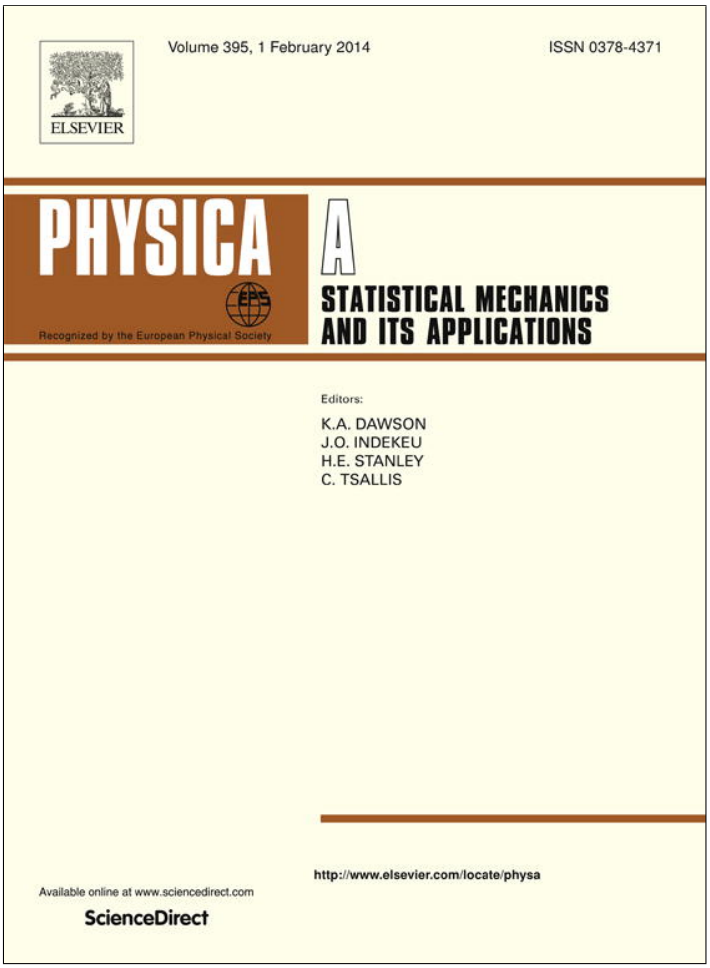

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Wavepacket dynamics of coupled particles in aperiodic chains: Weakening of Anderson localization and local field effects

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HIGHLIGHTS

- Dynamics of two electrons in $1d$ aperiodic systems.
- Effect of electron–electron interaction.
- Effect of electric field on aperiodic systems.

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ABSTRACT

We study the wavepacket dynamics of two interacting particles under an aperiodic potential that can be continuously tuned from a pseudo-random to a uniform regime. Assuming an on-site Hubbard interaction, we show that the influence of interaction is not strong enough to change the characteristic aperiodicity that signals the emergence of extended states. However, we unveil that the inter-particles interaction promotes a weakening of Anderson localization that is more prominent at intermediate couplings. The wavepacket dynamics in the regime presenting extended eigenstates show an oscillatory motion of the centroid while the wavepacket widens. We explain in detail the origin of these oscillations and discuss the characteristics of the Bloch oscillations of the two-particles wavepacket by exploring the relevance of bounded states to the dynamics of pair formation.

1. Introduction

Electronic transport in disordered systems has been a subject of much interest since Anderson [1] demonstrated the localization of electronic wave functions by disorder. The single-parameter scaling hypothesis [2] predicts that all states are localized in systems with dimension $d < 2$ and, consequently, no metallic phase survives in low-dimensional disordered systems. However, some systems do not obey the single-parameter scaling framework. Among these systems, we highlight those incorporating a pseudo-random aperiodic potential [3,4]. The experimental discovery of quasi-crystals and their role in different domains of science and technology [5–11], with applications in photonic devices, has resulted in the engineering of a number of novel devices with new functionalities [12,13].

It is noteworthy that many models devoted to study the Anderson localization problem are restricted to non interacting particles. Even within the on-site Hubbard-like interaction framework, the analytical or numerical study of many body systems represents a hard task due to the fact that the number of configurations grows exponentially with the system size. Within this context, a simple model with only two interacting particles has been considered in Refs. [14,15], which was able

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to rescue the important aspects of many particles systems [16,17]. These studies have shown that the presence of interaction promotes an increase in the localization length compared to that in the absence of interaction. The competition between disorder and inter-particles interaction has raised new questions, with some controversial results concerning the possible weakening of the Anderson localization due to interaction [14,18–20].

Within the context of two particles moving in a quasi-periodic potential some discrepancies were observed concerning the degree of localization. More specifically, within the Aubry–André framework [21,22], some results propose that a Hubbard-like interaction provides a decrease of the localization length in the localized phase [23,24]. On the other hand, a propagation enhancement for small interaction and strong localization for large interaction have also been reported [25,26]. In addition, for the Harper potential, a recent work suggested that two-particle states can change from being localized to delocalized by tuning the interaction strength [27]. It was also observed that the wavepacket becomes localized again in the regime of strong interaction. This result was attributed to the resonant mixing of the non-interacting two-particles eigenstates, consistent with the previous studies on the dynamics of coupled particles [28].

