Wavepacket dynamics of the nonlinear Harper model

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The destruction of anomalous diffusion of the Harper model at criticality, due to weak nonlinearity $\chi$, is analyzed. It is shown that the second moment grows subdiffusively as $\langle m_2 \rangle \sim t^\alpha$ up to time $t^* \sim \chi^\gamma$. The exponents $\alpha$ and $\gamma$ reflect the multifractal properties of the spectra and the eigenfunctions of the linear model. For $t > t^*$, the anomalous diffusion law is recovered, although the evolving profile has a different shape than in the linear case. These results are applicable in wave propagation through nonlinear waveguide arrays and transport of Bose-Einstein condensates in optical lattices.

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I. INTRODUCTION

The spreading of a quantum mechanical wavepacket for a particle moving in a periodic lattice is a textbook example. One finds that the width increases ballistically with time and the corresponding eigenstates are extended (Bloch states). In the opposite case of strongly disordered systems, the eigenstates are exponentially localized, resulting in a total halt of the wavepacket spreading in the long-time limit. Between these extremes flourishes the world of quantum systems with anomalous diffusion. These include systems studied in the early days of quantum mechanics, such as Bloch electrons in a magnetic field as well as quasicrystals and disordered systems at the metal-insulator transition. In these cases, the eigenfunctions (or even the spectrum) show a fractal structure which dictates the wavepacket spreading.

The physical motivation to study such systems, along with the mathematically intriguing nature of their spectra, led to a series of works that eventually advanced our understanding of their dynamical properties. Most of these works have focused on the analysis of the temporal decay of the survival probability $P(t)$ at the initial position $n_0$ and the growth of the wavepacket second moment $m_2(t)$.\cite{1,2,3,4,5,6}

Despite all this activity, nothing is known about the effect of nonlinearity in the wavepacket spreading for systems with fractal spectra and eigenfunctions. Noticeable exceptions are Refs. 9 and 10 which numerically studied the wavepacket dynamics for the prototype one-dimensional (1D) tight-binding Harper model with nonlinearity. Their conclusions, however, are contradictory. Although both studies conclude that infinitesimal nonlinearity results in a short-time subdiffusive spreading of the variance $m_2 \sim t^\alpha$, they give different values for the power-law exponent. While Ref. 10 concludes that the subdiffusive spreading persists for longer time, Ref. 9 reports a saturation of the second moment. Moreover, they both fail to identify traces of the underlying linear model’s multifractality in the dynamics generated by the corresponding nonlinear one.

In the present paper, we address the nonlinearity-induced destruction of the anomalous diffusion. Our focus is on the 1D Harper model at criticality but we expect that our results will be applicable for other critical models (such as Fibonacci lattices) as well. Our detailed numerical calculations and theoretical arguments show that there is a critical nonlinearity $\chi^*$, above which the nature of anomalous diffusion (associated with the linear model) is altered. In particular, we found that for parametrically large time, the average (over initial sites) spreading of an initially localized $\delta-$like wavepacket spreads as

$$\langle m_2(t) \rangle \propto t^\alpha \quad \text{with} \quad 2 - 1/\alpha \leq \alpha \leq 2$$

(1)

where $D_2^\mu$ is the fractal dimension of the Local Density of States (LDoS) and $\alpha$ is independent of the nonlinearity $\chi$. The time scale $t^*$ up to which Eq. (1) is observed depends on $\chi$ as

$$t^* \sim \chi^\gamma \quad \text{with} \quad \gamma = 1/D_2^\mu$$

(2)

Beyond this time scale, the effects of nonlinearity diminish and we recover the spreading of the linear model i.e. $\langle m_2(t) \rangle \propto t^{2\beta}$. However, other moments still behave differently with respect to the linear (i.e. $\chi = 0$) case. Finally, we show that for any $\chi \neq 0$, the core of the evolving profile satisfies the scaling behavior,

$$P_x(n,t) = \sqrt{\langle m_2(t) \rangle} P_x(n,t), \quad x = \frac{n - n_0}{\sqrt{\langle m_2(t) \rangle}}$$

(3)

This paper is structured in the following way. In Sec. II an overview of the linear Harper model is presented. The nonlinear Harper model will be introduced in Sec. III and the effects of nonlinearity on the spreading and the evolving profile will be investigated both numerically and analytically. Finally, we will draw our conclusions in Sec. IV.

