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Research paper

Nonlinear wave-packet dynamics resonantly driven by AC and DC fields

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ABSTRACT

The dynamics of a charged single-particle placed in a chain under the simultaneous action of local non-linearity and superposed harmonic AC and static fields (DC field) is considered. The non-linearity is represented as a diagonal potential proportional to the square modulus of the local wave-function. We unveil a rich dynamics with the wave-packet fronts displaying either a continuous spreading or a solitonic-like evolution depending on a delicate balance between the non-linearity strength and the phase of an AC field in resonance with the Bloch oscillations induced by a DC field. In particular, the non-linearity induces a unidirectional motion of the wave-packet centroid of an initially fully localized wave-packet which is absent in the linear regime.

1. Introduction

The dynamics of electrons under the influence of electric fields consists of an interesting research field within solid state physics. The dynamics of one-electron wave-packets under the action of a static (DC) electric field exhibits the so called Bloch oscillations (BO). In general, BO represents an oscillatory motion of wave-packets whose frequency is proportional to the amplitude of the applied DC electric field [1–9]. From the experimental standpoint, this phenomenon was observed in quantum electronic wave-packets in semiconductors superlattices [10], as well as in analogue systems including ultra-cold atoms [11–13], optical [14] and acoustic waves [15]. Moreover, when considering the wave-packet dynamics under influence of superposed static (DC) and harmonic (AC) electric fields, unidirectional transport and super-bloch oscillations (SBO) can be developed [16–23]. When the AC harmonic field is resonant with the Bloch frequency, the wave-packet centroid can acquire a unidirectional motion whose velocity depends on the initial wave-packet width. A small detuning from the resonant condition leads to Bloch oscillations with giant amplitudes (also called super bloch-oscillations). It is important to emphasize that these phenomena have been experimentally demonstrated in a weakly interacting Bose–Einstein condensate of Cs atoms placed in a tilted one-dimensional optical lattice under a forced driving, achieving matter-wave transport over macroscopic distances [19].

Another relevant aspect that influences the one-electron wave-packet dynamics is its effective interaction with lattice's phonons [24–27]. In particular, it has been shown that the interaction between electrons and optical phonons can be well described by a nonlinear Schrödinger equation (NLSE) [28]. A NLSE has also be widely used to describe the wave-packet dynamics of Bose–Einstein condensates where the nonlinear contribution arises from the underlying inter-particle inter-

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action [29–31]. One of the most prominent phenomena related to the wave-packet dynamics in nonlinear systems is the self trapping (ST). In general, ST occurs when the non-linearity strength exceeds the magnitude of the energy bandwidth [32–39]. Moreover, the competition between disorder and non-linearity was investigated in detail in Refs. [33,40,41]. It was shown that in 1D disordered systems, the Anderson localization is destroyed for a specific range of values of the non-linearity parameter [40,41]. A similar result was found by studying the spatio-temporal evolution of a wave-packet in disordered nonlinear anharmonic chains [33]. Several aspects related to transport properties in nonlinear lattices have been widely explored in the recent literature [42–50].

In this work we will address to the question of how a nonlinear contribution affects the dynamics of a one-particle wave-packet driven by AC field in resonance with the Bloch oscillations promoted by a DC field. We emphasize that the effects of these terms on the electronic dynamics was investigated separately in the previous literature. The combination of AC and DC electric fields acting on an ordered chain (without nonlinearity) promotes the emergence of an unidirectional electronic propagation. The electronic dynamics in a chain with diagonal nonlinearity (without electric fields) can exhibit electronic self-trapping depending on the magnitude of the nonlinear interaction. However, a detailed description about competition between electric fields (AC plus DC) and nonlinearity is completely absent and it can not be directly infered from their separate actions because the linear superposition principle can not be applied. This is the main focus of our work. By solving the effective nonlinear Schrödinger equation, we will follow the wave-packet time-evolution and compute some representative quantities associated with the wave-packet dynamics such as the participation function, centroid velocity and its dispersion with respect to the AC field phase. We will be particularly interested in the dynamics of an initially fully localized wave-packet which has no net drift of its centroid in the linear regime. We will report a new phenomenology associated with a nonlinear induced unidirectional motion of the centroid due to the distinct dynamics acquired by the left and right wave-fronts. The ultimate self-trapping transition will also be identified.