Given the aspects mentioned above, we advance in the study on two interacting particles by considering an aperiodic chain on which the underlying potential is a harmonic function governed by three parameters ($\epsilon_n = Q\cos(2\pi\alpha n^\nu)$). Within this model system, its possible to continuously tune from a periodic Bloch potential up to a pseudo-random potential [4]. We study the stationary eigenstates and dynamical aspects of this system in the presence of an on-site Hubbard interaction. We will show that the presence of interaction always promotes a weakening of Anderson localization, being more prominent for intermediate values of the interaction strength. The dynamical aspects of the system reveal that in the regime depicting extended states, the wavepacket centroid shows an oscillatory behavior around the initial position while the wavepacket widens. We explain in detail the origin of these oscillations and their influence on the Bloch oscillations frequencies of two-particles wavepackets driven by an external field. Finally, We also explore the effects of bounded states on the dynamics of correlated two-particles states.

2. Model

In the present work, we will consider a simple model for two interacting particles whose Hamiltonian operator is given by

$$H = \sum_n \sum_{p=1,2} J(\hat{b}^\dagger_{n+1,p}\hat{b}_{n,p} + \hat{b}^\dagger_{n,p}\hat{b}_{n+1,p}) + \sum_n \left[\sum_{p=1,2} \epsilon_n \hat{b}^\dagger_{n,p}\hat{b}_{n,p} + U\hat{b}^\dagger_{n,1}\hat{b}_{n,1}\hat{b}^\dagger_{n,2}\hat{b}_{n,2}\right] \tag{1}$$

where $\hat{b}_{n,s}$ and $\hat{b}^\dagger_{n,s}$ are the annihilation and creation operators for the particles at site n, J is the hopping amplitude, ϵ_n is the on-site energy at site n, and U is the on-site Hubbard interaction. We used units of $\hbar = J = 1$ without any loss of generality.

In the following, we will restrict our analysis to the case of two particles with different spins. As the Hamiltonian does not contain any spin exchange term, the particles can be considered as distinguishable. Additional quantum correlations would develop for the case of indistinguishable particles. Therefore, the assumption of distinguishable particles allows us to probe the correlations that are due to the underlying inter-particles interaction. In order to characterize the nature of the eigenstates $|\Phi\rangle$ of two distinguishable particles, we solve the time-independent Schrödinger equation to obtain the coefficients f_{n_1,n_2} in the expansion over the localized basis set $|\Phi\rangle = \sum_{n_1,n_2} f_{n_1,n_2}|n_1, n_2\rangle$. The sequence of on-site energies ϵ_n obeys the relation

$$\epsilon_n = Q\cos(2\pi\alpha n^\nu), \quad Q > 0 \tag{2}$$

with parameters Q, α and ν being variables which completely define the problem [4]. If α is rational and ν an integer, one results with a periodic Bloch potential. For $\nu = 1$ and α irrational, it is just Harper's equation, whereas for α irrational and $\nu \geq 2$, it is statistically equivalent to the random Anderson model. Taking α irrational, this one-dimensional deterministic potential shows a mobility edge for $0 < \nu < 1$ and $Q < 2$. There is a phase of extended states near the band center, which is separated by two mobility edges $\pm E_c = \pm(2 - Q)$ from the localized states at the band edges. All states are found to be localized whenever $Q > 2$ or $\nu > 1$, although the Lyapunov exponent approaches zero slowly at the band center for the latter [4].

3. Eigenstates

We start by applying a numerical diagonalization procedure of the complete Hamiltonian to obtain all eigenvectors $|\Phi\rangle$ and their corresponding eigenenergies E. In order to estimate the number of sites over which the wavefunction of energy E is spread, we compute the participation function