II. THE HARPER MODEL: OVERVIEW

In this section, we will briefly review the basic properties of the linear Harper Model. Its dynamics is described
by the standard 1D tight-binding model,

\[ \frac{i}{\hbar} \frac{\partial \psi_n(t)}{\partial t} = \psi_{n+1}(t) + \psi_{n-1}(t) + V_n \psi_n(t) \]  

(4)

Above, \( \psi_n(t) \) denotes the probability amplitude for a particle to be at site \( n \) at time \( t \) and we will assume that the on-site potential \( V_n \) takes the form:

\[ V_n = \lambda \cos(2\pi \sigma n + \phi) \]  

(5)

When \( \sigma \) is an irrational number, the period of the on-site potential \( V_n \) is incommensurate with the lattice period. In such cases, the eigenstates of the linear system are extended when \( \lambda < 2 \) and the spectrum consists of bands (ballistic regime). For \( \lambda > 2 \), the spectrum is point-like and all states are exponentially localized (localized regime). The most interesting case is the critical point \( \lambda = 2 \), where we have a metal-insulator transition. At this point, the spectrum is a zero measure Cantor set \( \lambda^2 \) and all states are exponentially localized (localized regime).

For the critical case, where \( \lambda = 2 \), previous studies show that the temporal decay of the probability to remain at the original site \( n_0 \) up to time \( t \) goes as

\[ P(t) \equiv |\psi_{n_0}(t)|^2 \sim 1/t^{D^2_2} \]  

(6)

while the wavepacket second moment grows as

\[ m_2(t) \equiv \sum_n (n - n_0)^2 |\psi_n(t)|^2 \sim t^{2\beta} \]  

(7)

with \( \beta \geq D^2_2 / D^2_2 \) where the exponent \( \beta \) depends on both \( D^2_2 \) and the correlation dimension of the fractal eigenfunctions \( D^2_2 \).

In fact, recent studies were able to demonstrate that the center of the wavepacket spatially decreases as \( |n - n_0|^{D^2_2 - 1} \) for \( |n - n_0| \ll t^\beta \) while the front shape scales as

\[ P(n, t) = A(t) \exp\left(-|n-n_0|/\sqrt{m_2(t)}\right)^{1/(1-\beta)} \]  

(8)

where \( A(t) \) is the height of the wave profile at time \( t \).

III. THE NONLINEAR HARPER MODEL

Introducing an on-site nonlinear term into Eq. (4), we come out with the nonlinear Harper model (NLHM). Mathematically, it is described by the following discrete nonlinear Schrödinger (DNLS) equation,

\[ i \frac{\partial \psi_n(t)}{\partial t} = \psi_{n+1}(t) + \psi_{n-1}(t) + V_n \psi_n(t) - \chi |\psi_n(t)|^2 \psi_n(t) \]  

(9)

We want to investigate the temporal behavior of the variance \( \langle m_2(t) \rangle \) for the NLHM at the critical point \( \lambda = 2 \). The initial condition is always taken to be a \( \delta \)-like localized state i.e. \( \psi_n(t = 0) = \delta_{n,n_0} \). An averaging \( \langle \cdot \rangle \) over different initial positions \( n_0 \) (at least 50) of the \( \delta \) function [or equivalently over a random distribution of the phase \( \phi \) in Eq. (3)] is done. In our calculations, we assume \( \sigma \) to be equal to the golden mean \( \sigma_G = (\sqrt{5} - 1)/2 \). Equation (9) has been integrated numerically using a finite-time-step fourth order Runge-Kutta algorithm on a self-expanding lattice in order to eliminate finite-size effects.\(^{11}\) Whenever the probability of finding the particle at the edges of the chain exceeded \( 10^{-10} \), ten new sites were added to each edge. Numerical precision is checked by monitoring the conservation of probability (norm) \( \sum_n |\psi_n(t)|^2 = 1 \). In all cases, the deviation from unity was less than \( 10^{-6} \).

