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Sub-diffusive spreading and anomalous localization in a 2D Anderson model with off-diagonal nonlinearity

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ABSTRACT

We study the electronic wavepacket dynamic in a two-dimensional lattice under the influence of off-diagonal nonlinearity in the regime of diagonal disorder larger than the crystalline bandwidth. By using numerical calculations of the participation function, the mean square displacement and the return probability, we show that the nonlinearity induces a sub-diffusive spreading of the wavepacket. We also report the existence of an anomalous nonlinear strength at which the wavepacket remains strongly localized.

1. Introduction

One of the fundamental phenomenon in solid state physics is related to the electronic wavepacket propagation in disordered structures. The localization theory, pioneered by P.W. Anderson, points out the localized nature of a non-interacting electron wavepacket due to a strong diagonal disorder [1–3]. Although the initial proposal has been devoted to electronic properties, the phenomenon of wave localization in disordered media has been observed in several other branches, such as electromagnetic [4,5] and acoustic [6] waves.

In particular, studies of matter waves localization [7] have provided an excellent framework to answer challenging open questions of condensed matter. A remarkable characteristic in these systems is the relevance of nonlinear effects. In particular, the evolution of a Bose-Einstein Condensate can be described by using the nonlinear Gross-Pitaevskii equation [8]. On the other hand, the nonlinearity in the Schrödinger equation of electronic systems has its origin in the electron interaction with the vibrational modes of the lattice [9,10]. This mechanism is of great interest in state solid physics, since the presence of nonlinearity may trap a wavepacket in a finite fraction of the lattice, a phenomenon called self-trapping [9,10]. It occurs when the strength of the nonlinearity exceeds a critical value. In addition, it is worth mentioning that a similar scenario holds for the propagation of nonlinear waves in photonic lattices [5,11]. As such, the study of wave dynamics in media involving simultaneously nonlinearity and disorder plays a relevant role in condensed matter, both in the theoretical [7,9,12–16] and experimental frameworks [7,11,17,18].

The competition between disorder and nonlinearity leads to a series of interesting features. It was demonstrated that in 1D disordered systems, the Anderson localization is destroyed for a specific range of values of the nonlinearity parameter [12,19]. A similar result was reported for the spatio-temporal evolution of a wavepacket in disordered nonlinear Schrödinger and anharmonic chains [20]. A systematic investigation of wave propagation in nonlinear disordered systems can be found in Refs. [21–27]. By considering the disordered discrete nonlinear Schrödinger equation and a quartic Klein-Gordon chain of coupled anharmonic oscillators, a general description of the one-particle propagation within disordered nonlinear chains was obtained [21]. Moreover, the propagation of nonlinear waves in two-dimensional disordered lattices with tunable diagonal nonlinearity was reported in Ref. [22]. It was demonstrated that nonlinear wavepackets spread sub-diffusively. The authors also showed that the degree of localization decreases as the strength of nonlinearity increases. In Ref. [23], a general theory of localization in nonlinear disordered systems at the zero-temperature limit was developed, firmly establishing that nonlinear waves can indeed propagate in nonlinear disordered systems. It is interesting to mention that, in spite of the literature has pointed out the absence of Anderson localization in nonlinear disordered systems, the kind of diffusion was a controversial issue. In general lines, some authors showed that the spread of a wavepacket starting from a single-site excitation grows as $t^{0.15}$ [21]. However, distinct time evolutions were also obtained: $t^{0.2}$ [12] or $t^{0.25}$ [25] for example. This controversy was clarified in Ref. [26]. The authors demonstrated that, depending on the disorder strength and nonlinearity intensity, three dis-

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tinct regimes can appear: strong chaos, weak chaos and self-trapping. Each regime exhibits distinct temporal behavior for the wavepacket spreading [26]. Further, it has been recently unveiled the probabilistic nature of the break up of Anderson localization in nonlinear disordered systems with the spreading dynamics being strongly dependent of the disorder configuration [23]. Ref. [27] contains an interesting and motivational review about the recent theoretical trends within this field. Within the experimental context, a one-dimensional lattice of coupled optical waveguides patterned on an ALGaAs substrate was considered to investigate the evolution of linear and nonlinear waves in a realization of the Anderson model. By exciting a pure localized mode and increasing the input beam power, the authors reported that the nonlinearity tends to promote the propagation of nonlinear modes [11]. Another experimental work showed that the dynamics of matter waves in the presence of disorder and nonlinearity also reveals a sub-diffusive behavior when a controllable repulsive atom-atom interaction is added to an atomic Bose-Einstein Condensate [28].