$$P(E) = \frac{1}{\sum_{n_1,n_2} |f_{n_1,n_2}(E)|^4} \tag{3}$$

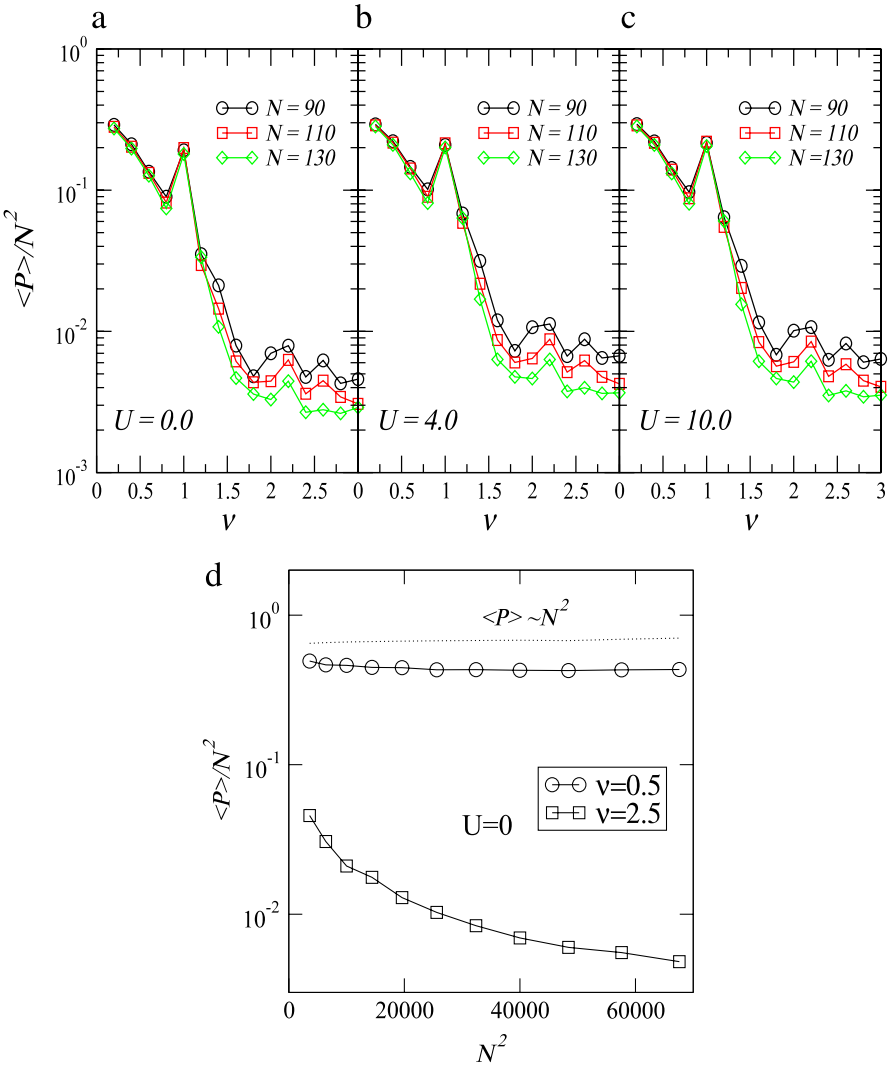

Fig. 1. Scaled average participation number $\langle P\rangle/N^2$ versus ν for $N = 90$, 110, 130 and (a) $U = 0.0$, (b) $U = 4.0$ and (c) $U = 10.0$. (d) Finite size scaling of the scaled participation number $\langle P\rangle/N^2$ versus N^2 for $\nu = 0.5$ and 2.5. Our calculations indicate that for $\nu \leq 1$, $\langle P\rangle$ is proportional to the volume of Hilbert space (N^2), thus indicating the extended states for any value of the interaction strength U.

In Fig. 1, we show the scaled average participation near the band center $\langle P\rangle/N^2 = (\sum_{|E|<0.5} P(E))/(N_E N^2)$ where N_E is the number of eigenstates within interval $|E| < 0.5$. Restricting the average only to the states located near the band center allows to more clearly signal the set up of the delocalization. The choice of the energy range to compute the average participation is arbitrary. The results remain mainly the same if this range is large enough to contain many states much smaller than the total bandwidth. We stress that the center of band $E = 0$ was avoided in this sum because the localization length of this eigenstate is large even in the strong disordered case. Calculations in figures $(a - c)$ were obtained using $N = 90$, 110, 130 sites, $Q = 1.5$, $2\pi\alpha = 1.0$, $\nu = 0.2, \ldots, 3.0$ and (a) $U = 0.0$, (b) $U = 4.0$, (c) $U = 10.0$. For $\nu \leq 1.0$ the scaled average participation seems to be size independent, i.e., the participation function is proportional to N^2. In Fig. 1(d) we provided a finite size scaling for two values of $\nu = 0.5$ and 2.5. Our calculations indicate that for $\nu < 1$ the participation number is proportional to N^2 thus indicating the extended two-particles modes. This feature is also obtained in the presence of inter-particles interaction U, which represents a clear signature of the presence of extended states in the center of the band. For $\nu > 1$ the system displays a localized regime. It is observed that the transition from localized to extended states agrees with the result obtained for the single particle problem [4], even in the presence of interaction. This indicates that the influence of interaction at this particular type of Anderson transition is not strong enough to change the characteristic value $\nu = 1$ below which the extended states appear [4,20,29].

In the Fig. 2(a), we compare the scaled participation number for non-interacting and interacting particles. We observe that the interaction does not modify substantially the low energy states in the regime presenting extended states. However, in the localized regime ($\nu > 1$), the scaled participation number indicates that interacting particles become less localized, in good agreement with the study of two interacting particles in a random potential [14]. When plotting the average participation versus U (see Fig. 2(b)), it is observed that $\langle P\rangle$ initially increases up to intermediate values of U and decreases slowly as U is further increased. The presence of interaction always promotes a weakening of Anderson localization, which is more prominent for intermediate interaction strengths.