2. Model and formalism

We consider a single-particle wave-packet moving in a nonlinear chain with N sites. The particle is driven by an external field. The nonlinear contribution will be considered as instantaneous, which results from the adiabatic approximation [40] of a more fundamental model including the particle's interaction with other degrees of freedom. The nonlinear diagonal potential is proportional to the square modulus of the local wave-function with χ representing the strength of the local nonlinear coupling. Within a tight-binding approach and considering a localized orbital basis, the wave-packet dynamics can be described by

$$i\dot{\psi}_n(t) = \psi_{n+1}(t) + \psi_{n-1}(t) + \left[F(t)(n-n_0) - \chi|\psi_n(t)|^2\right]\psi_n(t) \tag{1}$$

where we used units of $\hbar = 1$, particle charge $e = 1$, lattice spacing $a = 1$ and hopping amplitude $J = 1$. The external field will be assumed to be given by $F(t) = F_0 + F_\omega \cos(\omega t + \phi)$, i.e., a superposition of a DC field of magnitude F_0 and an AC field of magnitude F_ω, frequency ω and phase ϕ [16,19,22]. Following the previous literature [16,19,22], we will explore the case in which that $\omega = F_0$, i.e., the resonant condition for the Bloch frequency. Time is expressed in units of $\hbar/J$. In what follows, we will solve the above nonlinear dynamical equation for initially localized wave-packets $\psi_n(t=0) = \delta_{n,n_0}$, as well as Gaussian wave-packets with width σ defined as

$$\psi_n(t=0) = A(\Sigma)\exp\left[\frac{-(n-n_0)^2}{\Sigma}\right]. \tag{2}$$

where $\Sigma = 4\sigma^2$ represents the generalized square width of the wave-packet and $A(\Sigma)$ is a normalization constant. We emphasize that the case with a fully localized wave-packet at the position n_0 is equivalent to case with $\Sigma = 0$. The initial central position of the wave-packet (n_0) is the chain's center ($n_0 = N/2$). The set of equations (Eq. (1)) were solved numerically by using the fourth order Runge–Kutta method with step-size of the order of 10^{-5} in order to keep the wave-function norm conservation ($|1 - \sum_n |\psi_n(t)|^2| \le 10^{-12}$) along the entire time interval considered. After solving the set of equations, we computed some typical quantities to characterize the wave-packet time-evolution, such as its centroid

$$\bar{x}(t) = \sum_n n|\psi_n(t)|^2, \tag{3}$$

and the participation function

$$P(t) = 1/\sum_n |\psi_n(t)|^4. \tag{4}$$

The centroid $\bar{x}(t)$ represents the mean particle's position, while the participation function $P(t)$ gives an estimate of the number of sites over which the wave-packet is spread at time t. By using the numerical calculations of the mean position, we also estimate the centroid's velocity through the numerical linear regression of curves $\bar{x}(t) \times t$ in the long-time regime. In addition, we also analyzed the wave-function profile $|\psi_n(t)|^2$ versus t and n in order to better analyze the effect of the non-linearity on the wave-packet dynamics.