A. Wavepacket Spreading

In Fig. 1, we report our numerical results for some representative \( \chi \) values in a double logarithmic plot. In all cases, the variance displays a power-law behavior \( \langle m_2(t) \rangle \sim t^\alpha \). Leaving aside the very initial spreading \( t \leq 1 \) (which in all cases is ballistic), we observe that for \( \chi \geq \chi^* \sim 5.5 \times 10^{-4} \) the spreading is subdiffusive with \( \alpha < 2\beta \). This spreading is valid up to time \( t < t^* \) and then relaxes to the anomalous diffusion \( \alpha = 2\beta \) that characterizes the linear Harper model.

To obtain the law of spreading of Eq. (11) for \( t < t^* \), we consider the following simple model: The initial site together with the nearby sites \( n = n_0 \pm \delta n \) is considered as a confined source.\(^{25-27}\) Anything emitted from them moves according to the spreading law of the linear Harper i.e. \( s(t) = |\langle m_2(t) \rangle|_\phi = vt^{1/2} \) since for \( t < t^* \) the leaking norm is small and therefore the nonlinear term in Eq. (9) is negligible with respect to the on-site potential \( V_n \).

Initially, all probability is concentrated at the source. Due to the nonlinear nature of the system, the decay rate is not constant but depends on the remaining norm. Thus, the decay process is characterized by the nonlinear equation,

\[ \frac{dP(t)}{dt} = -\Gamma P(t) \]  

(10)

which leads to non-exponential decay.\(^{25-27}\) On the other hand, for \( \chi = 0 \), the decay is power-law

\[ P(t) \sim 1/t^{\delta} \]  

(11)

with \( \delta = D^2_2 \) [see Eq. (6) above]. It is, therefore, natural to expect that for \( \chi \neq 0 \), we will have a slower decay with \( \delta \leq D^2_2 \) due to self-trapping.\(^{27,28,29}\) The variance of the confined-source model is then given by

\[ M_{PS}(t) \approx \int_{-\infty}^{+\infty} ds s^2 \left( \int_{0}^{t} dt' (-\dot{P}(t')) \delta(s - v(t-t'))^{\beta} \right), \]  

(12)

where \(-\dot{P}(t)\) is the flux emitted from the confined source. Substituting Eq. (11) for \( P(t) \) we get

\[ M_{PS}(t) \sim v^2 \int_{0}^{t} dt' \left( \frac{1}{t'} \right)^{\delta+1}(t - t')^{2\beta}. \]  

(13)
If we do a variable substitution $\bar{t} = t'/t$, we will get

$$M_{PS}(t) \sim v^2 t^{2\beta-\delta} \int_0^1 d\bar{t} \bar{t}^{\delta+1} (1 - \bar{t})^{2\beta},$$

or Eq. (14) which leads to Eq. (1) with $\alpha = 2\beta - \delta \geq 2\beta - D_2^\mu$.

In order to compare the results of the numerical simulations with the theoretical predictions of Eq. (1) we have calculated for the linear Harper model the decay exponent $<m_2(t)>_\phi$ of the survival probability (see inset of Fig. 1) and the power-law exponent of the variance $<\chi_m(t)>_\phi$.

The least-squares fit gives the values $<m_2(t)>_\phi \approx 0.30 \pm 0.03$ and $2\beta \approx 1.00 \pm 0.03$. The numerically extracted value of $\alpha = 0.71$ fulfills nicely the bound $2\beta - D_2^\mu = 0.70$ given by Eq. (1).

To further test the validity of Eq. (1), we have also performed simulations with the Fibonacci model, where $D_2^\mu$ and $D_2^\nu$ (and, therefore, $\beta$) can be varied according to the on-site potential $V_n$. The latter takes only two values $\pm V (V \neq 0)$ that are arranged in a Fibonacci sequence. Again, we find a power-law spreading $<m_2(t)>_\phi \sim t^\alpha$. The extracted exponents $\alpha$ corresponding to various $V$’s are reported together with the theoretical predictions in Fig. 2 and they confirm the validity of Eq. (1).