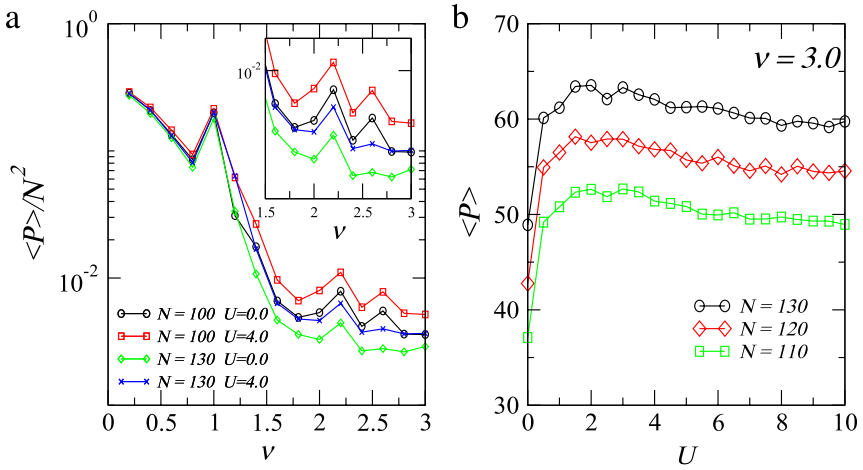

Fig. 2. (a) Scaled average participation number $\langle P\rangle/N^2$ versus ν for $N = 100, 130, U = 0.0$ and $U = 4.0$. In the localized regime, the weakening of Anderson localization due to the inter-particles interaction is identified. (b) The presence of interaction always promotes a weakening of Anderson localization, which is more prominent for intermediate values of the interaction strength.

4. Wavepacket dynamics

Although the results presented above indicate that, in the presence of extended states, the inter-particle interaction does not change significantly the average participation function of the eigenstates near the band center, the emergency of bounded states for $U > 0$ is expected to influence the dynamics of the two-particles wavepacket [30,31].

In order to follow the time evolution of wavepackets, we solve the time dependent Schrödinger equation by expanding the wave-function in the Wannier representation $|\Phi(t)\rangle = \sum_{n_1,n_2} f_{n_1,n_2}(t)|n_1, n_2\rangle$, where the ket $|n_1, n_2\rangle$ represents a state with one particle at site n_1 and the other particle at site n_2. According to the Hamiltonian (1), the time evolution of the wave-function in the Wannier representation can be obtained from

$$i\frac{\mathrm{d}f_{n_1,n_2}(t)}{\mathrm{d}t} = f_{n_1+1,n_2}(t) + f_{n_1-1,n_2}(t) + f_{n_1,n_2+1}(t) + f_{n_1,n_2-1}(t) + \left[\epsilon_{n_1} + \epsilon_{n_2} + \delta_{n_1,n_2}U\right]f_{n_1,n_2}(t) \tag{4}$$

The above set of equations (Eq. (4)) were solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $V(\Delta t)$:

$$V(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{n_o}\frac{(-iH\Delta t)^l}{l!} \tag{5}$$

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 method can be used recursively to obtain the wave-function at time t. The following results were taken by using $\Delta t = 0.05$ and the sum was truncated at $n_o = 22$. This cutoff was sufficient to keep the wave-function norm conservation along the entire time interval considered. Finally, we followed the time-evolution of an initial wavepacket composed of a product of Gaussian wavepackets of width σ:

$$\langle n_1, n_2|\Phi(t = 0)\rangle = \frac{1}{A(\sigma)}\exp\left[\frac{-(n_1 - n_1^0)^2}{4\sigma^2}\right]\exp\left[\frac{-(n_2 - n_2^0)^2}{4\sigma^2}\right] \tag{6}$$

where the particles initial positions are n_1^0 and n_2^0 respectively. We computed the centroid of both electrons defined as:

$$\langle n_i(t)\rangle = \sum_{n_1,n_2}(n_i - n_i^0)|f_{n_1,n_2}(t)|^2, \quad i = 1, 2 \tag{7}$$

In Fig. 3, we report the temporal evolution of the spacial extent defined by

$$\xi(t) = \sum_{n_1,n_2}\sqrt{[n_1 - \langle n_1\rangle_t]^2 + [n_2 - \langle n_2\rangle_t]^2}|f_{n_1,n_2}(t)|^2. \tag{8}$$

This function measures the wavefunction spread on the $n_1 \times n_2$ plane. Here we considered $N = 1800, 2\pi\alpha = 1, Q = 1.5, \nu = 0.5, \sigma = 1$ and $n_i^0 = 882$ (both particles at the same site). Associated with the Bloch-like nature of the extended states, the wavepacket presents a ballistic spread $\xi(t) \propto t^{1.0}$ even in the presence of inter-particles interaction. The initial ballistic spread is followed by a saturation related to multiple reflexions of the wavepacket at the chain boundaries.