In general, the coupling between electrons and lattice vibrational modes is expressed by diagonal nonlinearity on a tight binding approach [12,19,29,30]. However, the electron-lattice coupling can also result in off-diagonal terms [31–33]. Originally developed to study electrical properties of polymers [31], the Su-Schrieffer-Heeger Hamiltonian was used to analyze a one-dimensional nonlinear Schrödinger equation containing off-diagonal nonlinearity and diagonal disorder [32]. Recent results showed that the wavepacket displays a long-time sub-diffusive regime promoted by the nonlinear off-diagonal term [33]. The authors also showed that only those states around the band center are susceptible to the presence of an off-diagonal nonlinear contribution.

Aiming to understand the competition between nonlinearity and diagonal disorder on the electronic wavepacket dynamics, we provide a detailed study of the wavepacket propagation in a 2D disordered nonlinear square lattice. The existing disorder in the lattice has compositional origin, i.e., it is represented on the diagonal term of the Hamiltonian. We take into account the coupling of the electronic wavepacket with the acoustic phonons, originating the off-diagonal nonlinear term. Through the participation function and mean square displacement, we show that the nonlinearity induces a sub-diffusive spreading of the wavepacket. However, the sub-diffusive regime only develops after a long waiting time for small nonlinearities. We also report the existence of an anomalous point at which the wavepacket remains trapped at the initial position.

2. Model and formalism

We consider an electron moving in a two-dimensional (2d) square lattice with diagonal disorder and coupled with the atomic vibrations. Following the Su-Schrieffer-Heeger approach [31], we write the Hamiltonian of the electronic tight binding system, where the hopping integrals depends on the relative molecular displacements [30,32]:

$$H = \sum_{m,n}\left[\frac{(\dot{q}_{m,n})^2}{2} + \frac{K}{2}(q_{m,n} - q_{m-1,n})^2\right] + \sum_{m,n}\epsilon_{m,n}c^{\dagger}_{m,n}c_{m,n} + \sum_{m,n}\Big\{\Big(V_{m+1,n}c^{\dagger}_{m+1,n}c_{m,n} + V_{m,n+1}c^{\dagger}_{m,n+1}c_{m,n} + V_{m-1,n}c^{\dagger}_{m-1,n}c_{m,n} + V_{m,n-1}c^{\dagger}_{m,n-1}c_{m,n}\Big)\Big\}, \quad (1)$$

Here, $V_{m+\nu,n+\pi} = [V_0 + \tau(q_{m,n} - q_{m+\nu,n+\pi})]$ (ν and π assume values −1,0 or 1), $q_{m,n}$ is the atomic displacement, V_0 is the intrinsic hopping integral, τ is the electron-phonon coupling constant, $\epsilon_{m,n}$ is the on-site energy of element (m,n) randomly distributed in the interval $[-W/2, W/2]$ with uniform probability and $c^{\dagger}_{m,n}$ and $c_{m,n}$ are the creation and annihilation operators for the electron at the site m,n.

We assume that the electron is treated in the adiabatic approximation. Therefore lattice vibrations reach equilibrium on a time scale much smaller than the evolution time of the electronic wavepacket. In this regime ($\tau q_{m,n} \sim \chi|\psi_{m,n}|^2$). Once stated these preliminary considerations, we take the wavefunction in the Wannier representation $|\Psi(t)\rangle = \sum_{m,n}\psi_{m,n}(t)|m,n\rangle$ to write the Schrödinger equation with a nonlinear hopping term

$$i\hbar\frac{d\psi_{m,n}}{dt} = \epsilon_{m,n}\psi_{m,n} + [V_0 + \chi(|\psi_{m,n}|^2 + |\psi_{m+1,n}|^2)]\psi_{m+1,n} + [V_0 + \chi(|\psi_{m,n}|^2 + |\psi_{m,n+1}|^2)]\psi_{m,n+1} + [V_0 + \chi(|\psi_{m,n}|^2 + |\psi_{m-1,n}|^2)]\psi_{m-1,n} + [V_0 + \chi(|\psi_{m,n}|^2 + |\psi_{m,n-1}|^2)]\psi_{m,n-1} \quad (2)$$

where the parameter χ controls the degree of nonlinearity, describing the effective electron-phonon coupling. Using a predictor-corrector Adams-Bashforth-Moulton algorithm initialized by the Dormand-Prince Runge-Kutta method of order eight [35], we solve this set of nonlinear coupled differential equations. Our calculations for long times were done by using the tenth-order Adams-Bashforth formalism as the pre-