From Fig. 1 we see that the time scale $t^*$ up to which the power law of Eq. (1) applies depends on the strength of the nonlinearity parameter $\chi$. One can estimate the time $t^*$ from the fact that the effective potential $V_\chi = -\chi |\psi_{n_0}(t)|^2$ is comparable with the on-site potential $V_{n_0} \sim \lambda$ of the linear model at $t^*$. After this time, one expects that the effect of nonlinearity on the wavepacket spreading is negligible and, therefore, the survival probability should decay as $P(t) = |\psi_{n_0}(t)|^2 \sim 1/t^{D_2^\mu}$. Following this line of argumentation, we have that

$$V_{n_0} \sim \chi |\psi_{n_0}(t^*)|^2 \rightarrow V_{n_0} \sim \chi (1/t^*)^{D_2^\nu},$$

or Eq. (15) leading to Eq. (2). To test this theoretical prediction, we have manually scaled the time axis so that the variance curve where Eq. (11) applies overlaps for various $\chi$ values. The extracted scaling parameters $t^*(\chi)$ are plotted in the inset of Fig. 3. One can clearly see that the numerical data confirms the theoretical prediction of Eq. (2).

Finally, we will discuss the shape of the evolving wavefunction for $\chi \geq \chi^*$. Although for $t > t^*$ the temporal behavior of the variance becomes the same as that of the linear Harper model, other moments differ. The profiles...
inset the probability distribution
the behavior near the origin. The blue solid line is the fitting
between the data and the model. The scaling is lost for
\( t > t^* \) and for various \( \chi > \chi^* \). The nice overlap of the curves
at the core \(|x| \leq 8\) confirms the validity of the scaling law
Eq. (3). The scaling is lost for \(|x| > 8\). The lower inset shows
the behavior near the origin. The blue solid line is the fitting
curve Eq. (16). For comparison we also report in the upper
inset the probability distribution \( P_s(x) \) of the linear Harper model.

reported in Fig. 4 are snapshots of the average wavefunction
at various times and for three representative values of \( \chi = 1, 3 \) and 5 (the linear case \( \chi = 0 \) is also plotted in
the upper inset for comparison). They are plotted with the scaling assumption in Eq. (3). The data collapse for
\(|x| \leq 8\) (different curves corresponding to various times
\( t \) and nonlinearity strengths \( \chi \)) reveals that this representation is not affected much by finite-\( \chi \) corrections, although the tails of the profile are \( \chi \)-dependent. In fact, we found that the probability distribution near the center can be described by the formula:
\[
P_s(x) \sim |x|^{-\gamma} \exp(-|x|/l_\infty), \quad |x| \leq 8,
\]
where \( \gamma \approx 0.7 \) and \( l_\infty \approx 1.82 \). We note that a similar expression for the core of the probability distribution applies for 1D and quasi-1D disordered models with zero nonlinearity.\(^{14,27}\)

B. Critical Nonlinearity

Going back to Fig. 1 we observe that the destruction of the anomalous diffusion of the linear model takes place
for \( \chi \geq \chi^* \). To quantify \( \chi^* \), we evaluate the time- average survival probability \( \langle P(T) \rangle_T \), defined as\(^{18,19,22}\)
\[
\langle P(T) \rangle_T \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T |\psi_{n_0}(t)|^2 dt
\]
for various values of the nonlinearity strength \( \chi \). In our numerical calculations, we took an average over a time interval of \( T = 20000 \). Our numerical results are reported
in Fig. 5. We see that up to \( \chi^* \approx 5.5 \times 10^{-4} \), the time average survival probability \( \langle P(T) \rangle_T \) remains unchanged.
As the nonlinearity strength \( \chi \) is increased further, a fraction of the excitation begins to localize at the initial site.
As a result, the fraction of the excitation that can propagate is now effectively smaller, leading to smaller values of \( \langle m_2(t) \rangle \) as \( \chi \) is increased. We note that a similar type of self-trapping phenomenon\(^{17,18}\) was observed in various nonlinear lattices\(^{3,10,19,21,22,24,25}\) though in all these cases the value of \( \chi^* \) was much larger, i.e. \( \chi^* \sim O(1) \).