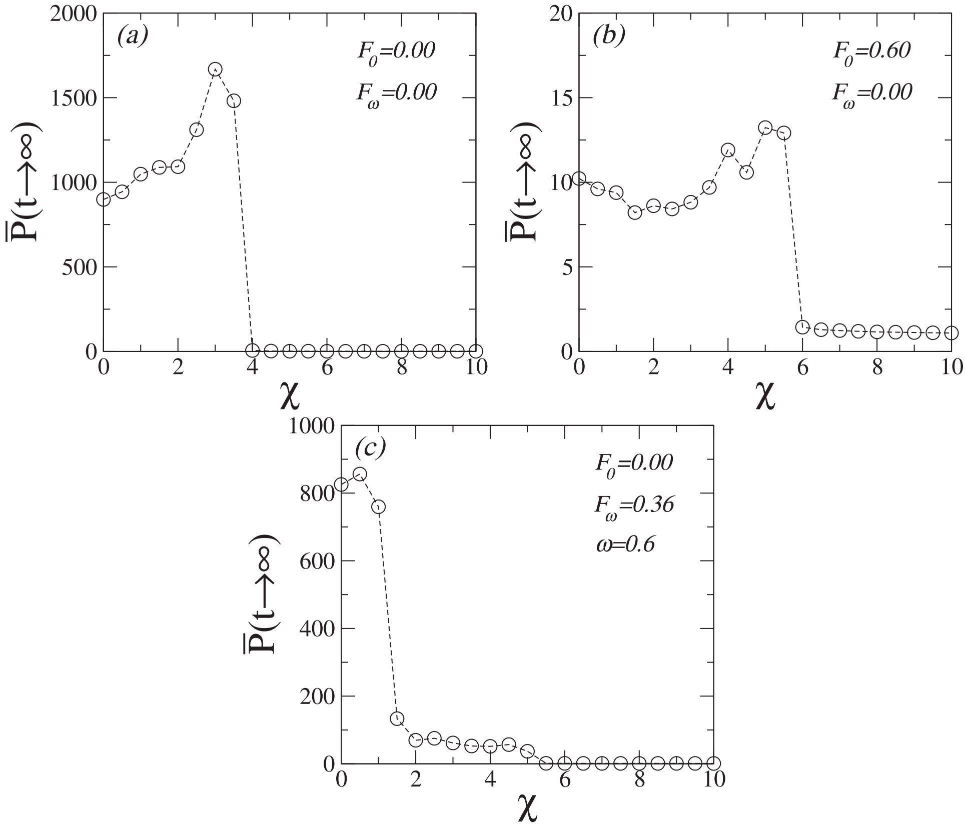

Fig. 1. Long-time Participation number ($P(t \to \infty)$) versus χ considering (a) $F_0 = F_\omega = 0$ (i.e. the case without DC and AC electric fields). (b) $F_0 = 0.6$ and (c) $F_\omega = 0.36$. In the absence of electric fields one has the "self-trapping" phenomenon induced by nonlinearity. In the presence of a DC field there is a transition form the regime of dynamic localization to full localization. Under an AC field, the wave-packet remains extended at weak nonlinearities. In this case, the regime of dynamic localization occurs in a finite range of nonlinear strengths.

3. Results and discussion

Our results were obtained through the numerical solution of the Eq. (1) using the fourth order Runge–Kutta method with step-size of the order of 10^{-5}. The wave-function norm conservation ($|1 - \sum_n |\psi_n(t)|^2| \leq 10^{-12}$) was checked along the entire time. We also emphasize that all calculations here were done for an open chain with $N = 2000$ sites.

Before showing our results on the effect of nonlinearity under the action of both DC and AC electric fields on the electronic propagation, we briefly summarize some aspects related with the electronic propagation in nonlinear systems without either DC or AC electric fields. In Fig. 1 we plot the long time participation number $P(t \to \infty)$ versus χ considering $F_0 = F_\omega = 0$ (i.e. the case without DC and AC electric fields). Our results illustrate the well know "self-trapping" phenomena [35,39,44]. When the nonlinearity χ exceeds the width of the energy band, the electron remains localized around the initial site. In Fig. 1(b) and (c) we plot $P(t \to \infty)$ versus χ for the cases with a DC field (Fig. 1(b)) and an AC field (Fig. 1(c)). A DC field promotes the localization of the wave-packet which develops Bloch oscillations. This picture remains in the presence of weak nonlinearities, with the ultimate full localization taking place above a critical threshold. An AC field can lead to a dynamic localization. The field intensity we are using is not sufficient to promote dynamic localization in the linear regime and the participation remains large. Nonlinearity enforces the dynamic localization above a first threshold, with full localization also being reached above a second critical nonlinearity.

We show in Fig. 2 the time evolution of the average particle's position (wave-packet centroid), for some representative values of the initial wave-packet width and nonlinear strengths. We considered the particular case of $\omega = F_0 = 0.6$ and $F_\omega = 0.6F_0$. In the absence of non-linearity ($\chi = 0.0$) only wave-packets with $\Sigma > 0$ display unidirectional motion. This feature has been previously demonstrated theoretically and numerically. It is directly related to the fact that the average velocity is proportional to the average value of the kinetic operator of the initial state which vanishes for a delta-like state [22,51]. In this case, the wave-packet spreads while developing two fronts that propagate in opposite directions. When the non-linearity is turned on, a new phenomenology emerges: Some degree of unidirectional motion takes place even for a fully localized initial state.

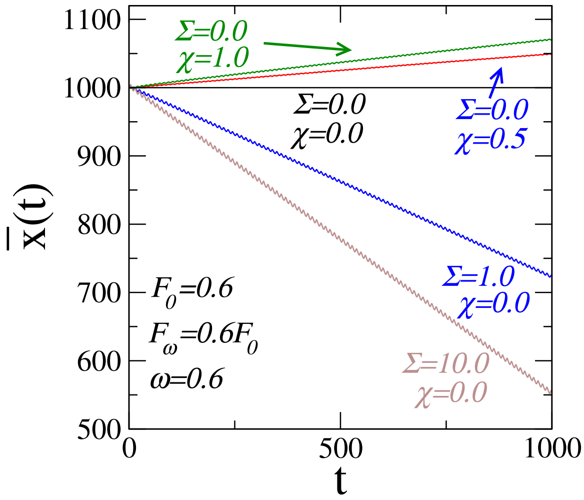

Fig. 2. Time evolution of the average position (wave-packet centroid) of the particle subjected to AC and DC fields satisfying the resonance condition $\omega = F_0$. Three distinct initial wave-packets widths ($\Sigma = 0.0, 1.0, 10.0$) were considered. In the absence of non-linearity ($\chi = 0.0$), only wave-packets with finite initial widths exhibit unidirectional motion of their centroid. The presence of non-linearity provides a finite drift velocity to initially fully localized wave-packets ($\Sigma = 0.0$).