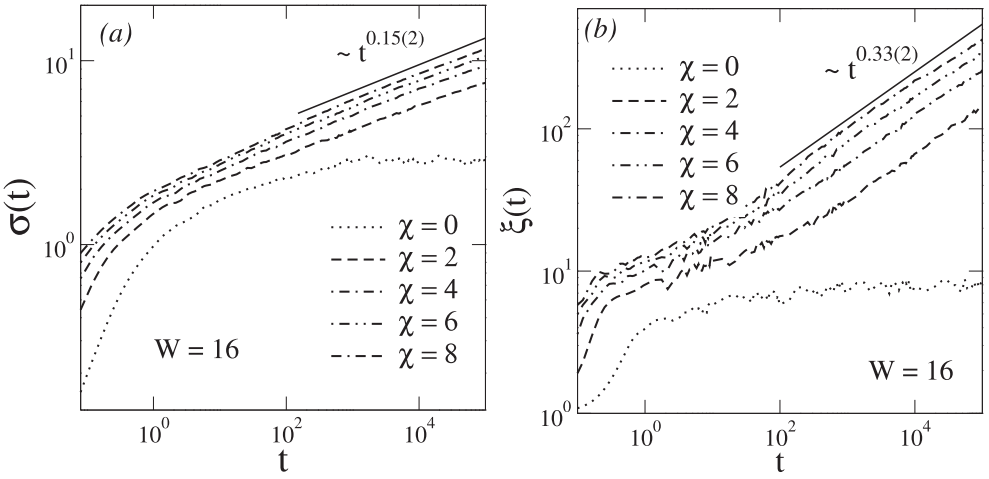

Fig. 1. (a) Root-mean-square displacement and (b) participation function versus time, for diagonal disorder $W = 16$ and nonlinearity parameter $\chi = 0$, 2, 4, 6 e 8. These two quantities show a non-localized wavepacket in the Anderson sense when a nonlinear hopping is present, depicting a sub-diffusive spreading.

dictor formula and the ninth-order Adams-Moulton procedure as the corrector. The time step used here ($\Delta t = 0.004$) is satisfactory to solve the set of nonlinear coupled differential equations with good precision. We checked at each time step the norm conservation, obtaining ($|1 - \sum_{n,m}|\psi_{m,n}|^2| < 10^{-9}$) even for long times. We observed the time-evolution of an initially localized wavepacket, i. e., $|\Psi(t=0)\rangle = \sum_{m,n}\psi_{m,n}(t=0)|m,n\rangle$, where $\psi_{m,n}(t=0) = \delta_{m,N/2}\delta_{n,N/2}$.

In order to analyze some aspects related to the electronic wavepacket dynamics, we first set it localized in the middle of the alloy at $t = 0$, i. e. $|\Psi(t=0)\rangle = \sum_{m,n}\psi_{m,n}(t=0)|m,n\rangle$, where $\psi_{m,n}(t=0) = \delta_{m,N/2}\delta_{n,N/2}$. Then we used some standard tools as the return probability [29,36], the participation number and the root-mean-square displacement. The return probability $R(t)$ is defined as:

$$R(t) = |\psi_{N/2,N/2}(t)|^2, \tag{3}$$

where $R(t)$ gives the probability of finding the electron at the position corresponding to the center of the initial wavepacket. Thus, in the long-time regime (we have used $t_{\max} \approx 10^5$ in our calculations), $R(t_{\max}) \to 0$ means that the electronic wavefunction escapes from its initial localization $(N/2, N/2)$. Otherwise, at least a fraction of the electronic wavepacket remains localized in a self-trapped state when $R(t_{\max})$ saturates at a finite value. The participation number ξ is defined as [30,37],

$$\xi(t) = 1\Big/\sum_{m,n}|\psi_{m,n}(t)|^4. \tag{4}$$

This measure provides an estimate of the number of base states where the wavepacket is spread in time t. In particular, the asymptotic participation number becomes size-independent for localized wavepackets. Conversely, $\xi(t_{\max}) \propto N^2$ corresponds to the regime where the packet is delocalized over the lattice [37].