By following directly the temporal evolution of the one-particle wavepacket profile $|f_n(t)|^2 = \sum_m |f_{n,m}(t)|^2$ for the same systems used in Fig. 3, it is observed that the centroid shows an oscillatory behavior around the initial position while the wavepacket widens (see Fig. 4). This oscillatory behavior has its origin in the aperiodic potential distribution. The harmonic

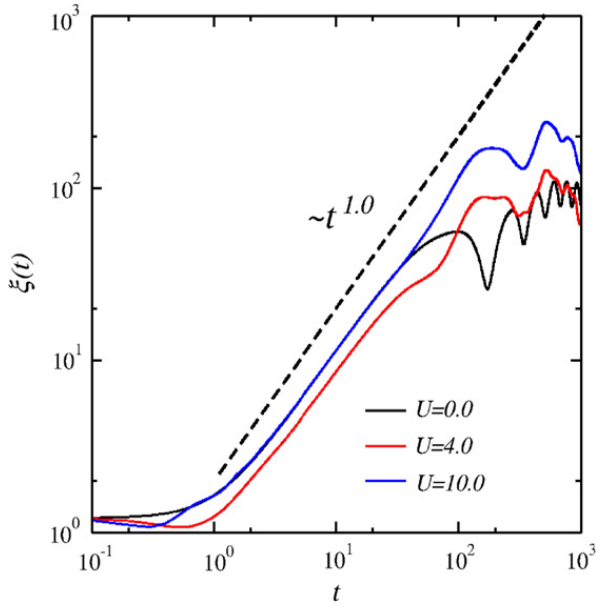

Fig. 3. Temporal evolution of the spacial extent $\xi(t)$ in the regime exhibiting extended states. Here we considered $N = 1800$, $2\pi\alpha = 1$, $Q = 1.5$, $\nu = 0.5$, $\sigma = 1$ and $n_i^0 = 882$. The wavepacket presents a ballistic spread $\xi(t) \propto t^{1.0}$ even in the presence of inter-particles interaction.

profile of the on-site potential works as a local effective field acting on both particles. This feature promotes an oscillatory behavior around the starting point n_i^0 similar to Bloch oscillations under the presence of an external uniform field. It is observed that the presence of interaction inhibits the centroid oscillation. In the absence of particle–particle interaction, the wavepacket spreads ballistically displaying a single peak structure, while in the presence of inter-particles interaction, the wavepacket develops two main structures. The first one is concentrated at the particles initial position and the second one has a strong amplitude at the wavefront [32]. The competition between these two components promotes a maximum correlation between the particles for intermediate values of U. This statement is consistent with the re-amplification of the particles oscillation for $U = 10$ (see Fig. 4(c)).

The analysis of these last results directed us to study the dynamics of two-particles wavepacket when subjected to an external uniform field. Bloch oscillation is a fundamental quantum-mechanical problem in solid state physics [33] experimentally observed in semiconductor super-lattices [34]. They have also been observed in ultra-cold atoms [35], Bose–Einstein condensates [36] and non-interacting fermions in tilted optical lattices [37]. The wave nature of light and some analogies between Maxwell and Schrödinger wave equations in periodic media, has been explored to expose the similarity between optical and electronic transport [38]. As a result, analogues of Bloch oscillations have been proposed using light beams in arrays of waveguides [39]. Circumventing the difficulties presented in drawing a comparative study involving the interacting particle systems, it was recently proposed that such systems are able to provide a test bed for an experimental demonstration of Bloch oscillations of correlated particles [40], corroborating the previous theoretical studies performed in the context of two interacting particles [28].

Before concluding, we will study the role played by the aperiodic potential acting concurrently with an external electric field on the two-electron dynamics. To include the external electric we will rewrite the original diagonal term of the Hamiltonian, i.e $\epsilon_{n_1} + \epsilon_{n_2} + U\delta_{n_1,n_2}$, in order to include the energy related to the electron-field interaction: $\epsilon_{n_1} + \epsilon_{n_2} + F(n_1 - n_1^0) + F(n_2 - n_2^0) + U\delta_{n_1,n_2}$ where F is the external electric field intensity. In Fig. 5 we show the time evolution of the one-particle wavepacket profile $|f_n(t)|^2 = \sum_m |f_{n,m}(t)|^2$, in the presence of a static external field with magnitude $F = 0.5$ and (a) $U = 4$ with $n_1^0 = 199$ and $n_2^0 = 283$ ($d_0 = n_2^0 - n_1^0 = 84$), (b) $U = 4$ with $d_0 = 0$ ($n_1^0 = n_2^0 = 199$) and (c) $U = 10$ with $d_0 = 0$ ($n_1^0 = n_2^0 = 283$), computed using a chain with $N = 500$ sites. The particle positions were chosen such that the local potential has distinct gradients. One clearly sees that the wavepacket becomes trapped around the initial position and a periodic coherent oscillation is observed. The results shown in Fig. 5(a) confirm the expectation of the semi-classical approach, since the amplitude of oscillation is inversely proportional to the magnitude of the external field ($A = \Delta/qE$, where Δ is the bandwidth). Since the interaction between them is on-site and the two particles are initially far apart, there is no influence of the inter-particle interaction on the wavepacket dynamics. In Fig. 5(b) it is observed that a small portion of the wavepacket has an oscillatory pattern consistent with that displayed by an independent particle, as seen in the Fig. 5(a). However, a significant part of the wavepacket has an oscillatory pattern with a smaller amplitude. The change of the oscillatory pattern from Fig. 5(a) to 5(b) is associated with the corresponding energy bandwidth of bounded states. It is known that the presence of an on-site Hubbard interaction gives rise to a band of extended bound states with width $\sqrt{U^2 + 16} - U$ [30,31]. The width of this band of bounded states is smaller than the non-interacting band. Just as it was observed in the absence of an external field, the oscillatory pattern of independent particles is amplified again for stronger interactions (see Fig. 5(c)).