In order to explore the unidirectional motion induced by the non-linearity, we plot the centroid's velocity as a function of the phase of the AC field, as shown in Fig. 3. In Fig. 3(a), we unveil that the non-linearity promotes a finite drift velocity of a fully localized initial wave-packet centroid with a non-trivial phase dependence. In Fig. 3(b), we show the corresponding phase dependence developed by a wide initial wave-packet in the linear regime. Such phase dependence has been fairly well described (see solid line) within a semi-classical approach [16,22],

$$v \propto \cos\left(\frac{F_\omega}{F_0}\cos(\phi) - \phi\right). \tag{5}$$

with the overall velocity amplitude depending on the initial wave-packet width.

To develop a deeper understanding of the origin of the nonlinear induced centroid's drift, we will provide a closer analysis of the wave-packet time evolution for the case of resonant driving and an initially fully localized state. Some representative values of the AC field phase will be considered to probe distinct regimes of the induced centroid's velocity.

We start our analysis with the resonant case $F_0 = 0.6$, $F_\omega = 0.6F_0$, $\omega = 0.6$, and the AC field phase $\phi = 2.6$. For this set of parameters, the wave-packet centroid develops a negative velocity, as shown in Fig. 3(a). Here, we show the time evolution of the wave-packet profile for the two values of the non-linearity used in Fig. 3(a). Surprisingly, the two wave-packet fronts exhibits quite distinct dynamics. While the front propagating to the left side displays a solitonic-like dynamics, the front evolving towards the right side spreads continuously. The spreading of the right-side wave-packet is directly related to the a radiating component, usually present in nonlinear dynamical systems. Actually, there is also a small radiation component on the left-side whose visualization is compromised by the presence of the strongly focused solitonic component. It is worthy to call attention that the solitonic waves are breathers with the main peak oscillating in time. Complimentary information concerning the wave-front dynamics is shown in bottom panels of Fig. 4. The corresponding time evolution of the participation function computed for each wave-packet branch is reported. Here, we see clearly that while the left branch remains localized with a finite participation number, the right branch displays a participation number that grows linearly in time, thus representing a front whose width spreads balistically.

As a second example, we follow the wave-packet evolution for the AC field phase $\phi = 4.4$ in Fig. 5. Under this condition, the wave-packet centroid is nearly stationary (see Fig. 3(a)). For a weak non-linearity, the wave-packet evolves similarly to the case shown before, with one branch spreading balistically while the other displays a solitonic-like dynamics. However, the two branches have the opposite behavior shown in Fig. 4. This feature shows that the out-coming dynamics of each branch depends on a delicate interplay between the AC field phase and the non-linearity strength. To further characterize this feature, one notices that the left branch turns into a solitonic wave superposed to a small radiation component, when the non-linearity increases, as shown in Fig. 5(b).

As a final example of the wave-packet dynamics, we show the case of $\phi = 5.4$ in Fig. 6 for which the wave-packet centroid has a positive velocity. Here, we can see that the right branch has a main solitonic-like evolution while the left one spreads. It is interesting to stress that stronger nonlinearities will ultimately promote the localization of the left branch. In Fig. 6(b) the non-linearity is close to the localization transition, which makes the spreading of the left branch to become slower (super-diffusive). We stress again the breathing character of the solitonic wave-packet fronts. This behavior is more clearly seen in Fig. 6(a) and (b). We emphasize that the oscillation of the main peaks is associated with a modulational instability that usually takes place in nonlinear dynamical systems (see Ref. [52] for a revision about the modulational