The following heuristic argument provides some understanding of the appearance of self-trapping phenomenon
for the NLHM. We consider successive rational approxi-
mants \( \sigma_i = p_i/q_i \) of the continued fraction expansion of \( \sigma \). On a length scale \( q_i \), the periodicity of the potential is not manifested and we may assume that for \( \chi < \chi^* \) the eigenfunctions preserve their critical structure as in the case of \( \chi = 0 \). In this case, the partitioning of the energy over the \( q_i \) sites is\(^{26}\)
\[
\mathcal{H} = -\frac{1}{2} \sum_{n=1}^{q_i} |\psi_n|^4 + \sum_{n=1}^{q_i} (\psi_n^* \psi_{n-1} + \psi_{n-1}^* \psi_n) + \sum_{n=1}^{q_i} V_n |\psi_n|^2
\]
(18)

Let us first estimate the energy \( \mathcal{H}_{\text{ext}} \) associated with the initial state \( \delta_{n_0,n_0} \). Since the probability distribution is located at a single site, we get an energy
\[
\langle \mathcal{H}_{\text{ext}} \rangle_{\phi} = -\frac{\chi}{2}
\]
(19)

Now we want to evaluate the partitioning of the energy \( \mathcal{H}_{\text{ext}} \) for a fractal wavefunction. In this case, the first term in Eq. (18) is the inverse participation number, which scales with the system size \( q_i \) as
\[
P_2 \sim q_i^{-D^*_f}
\]
(20)

Hence, in the thermodynamic limit where \( q_i \to \infty \), this term will go to zero. We define the sum of the two other terms as follows:
\[
S = \left( \sum_{n=1}^{q_i} (\psi_n^* \psi_{n-1} + \psi_{n-1}^* \psi_n + V_n |\psi_n|^2) \right)_{\phi}
\]
(21)

We found from numerical calculations (see inset of Fig. 5) that \( S \) goes to a finite value in the thermodynamic limit, and, therefore, arrive at the equation \( \langle \mathcal{H}_{\text{ext}} \rangle_{\phi} = S \).

If \( \mathcal{H}_{\text{ext}} \) is higher than the initial energy \( \mathcal{H}_{\text{ext}} \), then conservation of energy prevents the partitioning of energy over all \( q_i \) sites. Therefore, in the thermodynamic limit, we get for the critical nonlinearity \( \chi^* \) that
\[
\chi^* \sim -2S.
\]
(22)

The numerical data in Fig. 5 (inset) indicate that \( S \sim -2.2 \times 10^{-4} \), which is consistent with our numerical evaluation of \( \chi^* \sim 5.5 \times 10^{-4} \).
IV. CONCLUSIONS

In this paper, we studied the nonlinear Harper model at criticality and found bounds for the power-law exponent of the temporal spreading of the wavepacket variance. These bounds reflect the fractal dimension of the LDoS of the linear system. This nonlinear spreading appears for nonlinearity strength above some value and persists up to time $t^* \sim \chi^{1/D^2}$, which depends parametrically on the nonlinearity strength. After this time, the linear spreading of the second moment is restored; other moments, however, are still affected by the nonlinearity. For the central part of the evolving profile, we have also found a scaling relation that applies to any time and any nonlinearity strength.

The importance of these results lies in their applicability to quasiperiodic photonic structures (such as optical super-lattices\cite{supplref}) and arrays of magnetic micro-traps for atomic Bose-Einstein Condensates\cite{supplref} (BEC). In the latter case, nonlinear wave self-action appears due to atom-atom scattering in BEC, while in optical crystals, it appears due to light-matter interactions.

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We recall that the DNLS (9) can be derived from the Hamiltonian Eq. (18), using the Poisson brackets
\[ \{ \psi_m, \psi_n^* \} = i \delta_{mn}, \{ \psi_m, \psi_n \} = \{ \psi_m^*, \psi_n^* \} = 0, \]
and the equation of motion \( \dot{\psi}_n = \{ H, \psi_n \} \).