wave function after a long evolution time. Here, we used $N = 200$, $d_0 = 0$, (b) $U = 0$ and (c) $U = 4$. In the absence of electron–electron coupling, both electrons spread ballistically filling the $n \times m$ plane. For $U > 0$, the electrons become correlated due to the emergence of bounded states and, thus, the wave-packet concentrates along the diagonal $n = m$.

the electron–electron coupling is turned on, we obtain a slower divergence of the participation number, in the form ($P(t) \propto t$). In Fig. 2(b–c) we illustrate more clearly the time-evolution of both electrons through the lattice. These calculations were performed using $N = 200$, $d_0 = 0$, (b) $U = 0$ and (c) $U = 4$. In the absence of electron–electron interaction both electrons spread ballistically and independently, with the two-particles wave-packet filling isotropically the $n \times m$ plane. For $U > 0$, due to the appearance of bounded states within the energy band, the electrons spread become correlated and the wave packet concentrates around the $n = m$ region. These features also leave signatures in the one-electron wave-function $|f_n|^2 = \sum_m |f_{n,m}|^2$ (see Fig. 3). This figure shows snapshots of the wave-packet starting from the initial transient regime ($t = 5$) until longer time evolution periods ($t = 20$, 40, 100) for $U = 0$, 4, and 12. In the absence of electron–electron interaction, the wave-packet spreads ballistically displaying a single peak structure. In the presence of electron–electron interaction, the wave-packet develops two main structures. One of then is concentrated at the electron initial position. The other component has a strong amplitude at the wave front that resembles the wave packet spread of a single non-interacting electron initially localized at the chain center [20,21]. Both structures evolve ballistically.

2.2. Biased dynamics ($F \neq 0$)

Now, we consider the wave-packet dynamics of both electrons subjected to a uniform electric field ($F \neq 0$). It is well known that in disorder-free systems, a uniform electric field causes the dynamic localization of the one-electron and gives rise to an oscillatory motion of the wave-packet, the so-called Bloch oscillations [17,22]. Once Eq. (2) is solved for the initial condition (3), we compute the mean position of a given electron $\langle n \rangle(t)$

$$\langle n \rangle(t) = \sum_{n,m} n \left| f_{n,m}(t) \right|^2. \tag{6}$$

In Ref. [17] it was shown that the centroid of the two-electron wave-packet displays an oscillatory pattern with a predominant frequency close to $\omega = 2F$. This phenomenon was related to the emergence of bounded states with the electrons oscillating coherently with an effective charge $2e$ [17]. For much stronger interactions, the $\omega = F$ frequency is re-amplified. Here we analyse in detail the effect of Hubbard interaction on this unusual Bloch oscillation. We will explore the role played by bounded states on the amplitude of the wave-packet oscillation and also on the intensity of the doubled frequency mode. We numerically determine in Fig. 4 the average displacement of one electron from its average position as a function of the Hubbard coupling. Firstly, we analyzed the particular case on which both electrons are initially fully localized ($\sigma = 0$). In this case, no Bloch oscillation is observed for non-interacting electrons. As the interaction is turned on, the oscillation amplitude depicts a maximum at a finite interaction strength (of the order of $U = 4$), with the oscillation amplitude vanishing in the regime of strong couplings. Whenever the initial wave-packet has a finite width σ, a quite distinct picture emerges. At $U = 0$, the centroid oscillates with a relatively large amplitude. The oscillation amplitude initially decreases when increasing U, but slowly return to increase in the regime of strong couplings. Also, the asymptotic amplitude increases with the width of the initial wave-packet. All these features can be qualitatively understood by stressing that the initial wave-packet can be splited in two components composed of bounded and unbounded states. The band of bounded states is centered around $E = 0$, while the band of bounded states ranges from $U < E < \sqrt{16 + U^2}$ [14]. The Bloch oscillation due to the unbounded component has a larger amplitude than that due to the bounded states, according to the semi classical argument that predicts the oscillation amplitude to be directly proportional to the bandwidth and inversely proportional to the effective charge. Also, the relative role of these two components depends on the width of the initial wave-packet, with a larger contribution of unbounded states being present at larger values of σ. Further, the initial Gaussian wave-packet (Eq. (3)) has a spectral density centered at $E = 0$. As the coupling strength starts to increase, there is an increasing role played by the bounded component, which leads to the decrease of the oscillation amplitude. At very large couplings, the re-amplification of the $\omega = F$ oscillation mode as well as of the oscillation amplitude are related to the large displacement of the band of bounded states from the spectral distribution of the initial wave-packet.