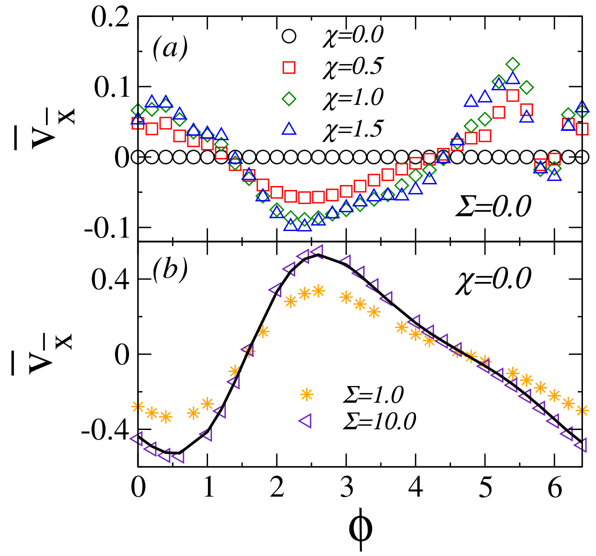

Fig. 3. Phase dependence of the centroid velocity for: (a) a fully localized initial wave-packet ($\Sigma = 0.0$); and (b) wave-packets with a finite initial width ($\Sigma = 1.0, 10.0$). The AC and DC fields are set in the same resonance condition as in Fig. 2. For weak nonlinearities ($\chi = 0.5, 1.0, 1.5$), the centroid of initially localized wave-packets develops a phase-dependence. In the linear regime ($\chi = 0.0$), the phase-dependence is well described by a semiclassical approach (solid line).

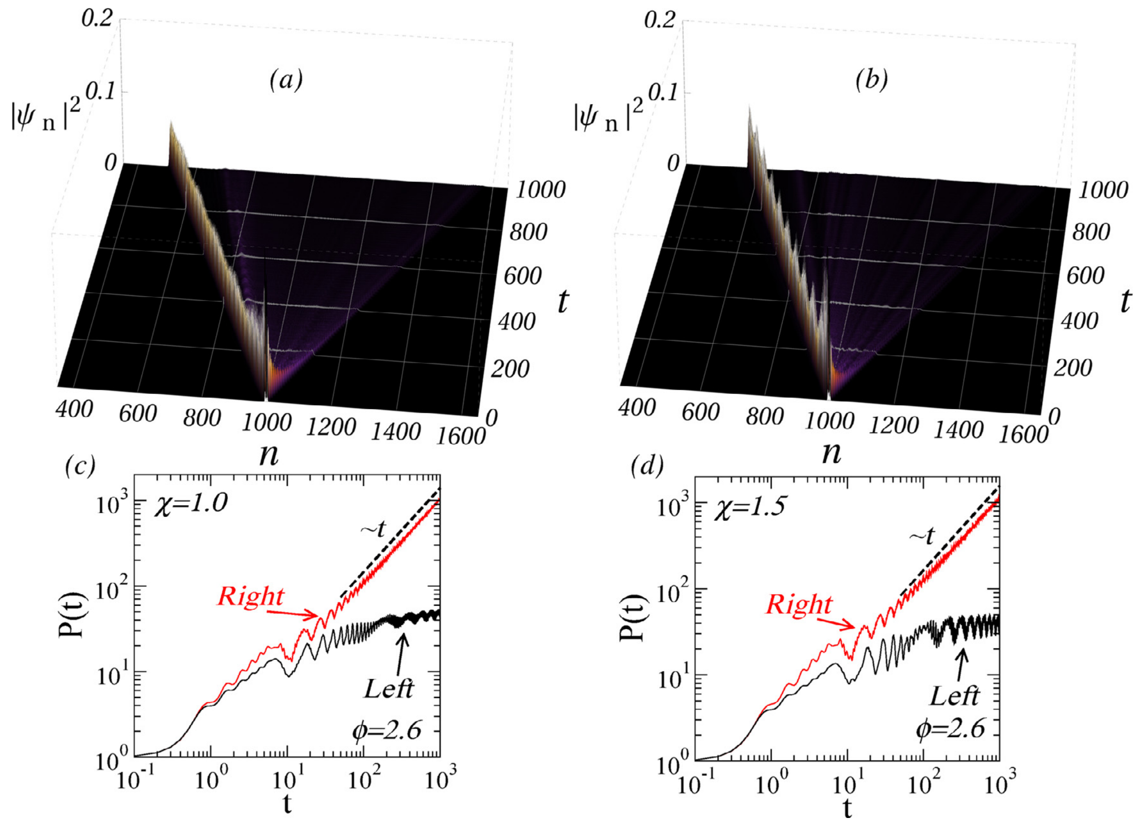

Fig. 4. (a) and (b) Time evolution of initially fully localized wave-packets, with $F_0 = 0.6$, $F_\omega = 0.6F_0$, $\omega = 0.6$, $\phi = 2.6$ and (a) $\chi = 1.0$ and (b) $\chi = 1.5$. (c) and (d) Participation function computed in the left and right sides of the chain (with respect to the initial wave-packet center) for the configurations shown in (a) and (b). The centroid's net velocity shown in Fig. 3 is related to a soliton-like branch which acquires a unidirectional drift to the left side. On the right side, the wave-packet spreads ballistically.