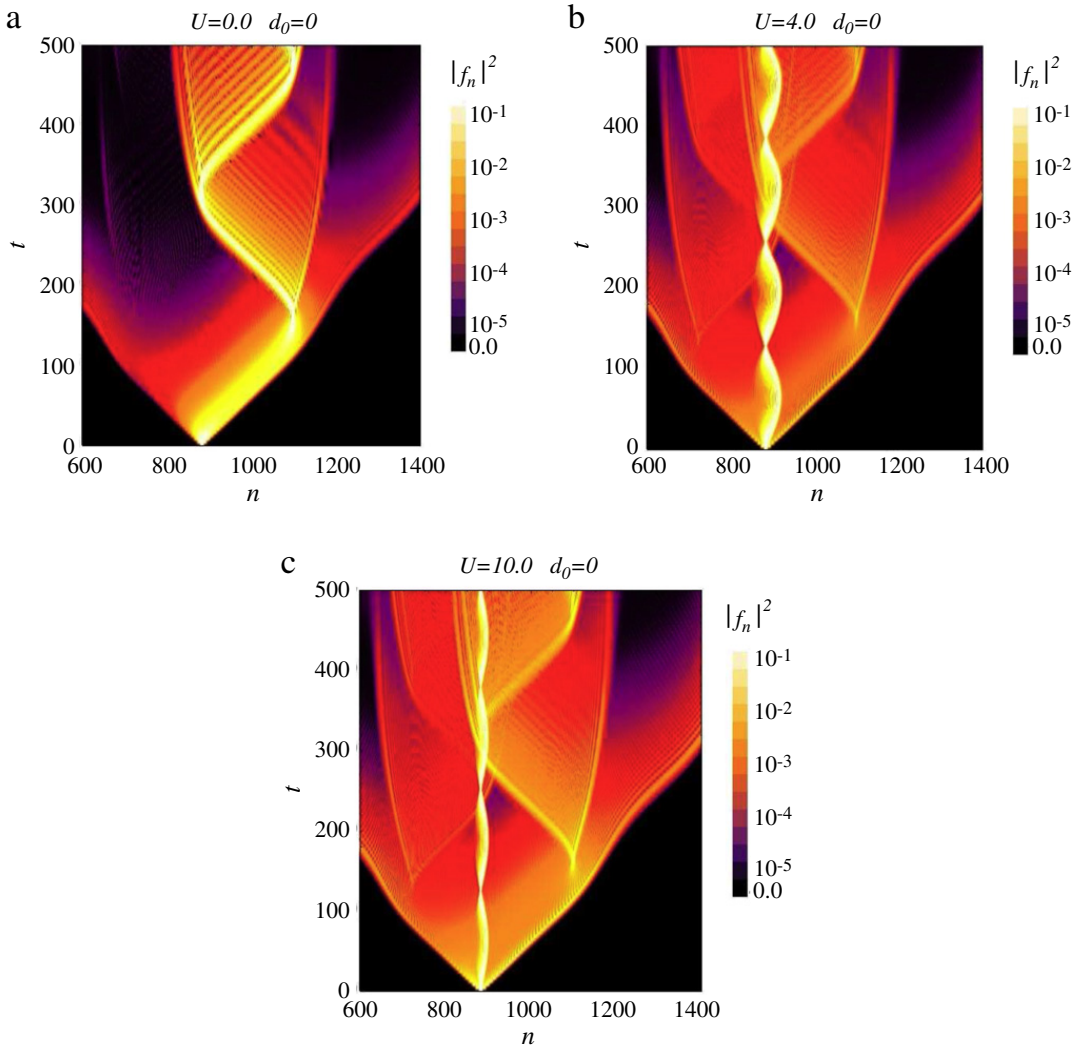

Fig. 4. Temporal evolution of the one-particle wavepacket profile $|f_n(t)|^2 = \sum_m |f_{n,m}(t)|^2$ for systems with $N = 2000$, $2\pi\alpha = 1$, $Q = 1.5$, $\nu = 0.5$, $\sigma = 1$, $n_1^0 = n_2^0 =$ and (a) $U = 0.0$, (b) $U = 4.0$ and (c) $U = 10.0$. We observe that the centroid shows an oscillatory behavior around the initial position while the wavepacket continues to widen. For strong interactions, the presence of bounded states components in the initial wavepacket promotes the trapping of a finite fraction of the wavepacket around the initial site.