The root-mean-square displacement $\sigma(t)$ [36,38,39] is obtained as:

$$\sigma(t) = \sqrt{\sum_{m,n}[(m - \overline{m(t)})^2 + (n - \overline{n(t)})^2]|\psi_{m,n}(t)|^2}, \tag{5}$$

with $\overline{m(t)} = \sum_{m,n} m|\psi_{m,n}(t)|^2$ and $\overline{n(t)} = \sum_{m,n} n|\psi_{m,n}(t)|^2$. We stress that σ ranges from 0 (a wavefunction fully localized in a single site) to $\sigma \propto N$ (a wavefunction extended over the entire lattice). The time evolution of the root-mean-square displacement usually follows a power law $\sigma(t) \propto t^{\alpha}$, characterizing the motion of the wavepacket as localized ($\alpha = 0.0$), sub-diffusive ($0 < \alpha < 1/2$), diffusive ($\alpha = 1/2$), super-diffusive ($1/2 < \alpha < 1$) and ballistic ($\alpha = 1$) [40–42].

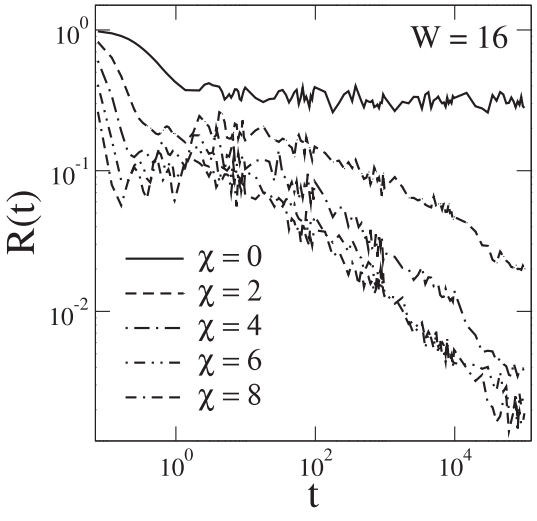

Fig. 2. Time evolution of the return probability $R(t)$. The decay of $R(t)$ with time t for all positive values of χ is a signal of the sub-diffusive spreading shown in Fig. 1. For $\chi = 0$ the wavepacket is localized in the Anderson sense, with the return probability remaining close to unit.

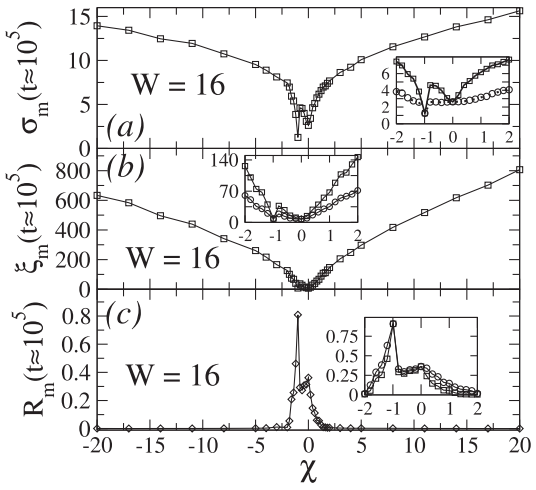

Fig. 3. (a) Average extension of the wavepacket $\sigma_m(t_{\max})$; (b) average participation number for long time $\xi_m(t_{\max})$; and (c) average return probability $R_m(t_{\max})$ calculated for different values of χ and disorder amplitude $W = 16$. Main plots are for $t_{\max} = 10^5$. The insets show data for $t_{\max} = 10^4$ and $t_{\max} = 10^5$, unveiling that wavepacket localization is only achieved in the linear limit of $\chi = 0$ and in the anomalous point with $\chi = -1$.