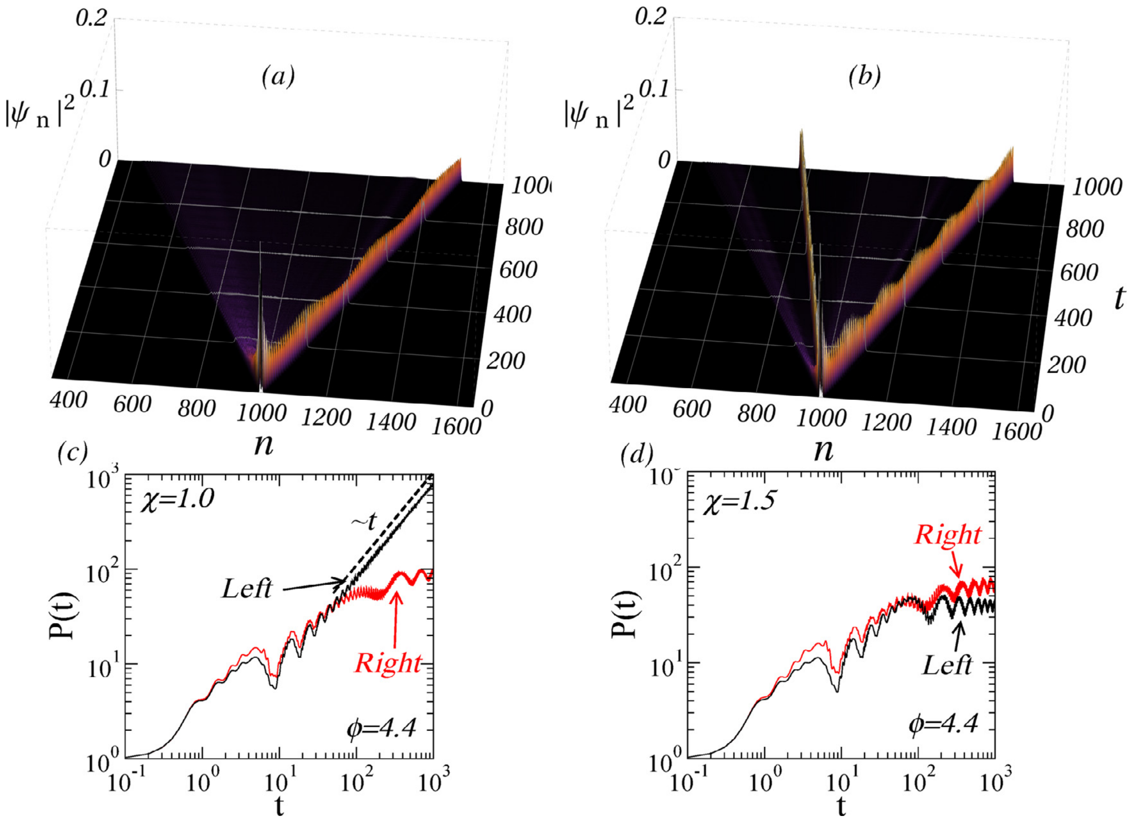

Fig. 5. (a) and (b) Time evolution of initially fully localized wave-packets, with $F_0 = 0.6$, $F_\omega = 0.6F_0$, $\omega = 0.6$, $\phi = 4.4$ and (a) $\chi = 1.0$ and (b) $\chi = 1.5$. (c) and (d) Participation function computed in the left and right sides of the chain for the same configurations shown in (a) and (b). Although both configurations have nearly zero centroid's velocity, only sufficiently strong nonlinearities promotes the emergence of two solitonic branches.

instability within the context of nonlinear Scrödinger equation). The frequency of these oscillation have no direct relation with the Bloch oscillations induced by a DC field.