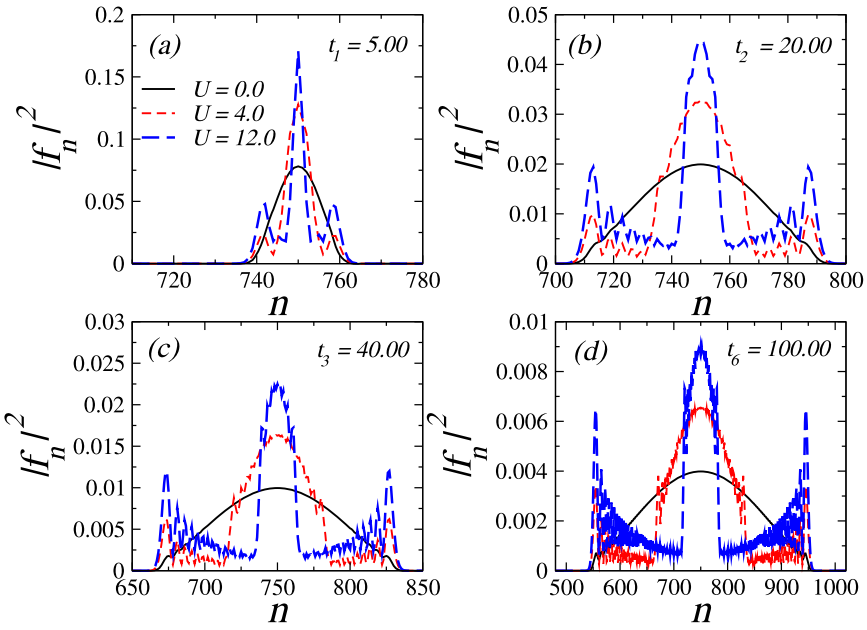

Fig. 3. The one-electron wave-function $|f_n|^2 = \sum_m |f_{n,m}|^2$ for times $t = 5$, 20, 40, 100, $N = 1500$ sites, $\sigma = 1$ and $U = 0$, 4, 10. In the absence of electron–electron interaction, the wave-packet spreads ballistically displaying a single peak structure. Two main structures develops in the presence of electron–electron interaction. One of them is concentrated at the electron initial position while the other has a strong amplitude at the wave front. Both structures evolve ballistically.

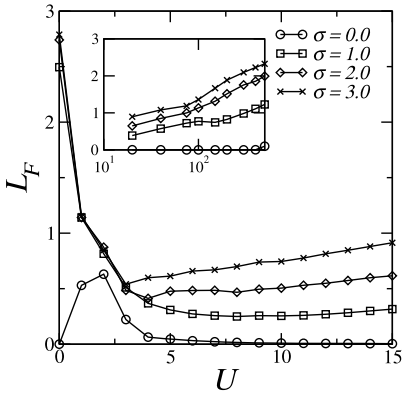

Fig. 4. The amplitude of the Bloch oscillation L_F versus the strength of the Hubbard interaction U for several initial wave-packet widths $\sigma = 0$, 1, 2, 3 and $F = 0.5$. For $\sigma = 0$, L_F vanishes for non-interacting electrons. As the interaction is turned on, the oscillation amplitude depicts a maximum at a finite interaction strength (of the order of $U = 2$), with the oscillation amplitude vanishing in the regime of strong couplings. For a finite width σ, the centroid oscillates with a relatively large amplitude at $U = 0$. The oscillation amplitude initially decreases when increasing U, but slowly returns to increase in the regime of strong coupling (inset).

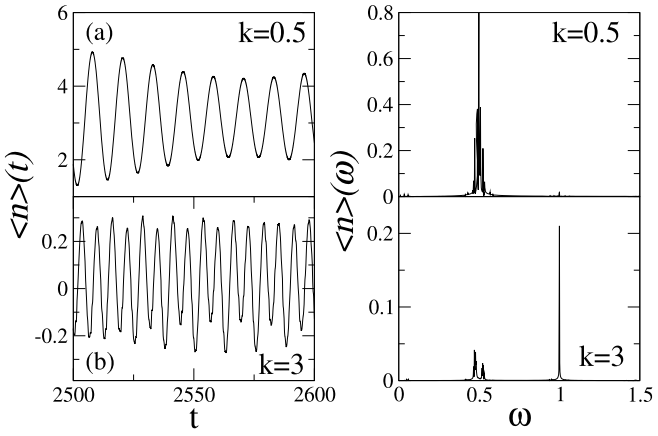

Fig. 5. Data for the mean position $\langle n(t)\rangle$ versus time t using a chain with $N = 100$ sites, $d_0 = 0$ (initially close electrons), $F = 0.5$, $U = 8$, $\sigma = 1$ and (a) $k = 0.5$ and (b) $k = 3$. For small k, the re-amplification of the mode with frequency $\omega = F$ is seen in this strong coupling regime. For $k = 3$ the frequency doubling persists.