3. Results

In Fig. 1(a) and (b) we plot, respectively, the time evolution of the root-mean-square displacement $\sigma(t)$ and participation function $\xi(t)$. We have considered, in both figures, several values of the off-diagonal electron-phonon coupling constant χ at the strong disorder regime i.e. the disorder width larger than the bandwidth ($W > 8V_0$). In particular, we have chosen $W = 16V_0$. In this strong disorder regime, the wavepacket dynamics in systems with diagonal nonlinearity can only show self-trapping or sub-diffusion, depending on the nonlinearity strength [22,26]. In the absence of nonlinearity ($\chi = 0$), the wavepacket does not spread. This is the signature of the usual Anderson localization regime [43]. However, when the nonlinear hopping term is switched on ($\chi > 0$), we get $\sigma(t) \propto t^{0.15(2)}$ and $\xi(t) \propto t^{0.33(2)}$, thus supporting an electronic sub-diffusive dynamics. The exponents in Fig. 1(a) and (b) are roughly of the same order of magnitude of those found in one-dimensional models with diagonal nonlinearity [13,21]. We also found good agreement with those results found for two-dimensional disordered models with diagonal nonlinearity [22]. Notice that the sub-diffusion develops after a finite waiting time. The waiting time grows when the nonlinearity strength is decreased. It diverges in the limit $\chi \to 0$ signaling the strong Anderson localization in the linear

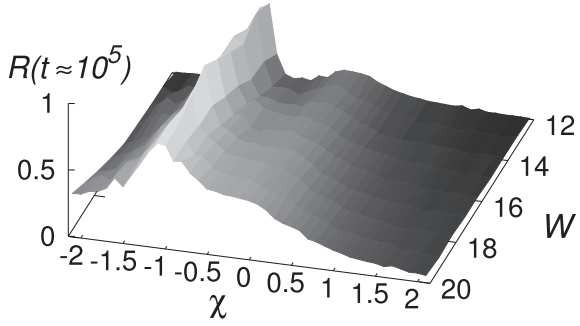

Fig. 4. Return probability after a long evolution time $R(t \approx 10^5)$ versus W and χ. The maximum at $\chi = 0$ stands for the usual Anderson localization in linear disordered systems. The narrow peak at $\chi = -1$ signals the anomalous localization point.

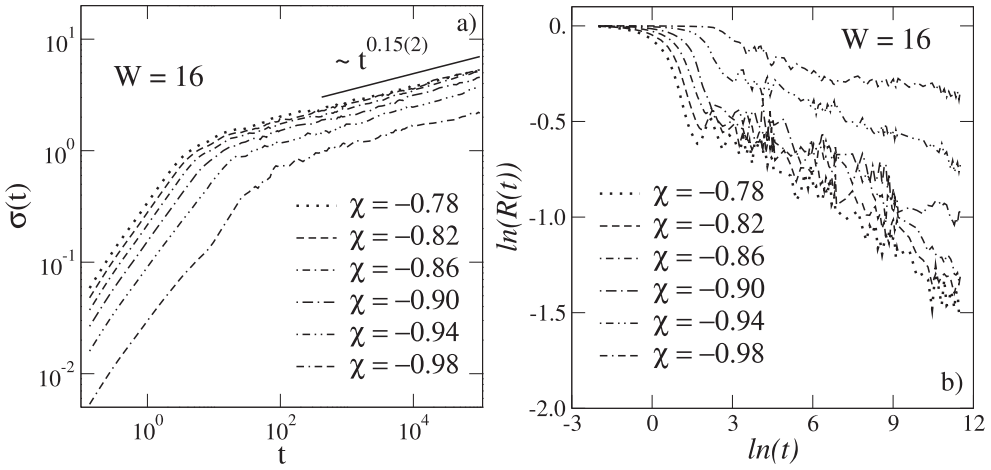

Fig. 5. (a) Root-mean-square displacement and (b) return probability versus time, for diagonal disorder $W = 16$ and nonlinearity parameter $\chi = -0.780, -0.82, -0.86, -0.9, -0.94$ and -0.98.