Further increasing the nonlinear strength will promote the ultimate self-trapping of the wave-packet near its initial position. In Fig. 7 we explicitly show the transition to the self-trapped regime of an initially fully localized wave-packet. In this case, the wave-packet centroid remains stationary for any phase of the DC field for non-linearity strengths above the critical value $\chi_c \simeq 7$. The self-trapping of an initially wide wave-packet is known to require stronger nonlinearities. To signal the self-trapping transition as a function of the non-linearity strength, we computed the standard deviation of the centroid's velocity with respect to the AC field phase defined as $\Delta\bar{v}_{\bar{x}} = \sqrt{<\bar{v}_{\bar{x}}^2>_\phi - (<\bar{v}_{\bar{x}}>_\phi)^2}$. The velocity standard deviation is finite whenever the centroid exhibits a phase dependent velocity, vanishing above the self-trapping transition. In Fig. 8 we plot $\Delta\bar{v}_{\bar{x}}$ as a function of the nonlinear strength for the same resonance condition explored before, namely $F_0 = 0.6$, $F_\omega = 0.6F_0$ and $\omega = 0.6$. For an initially localized state (Fig. 8(a)) the velocity standard deviation is zero in the linear regime ($\chi = 0$). It becomes finite when the non-linearity induces a centroid drift, resulting from the distinct dynamics developed by the wave-fronts. Finally, it vanishes again in the self-trapped regime of $\chi > \chi_c$. In Fig. 8(b) we consider a initial Gaussian wave-packet of width $\Sigma = 2$. In this case, the velocity dispersion is finite in the linear limit due to the finite average value of the kinetic operator. Self-trapping is only reached above a very large nonlinear strength of the order of $\chi_c = 60$.

4. Summary and conclusions

In summary, we showed that the presence of an underlying non-linearity has a significant impact on the dynamics of one-particle wave-packets driven by an AC field in resonance with the Bloch oscillations promoted by a DC field. The main new features are observed when the initial wave-packet is fully localized in a single site of a chain. In the absence of a nonlinear contribution, the wave-packet spreads symmetrically with no net displacement of its centroid. Unidirectional motion of the wave-packet centroid only takes place for wide wave-packets. The introduction of a cubic non-linearity breaks the symmetry of the wave-packet evolution. The left and right wave-fronts develop distinct dynamics, including ballistic and super-diffusive spreadings, solitonic-like drifting, as well as self-trapping. The actual wavefront dynamics depends on both the nonlinear strength and the AC field phase. As a result, the wave-packet centroid acquires a finite velocity with a nontrivial dependence on the AC field phase. According to the present results, a single localized state can be splitted