In Fig. 6, we show the results for the Fourier transform $\langle n_i(\omega)\rangle$ of the wavepacket centroid computed using a chain with $L = 500$ sites in the presence of a constant external field with magnitude $F = 0.5$ and (a) $U = 4$ with $d_0 = 84$ ($n_1^0 = 199$, $n_2^0 = 283$), (b) $U = 4$ with $d_0 = 0$ ($n_1^0 = n_2^0 = 199$) and (c) $U = 10$ and $d_0 = 0$ ($n_1^0 = n_2^0 = 283$), $\sigma = 1$,. We observe that for $d_0 \gg 0$ the Fourier transform $\langle n_i(\omega)\rangle$ shows that the predominant oscillation frequency is close to the semi-classical prediction $\omega = F$ [30,31]. For $U = 4$ and $d_0 = 0$ the Fourier transform $\langle n_i(\omega)\rangle$ clearly shows that the centroid displays an oscillatory pattern with a predominant frequency close to $\omega = 2F$. For much stronger interactions, the $\omega = F$ frequency is re-amplified. Therefore, our results suggest that the doubling frequency phenomenon for two-interacting particles previously reported for periodic chains [31] also takes place in aperiodic chains in the regime presenting extended Bloch-like states $\nu < 1$. However, by examining in detail the Fourier transform around the predominant frequencies (see inset), we can see that the frequencies found here are somewhat different from the predicted semi-classical value. In fact, the oscillation's frequency exhibits shifts which are associated to the local potential gradient. Using semi-classical arguments, the total field at position n_i^0 is given by

$$F_{ef} = \frac{d\epsilon_n}{dn} + F, \tag{9}$$

with $d\epsilon_n/dn$ representing the local field strength. For the sites $n = 199$ and $n = 283$ (initial position of particles) we have $d\epsilon_n/dn \approx -0.053$ and $d\epsilon_n/dn \approx 0.040$ respectively. The insets of Fig. 6 display a magnification, providing a greater detail of the oscillation frequency for each particle, corroborating the result proposed by Eq. (9). For $U = 4$ (Fig. 6(b)) the spectrum of frequencies displays a structure of multi-modes near of standard frequency of BO ($\omega = qEa/\hbar$) and a predominant mode related to the frequency doubling phenomenon [40,31,32]. Since the particles are clustered into an interacting cloud at time $t = 0$, the components associated with bounded states keep the particles paired and produces coherent hoppings,