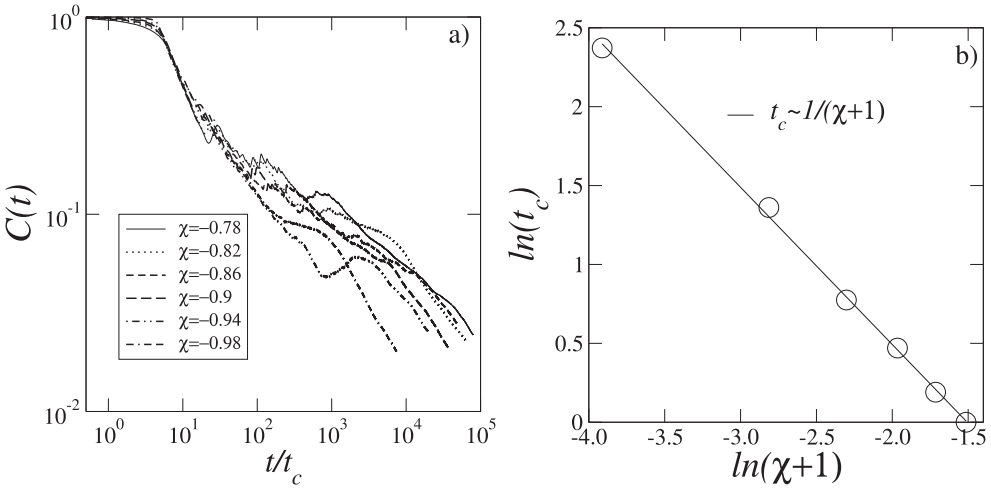

Fig. 6. (a) The autocorrelation function $C(t)$ versus t/t_c. We observe that all curves for distinct values of χ collapse into a single curve, except by random fluctuations in the very long-time regime. (b) Scaling behavior of the crossover time, indicating $t_c \propto 1/(1+\chi)$. Here, the crossover times were measured in units of $t_c(\chi = 0.78)$.

regime.

A complementary analysis of the sub-diffusive character induced by the nonlinearity is shown in Fig. 2, where we plot the return probability as a function of time for same cases considered in Fig. 1. When the electron-phonon interaction is absent, the return probability remains finite. This result is a direct consequence of the strong Anderson localization for $W = 16$. However, the presence of nonlinearity promotes the wavepacket spreading, with the probability of finding the electron close to the initial position vanishing as time evolves. It is important stress that models with diagonal nonlinearity can exhibit a regime with self-trapping above a nonlinearity threshold [26]. Within this self-trapping regime, a finite fraction of the initial wavepacket remains localized, while the remaining fraction spreads. This self-trapping regime was characterized by the saturation of the participation number co-existing with the sub-diffusive growth of the second moment [26]. In the present two-dimensional disordered model with off-diagonal nonlinearity such regime is absent, at least within the range of nonlinearities we explored. Both participation number and second moment show a sub-diffusive growth. In this sense, disordered systems with diagonal and non-diagonal nonlinear contributions display distinct wavepacket dynamical regimes.

In order to further characterize the suppression of Anderson localization due to the presence of a non-diagonal nonlinearity, we show in Fig. 3(a–c) respectively, the long-time behavior of the root-mean-square displacement $\sigma(t_{\max} \approx 10^5)$, participation function $\xi(t_{\max} \approx 10^5)$ and return probability $R(t_{\max} \approx 10^5)$ versus the nonlinear coupling. In the insets, we show a detail of these curves in the vicinity of $\chi = 0$ using two values for $t_{\max}$. These show that the wavepacket delocalizes (increasing values of $\sigma(t_{\max})$ and $\xi(t_{\max})$ with decreasing values of $R(t_{\max})$ as $t_{\max}$ increases) except at $\chi = 0$ and at the anomalous point $\chi = -1$ where the wavepacket remains strongly localized. For $\chi = -1$, the effective hopping vanishes, thus promoting the wavepacket trapping. This behavior was also reported in 1D systems (see Ref. [32]). Except in the close vicinity of $\chi \approx -1$, both $\sigma(t_{\max})$ curves and $\xi(t_{\max})$ show a monotonic growth as $|\chi|$ increases. In other words, the higher the value of $|\chi|$, the larger the anomalous diffusion coefficient is. In addition, the weak asymmetry observed in Fig. 3(a) and (b) suggests that the diffusion coefficient for positive values of χ is larger than in the case of negative values of χ. In the case of negative χ, the hopping term can be zero in some specific lattice sites, hence decreasing the diffusion coefficient.