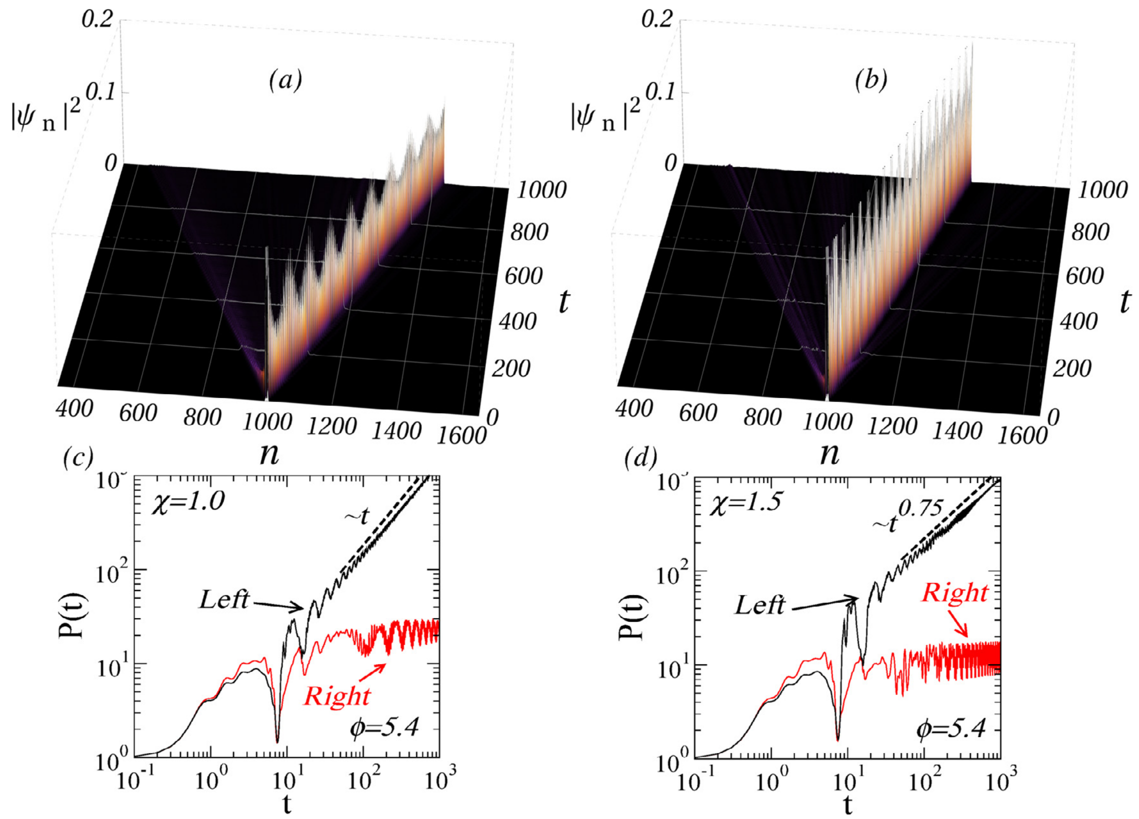

Fig. 6. (a) and (b) Time evolution of initially fully localized wave-packets, with $F_0 = 0.6$, $F_\omega = 0.6F_0$, $\omega = 0.6$, $\phi = 5.4$ and (a) $\chi = 1.0$ and (b) $\chi = 1.5$. (c) and (d) Participation function computed in the left and right sides of the chain for the same configurations shown in (a) and (b). The centroid's velocity shown in Fig. 3 is related to a soliton-like branch which has a unidirectional drift to the right side. A super-diffusive spreading of the left branch is observed at $\chi = 1.5$.

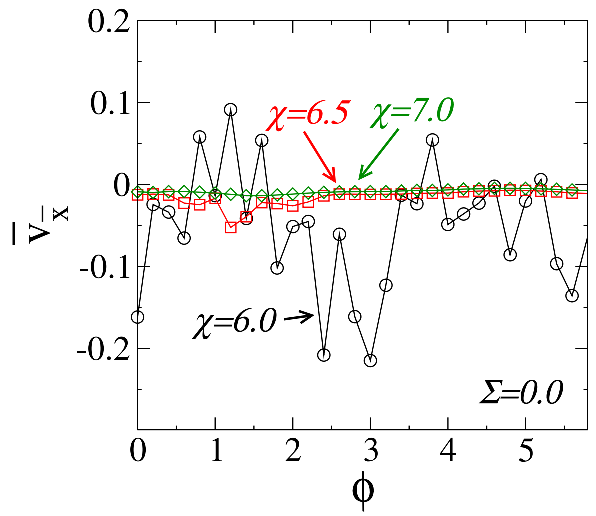

Fig. 7. Phase dependence of the centroid velocity for a fully localized initial wave-packets ($\Sigma = 0.0$). The AC and DC fields are set in the same resonance condition as in Fig. 2. Above a critical non-linearity of the order of $\chi_c \approx 7.0$ the centroid velocity vanishes irrespective to the AC field phase, a signature of the complete self-trapping.

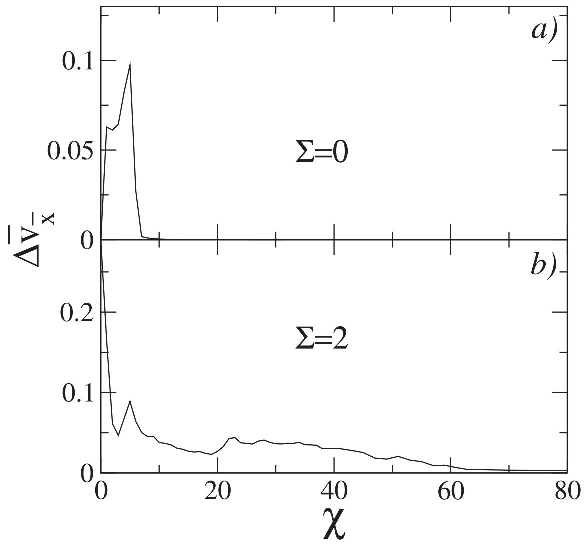

Fig. 8. The mean square deviation of the centroid velocity $\Delta\bar{v}_{\bar{x}} = \sqrt{<\bar{v}_{\bar{x}}^2>_\phi - (<\bar{v}_{\bar{x}}>_\phi)^2}$ with respect to the AC field phase. While the self-trapping with $\Delta\bar{v}_{\bar{x}} = 0$ takes place at $\chi_c \approx 7$ for a fully localized initial state (a), a much large non-linearity is required to obtain the self-trapping of a wider Gaussian initial wave-packet with width $\Sigma = 2$ (b). The field parameters were the same as in the resonance condition used in Fig. 2.

in components moving in opposite directions of a nonlinear media, with velocities that can be controlled by tuning the phase of an AC field in resonance with Bloch oscillations. This feature opens a new possibility for manipulating matter waves. Considering that several experiments with could atoms trapped in optical lattices have already been realized to demonstrate unconventional aspects of matter wave such as Bloch oscillations and unidirectional motion [19], we hope the here predicted phenomenology can be experimentally verified in the near future. However, it is important to have in mind that the strong sensitivity of the outcome wave-packet nonlinear dynamics on the physical parameters have to be carefully taken into account if one aims to use them as control parameters.

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