Before concluding, we provide additional evidence of the influence of bounded states in the frequency doubling phenomenology. We consider now the time-evolution of an initially Gaussian wave-packet with a finite initial velocity given by

$$\langle ns_1, ms_2 | \Phi(t=0)\rangle = \frac{1}{A(\sigma)} \exp i[k(n+m)] \times \exp\left[-(n-n^0)^2/4\sigma^2\right] \times \exp\left[-(m-m^0)^2/4\sigma^2\right] \quad (7)$$

where i is the imaginary unit. The phase factor $\exp[ik(n+m)]$ governs the initial velocity of the wave-packet (in the particular case of identical velocities of both electrons). It also can be used to displace the spectral density of the wave-packet away from the band center. In Fig. 5, we compute the mean position $\langle n\rangle(t)$ versus time t using a chain with $N = 100$ sites, $d_0 = 0$ (initially close electrons), $F = 0.5$, $U = 8$, (a) $k = 0.5$ and (b) $k = 3$. For small k, we recover the previous result showed above, the re-amplification of the mode with frequency $\omega = F$. This is in agreement with the general scenario described above because the band of bounded states is far from the band center around which the wave-packet spectral density is just slightly displaced. However, for $k = 3$ we obtain an oscillatory pattern with a predominant frequency close to $\omega = 2F$. It is important to stress that, in this case of large k, the frequency doubling persists even in the strong interaction regime for which this phenomenon is suppressed at low k. In fact, the initial state defined in Eq. (7) for $k = 3$ has a spectral decomposition which is quite displaced from the band center and exhibits a significant superposition with the band of bounded states. This feature promotes the emergence of coherent hoppings and the consequent frequency doubling of the Bloch oscillations.

3. Summary and conclusions

In summary, we studied the one-dimensional dynamics of two interacting electrons with opposite spins under the influence of a

static uniform electrical field F. Starting from an initial Gaussian wave-packet and keeping the electric field turned off, we showed a non-trivial dynamics of two-electrons wave-packet width and participation number. The time-evolution of wave-packet width is always ballistic, irrespective to the strength of the electron–electron interaction. However, the dynamics of the participation number of the two-electrons wave-packet displays a crossover from a ballistic-like growth ($P(t) \propto t^2$) for non-interacting electrons to a diffusive-like growth ($P(t) \propto t$) whenever the electron–electron coupling is turned on. Such crossover is related to the emergence of two-electrons bounded states that correlates the dynamics of the electronic wave-packet. The presence of an electron–electron coupling also imprints its signature in the one-electron wave-packet. In the regime of non-interacting electrons, an initially Gaussian one-electron wave-packet evolves ballistically displaying a single peak structure. The presence of an electron–electron coupling is reflected by the development of a doubled structure with the electronic density concentrated at the initial position as well as at the wave fronts.

In addition, the electric-field biased wave-packet dynamics was revisited. We numerically showed that the length of the segment over which the centroid of the electron wave-packet oscillates displays distinct features for delta-like and Gaussian initial wave-packets. In the case of delta-like initial wave-packets, the oscillation amplitude exhibits a maximum at a finite interaction strength and vanishes in both limits of $U \to 0$ and $U \to \infty$. The vanishing of the oscillation amplitude in these limits is in agreement with previous results that showed no Bloch oscillation for delta-like wave-packets of non-interacting electrons [20,21]. On the other hand, a reversed trend is found for initially Gaussian wave-packets. A finite oscillation amplitude in the regimes of weak and strong interaction is typical of non-interacting electrons with an initial Gaussian wave-packet distribution. The oscillation amplitude displays a minimum at a finite interaction strength where the band of bounded two-electron states plays a significant role in the wave-packet dynamics. Such reduced oscillation amplitude is related to the reduced width of the bounded states band and to the correlated dynamics of the two-electrons. In the intermediate coupling strength regime, the predominant role played by bounded states in the Bloch oscillations is supported by the emergence of a frequency doubled component in the spectral decomposition of the wave-packet centroid. We further showed that a re-amplification of the doubled frequency mode can be achieved in the regime of strong couplings by tuning the overall wave-vector of the initial two-electrons wave-packet in order to promote a stronger superposition between the wave-packet spectral distribution and the band of bounded states. The above features reveal that even a short-ranged electron–electron interaction has a strong influence on the field driven Bloch oscillations. It would be much valuable to extend the present analysis to the case of interacting many electron systems. We hope the present work can stimulate future developments along this line.

Acknowledgements

This work was partially supported by the Brazilian research agencies CNPq, CAPES and FINEP, Rede Nanobioestruturas, as well as by the Alagoas State research agency FAPEAL. We are grateful to H.N. Nazareno for useful discussions.

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