In order to obtain a complete description of the dependence of the electronic dynamics with disorder and nonlinearity, we compute the return probability after a long evolution time and for a wide range of W and χ values. We plot, in Fig. 4, $R(t \approx 10^5)$ versus W and χ. By analyzing Fig. 4 we observe that even for strong disorder ($W > 10$) the

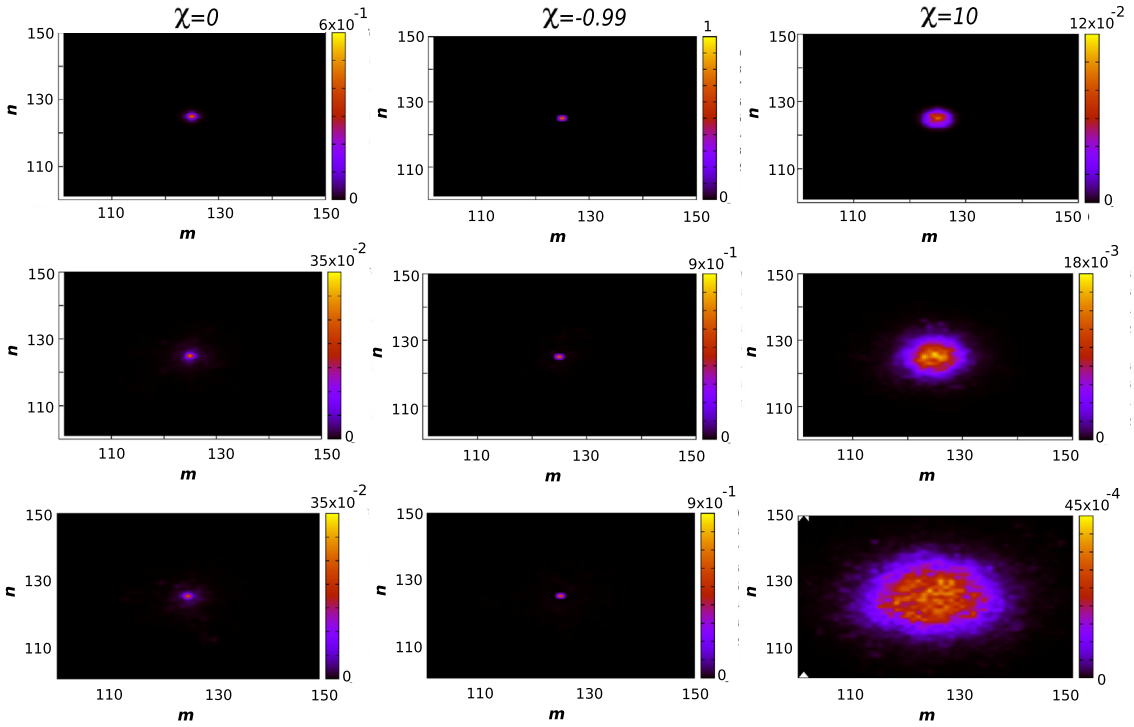

Fig. 7. Wavepacket snapshots at different stages of the time evolution, for $\chi = 0$, $\chi \approx -1$ and $\chi = 10$. From top to bottom, the pictures represent time instant $t = 0.5$, $t = 100$ and $t = 1000$. The off-diagonal nonlinearity pushes the suppression of Anderson localization even at very large nonlinearities, while the wavepacket remains trapped for $\chi = -1$.

nonlinearity promotes a decreasing return probability, thus suggesting the existence of a non-localized electronic dynamics. The wide peak around $\chi = 0$ accounts for the usual Anderson localization in linear disordered systems. For negative values of χ, the fingerprint of the anomalous point $\chi = -1$ is signaled by a narrow peak. We emphasize that at this special value of the nonlinearity, the effective hopping between the site at which the initial state is fully localized and its four nearest neighbor sites vanishes. Therefore the electron becomes fully trapped at its initial position. For negative values of χ such that $|\chi| > 1$, there is a nonzero probability of finding negative and positive hopping which results in the observed asymmetry.