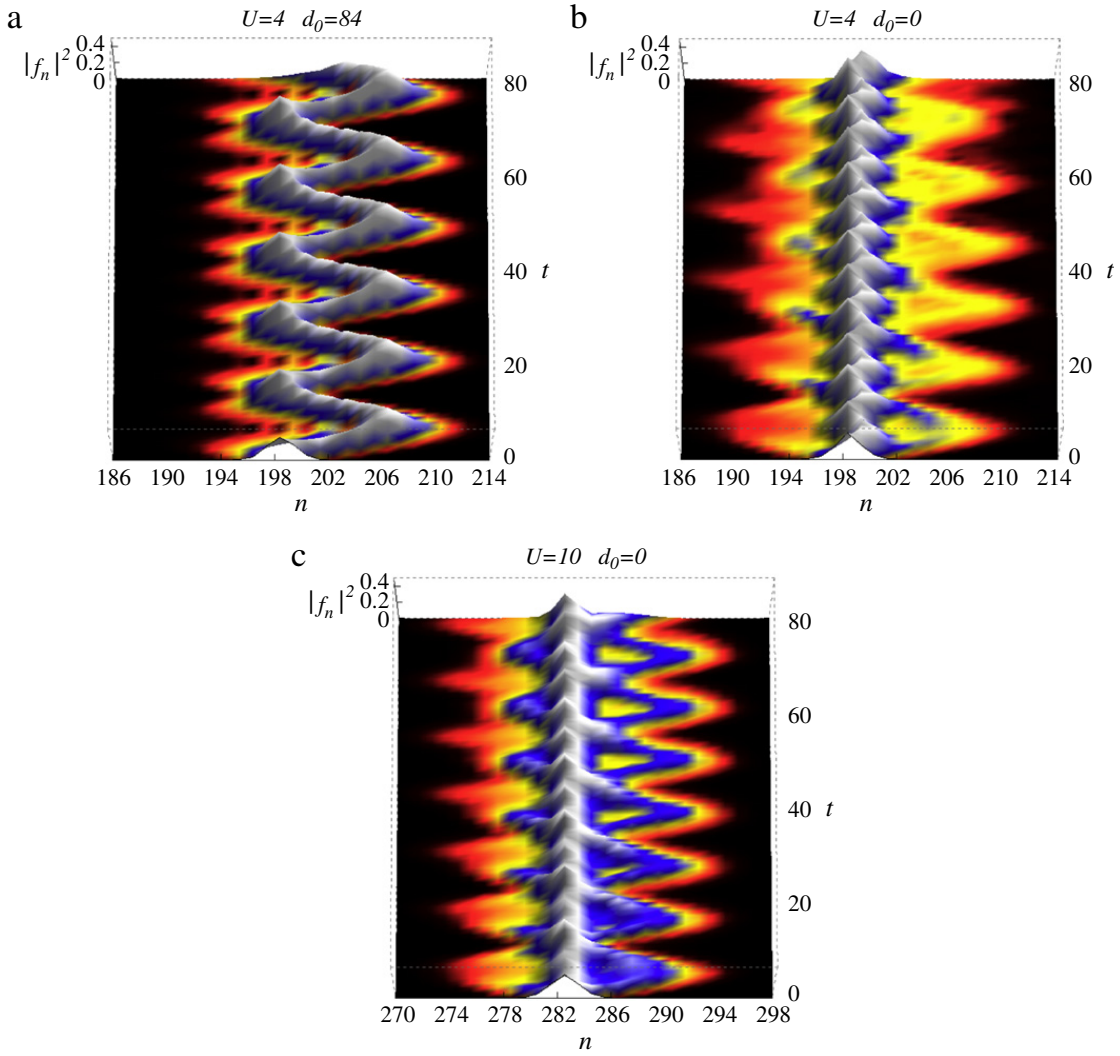

Fig. 5. Time evolution of the one-particle wavepacket profile $|f_n(t)|^2 = \sum_m |f_{n,m}(t)|^2$ in the presence of a uniform external field with magnitude $F = 0.5$ and (a) $U = 4$ with $n_1^0 = 199$ and $n_2^0 = 283$, (b) $U = 4$ with $n_1^0 = n_2^0 = 199$ and (c) $U = 10$ with $n_1^0 = n_2^0 = 283$. The inter-particle correlation promotes oscillations with much smaller amplitude when compared to the amplitude of an independent particle oscillation. The correlation is stronger for intermediate values of the interaction strength.

where two particles of charge q behave like a single particle of charge $2q$. The components associated with unbounded states produce independent hoppings, responsible by the frequency $\omega = qEa/\hbar$. The small splitting observed is due to the particle–particle interaction, which is also responsible for the emergence of an additional oscillation frequency of the drift velocity of bounded eigenstates [30]. Note also that the frequency shift is also connected to the effective particle number, since the shift for the doubling frequency peak is two times the local effective field (see inset of Fig. 6(b)). For strong interactions, the oscillatory pattern of independent particles is re-amplified, as a result of the competition between the trapped and travelling components of the wavepacket, as can be seen in Fig. 6(c).

5. Summary and conclusions

In this work, we studied the one-dimensional dynamics of two interacting distinguishable particles under the influence of an aperiodic potential and a static uniform external field F. To introduce aperiodicity, we assigned values to the on-site energies according to a deterministic rule $\epsilon_n = Q\cos(2\pi\alpha n^\nu)$, where α is an arbitrary rational number and ν and Q are tunable parameters [4]. The exponent ν controls the degree of aperiodicity in the on-site terms. By considering an on-site Hubbard interaction, we determined the stationary eigenstates which showed a localization–delocalization transition around the band center for $Q < 2$ and $\nu \leq 1$ irrespective to the coupling strength.

We reported that the presence of interaction always promotes a weakening of the degree of localization of the high energy modes which is more prominent for intermediate values of the interaction strength. Moreover, we studied some wavepacket dynamical aspects by solving numerically the time-dependent Schroedinger equation. In the presence of extended Bloch-like states, the centroid shows an oscillatory behavior around the initial position while the wavepacket widens. We explained

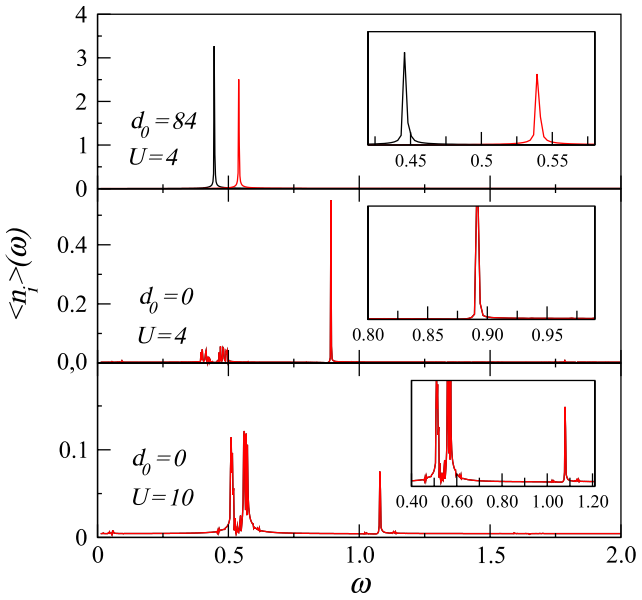

Fig. 6. Fourier transform of the centroid for the same conditions of Fig. 5, (a) $U = 4$ and $d_0 = 84$; (b) $U = 4$ and $d_0 = 0$; (c) $U = 10$ and $d_0 = 0$. The oscillation frequencies are somewhat different from the value predicted by the semi-classical approach ($\omega = F$). In fact, the oscillation's frequency found here exhibits shifts which are associated with the local potential gradient. The frequency shifts are also connected to the pair formation, since the shift on the doubling frequency peak is two times the one achieved by non-interacting particles (see inset).

the origin of these oscillations based on the particular features of the on-site potential and the existence of bounded states components on the initial wavepacket.

The effect of an external field was also discussed in detail. We analyzed the interplay of the effective local field related to the aperiodic potential and the external static uniform field. We found Bloch oscillations whose frequencies are strongly dependent on these two ingredients. We provided numerical predictions for the shift of the Bloch oscillation's frequencies based on the effective local field calculations. The results reported here provide additional evidences that the inter-particles interaction plays a major role in the wavepacket dynamics for intermediate values of the Hubbard coupling, leading to both frequency and frequency-shift doubling in aperiodic system with delocalized states.

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