To better characterize the behavior around $\chi = -1$, we plot the root-mean-square displacement $\sigma(t)$ and the return probability $R(t)$ versus time for diagonal disorder $W = 16$ and nonlinearity parameter $\chi = -0.780$, -0.82, -0.86, -0.9, -0.94 and -0.98 (see Fig. 5). We can observe that the spread σ decreases as $\chi \to -1$, displaying an increasing crossover time to the asymptotic sub-diffusive regime. Also, the waiting time for the return probability start to decrease becomes larger as this special nonlinearity value is approached. These results show that the escaping of the wavepacket from its initial position is suppressed as $\chi \to -1$ due to the vanishing of the effective hopping to the neighboring sites. To unveil the scaling behavior of the waiting time around the anomalous point $\chi = -1$, we will use an auxiliary tool called autocorrelation function defined as $C(t) = (1/t)\int_0^t R(t)dt$ where $R(t)$ represents the return probability. The autocorrelation function and the return probability display similar trends. However, $C(t)$ is less sensible to numerical fluctuations. For $\chi = -1$ the autocorrelation function remains $C(t) = 1$ in agreement with the strong localized behavior of the wavefunction. In the vicinity of $\chi = -1$ the autocorrelation function remains finite for a short time scale $t < t_c$ and decreases after long times $t > t_c$, thus suggesting electronic diffusion at the long-time regime. In order to estimate the dependence of the typical crossover time t_c with the nonlinear strength, we calculate the time evolution of $C(t)$ for several values of χ around -1. These curves shall exhibit a universal behavior when plotted against the dimensionless time scale t/t_c. Our results for the data collapse of the autocorrelation functions can be found in Fig. 6(a). We indeed can see that all curves of $C(t)$ collapse, except by the presence of random fluctuations in the very long-time regime due to the strong underlying nonlinearity. The estimated values of t_c are plotted in Fig. 6(b), normalized by $t_c(\chi = 0.78)$. Our calculations unveils a power-law scaling in the form $t_c \propto 1/(1 + \chi)$. We would like call attention that this anomalous behavior at $\chi = -1$ is a direct consequence of the nonlinear contribution to the effective hopping term we are using. In the case of an initial fully localized wavepacket, the electronic hopping between the initial site and its four nearest neighbor sites is zero and the electron remains trapped at this site. For an initial Gaussian wavepacket with a small width, the hopping between the initial position and its neighbors will be small for short times, although finite. This will result in an initial crossover during which the electronic wavepacket slowly leaks out from its initial position, becoming delocalized in the long-time regime.

The phenomenon of weakening of Anderson localization promoted by off-diagonal nonlinearity is illustrated in Fig. 7. In this figure, we provide wavepacket snapshots in three stages of its time evolution. From top to bottom, the frames represent times $t = 0.5$, $t = 100$ and $t = 1000$. For $\chi = 0$ (left column) we observe the Anderson localization regime. Due to strong disorder considered ($W = 16$), the wavepacket remains localized. For $\chi \approx -1$ (middle column), localization of the wavepacket is stronger than that of $\chi = 0$, since the nonlinearity is at the anomalous point $\chi = -1$. As discussed above, this behavior is related to the zero effective hopping between the initial site and the nearest-neighbor sites. For $\chi = 10$ (right column), we clearly see the size of the wavepacket increasing. We emphasize that this situation corresponds to a sub-diffusive wavepacket spreading, as shown in Fig. 3.

4. Summary

In this work, we studied the electronic transport in a two-dimensional disordered nonlinear lattice. We considered both the presence of compositional disorder i.e., a diagonal term of the Hamiltonian with random coefficients uniformly distributed in the interval $[-W/2,$

$W/2$] as well as the coupling between the electron wavepacket with the lattice vibrations originating an off-diagonal nonlinear term. By using numerical methods to solve the effective Schröedinger equation, we computed several quantifying function to characterize the electronic dynamics. We found that nonlinearity induces a sub-diffusive spread of the wavepacket. This result in agreement previous studies of light propagation in a two-dimensional square photonic lattice that reported that Anderson localization is always less pronounced in the presence of nonlinearity [44]. However no self-trapping dynamics was observed even for strong nonlinearities, contrasting with the behavior shown in disordered systems with diagonal nonlinearity [26]. Further, we reported strong localization in the vicinity of an anomalous point at which the effective hopping term becomes vanishingly small. The present results add to the general scenario supporting the suppression of Anderson localization by nonlinear contributions. It would be interesting to extend the present analysis to consider the influence of a superposed external field. The possibility of partial wavepacket trapping may lead to the field-control of the electronic localization in nonlinear media.

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