Abstract

The interplay between nonlinearity and disorder has been the subject of many recent studies. Due to Anderson localization, the normal modes of a 1-dimensional disordered lattice of linear oscillators are exponentially localized. When nonlinearities are also added to the model a natural question arises: Will the chaotic processes, induced by the nonlinear terms of the equations, enhance the localization or they will destroy it? The latest numerical results confirm a subdiffusive spreading of an initially localized wavepacket. The purpose of this thesis is to try to lighten the dynamics behind the diffusive behaviour. Using numerical techniques, like symplectic integrators and their extension to the tangent map method, not only we qualitatively observe the spreading process, but a quantitative approach is used with the aid of chaos detection indicators. For the first time systematic numerical calculations of finite Lyapunov exponents are reported for such systems. Our findings yield that the chaotic time-scale of the system is shorter than the spreading time scales, supporting the theories that the diffusion is a process driven by chaos.
To my parents.
Acknowledgements

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Introduction

In the dawn of the computer era, the problem of energy transportation in nonlinear lattices was among the first ones which were tackled by the computational horsepower provided by the first generation of computers. It was in the early 1950s, at the Los Alamos National Laboratory, when Enrico Fermi, Stanislaw Ulam, John Pasta and Maury Tsingou tried to explore the foundations of the statistical mechanics. The problem posed was whether the nonlinear coupling among the oscillators of a chain would lead to equipartition of energy among the degrees of freedom or not. The numerical results, not only did not provide a concrete answer to the problem, but continued to puzzle the researchers for more than half a century [Gallavotti, 2008].

Figure 1: Philip W. Anderson

A few years later, P.W. Anderson (figure (1)) was trying to understand the mechanisms underlying in the transport of electrons in crystals, when he came up with an unexpected result. In a seminal paper in 1958, he predicted
that the electronic wavefunctions in disordered crystals are exponentially localized and hence there is an absence of diffusion [Anderson, 1958]. However the concept of Anderson localisation is much more general and can be applied to a large variety of systems, including light waves, acoustic waves, microwaves and condensed matter (see [Bodyfelt et al., 2011] for a review on this topic). The impact of Anderson’s findings was so vast, that he has been awarded the Nobel prize in 1977.

While the Anderson’s theory has been indirectly proven by various experiments, the direct observation involving material particles such as electrons and atoms is hard to achieve. The main problems are the thermally excited phonons and the unavoidable interactions between particles. Researchers thus turned to localization of light or microwaves for which interactions are truly negligible.

It took almost fifty years for researchers to set up a controlled environment for the direct observation of Anderson localization. In an optics experiment [Schwartz et al., 2007], the transverse localization of light caused by random fluctuations on a two-dimensional photonic lattice was reported. A year after, the results were confirmed also for one-dimensional photonic lattices [Lahini et al., 2008] (figure (2)).

![Figure 2: Direct experimental observation of Anderson localisation in 1-dimensional photonic lattices (after [Lahini et al., 2008]).](image)

However, the breakthrough that made direct observation possible with material particles was the use of a ultracold atoms. The recent advances in the control over Bose-Einstein Condensates (BECs) in optical potentials made it possible to observe Anderson localization [Billy et al., 2008; Roati et al., 2008] (figure (3)).

![Figure 2: Direct experimental observation of Anderson localisation in 1-dimensional photonic lattices (after [Lahini et al., 2008]).](image)
The direct observation of Anderson localization was not only the outcome of the aforementioned works. It became also possible to study the interplay between localization and nonlinearity. The effect of weak nonlinearity in some cases caused the delocalization of localized modes, while in other enhanced their localization [Lahini et al., 2008]. The theoretical explanation of that observations became a hot topic among the material scientists.

The Discrete Nonlinear Schrödinger Equations (DNLS) and the Klein Gordon quartic lattice (KG) provided a proper framework, not only for numerical computations but also for analytical estimates. The first theoretical works were rather controversial [Shepelyansky, 1993; Kopidakis et al., 2008; Pikovsky and Shepelyansky, 2008], like the experimental results. Shortly after the fate of an initially localized wave packet under the effect of nonlinearities became clear. There are different evolution regimes defined by the frequency shifts introduced by the nonlinearities [Flach et al., 2009; Skokos et al., 2009]. Extensive numerical simulations confirmed the subdiffusive spreading of the wave packet for weak nonlinearities and the self-trapping of it for large nonlinearities [Flach et al., 2009; Skokos et al., 2009]. The subdiffusive behaviour was more carefully studied, revealing two different spreading laws. The crossover between the two, namely the ‘strong chaos’ and ‘weak chaos’ diffusion regimes, was also reported [Laptyeva et al., 2010; Flach, 2010].

In all previous works the wavepacket spreading was monitored by means of the second moment and participation number of its energy distribution. While this kind of analysis is rather qualitative, it does not provide an insight
of the underlying dynamics. The purpose of the current work is to quantitatively study the subdiffusion process by calculating the maximal Lyapunov Characteristic Exponent (mLCE) in the duration of the wavepacket evolution.

The thesis is organised in three chapters. In the first chapter the theoretical aspects of this work are covered. In the second chapter, a detailed description of the numerical techniques used to obtain our results is presented. In the third chapter, the results of the numerical simulations are reported. Finally, we also present a discussion of the main conclusions of this thesis and an outlook for further work.
Chapter 1

Theoretical Background

In this chapter the necessary theoretical background in order to study the energy spreading in nonlinear, disordered lattices is presented. In the first section the ground breaking work of Anderson and its implications to energy spreading is discussed. Then the two main models used in our work, the Discrete NonLinear Schrödinger equation (DNLS) and the Klein-Gordon (KG) chain of unharmonic oscillators are introduced. DNLS provides a fertile ground for theoretical considerations and all the results can be easily adapted to KG with a straightforward transformation, which holds for small wavepacket amplitudes. In Section 1.3, some useful theoretical estimations on the expected regimes of spreading are outlined. Finally, some rather intriguing open questions are discussed in Section 1.4, giving motivation for the work performed in this thesis.

1.1 Anderson Localization

The term Anderson Localization (AL) is used nowadays to describe the absence of wave diffusion in disordered mediums. It is a general wave phenomenon that applies to the transport of various types of waves, e.g. light waves, microwaves, acoustic waves and matter waves. Its origin is the wave interference between multiple scattering paths. The introduction of randomness can drastically disturb the constructive interference, leading to the halting of waves.

Theoretical and numerical approaches of localization start with the Anderson model: a standard tight-binding (nearest-neighbour interaction) with
on-site potential disorder model. In 1-dimension the model can be represented with the Hamiltonian:

\[ H_A = \sum_l \epsilon_l |\psi_l|^2 - (\psi_{l+1}\psi_l^* + \psi_{l-1}\psi_l) \] (1.1)

with \( \psi_l \) complex variables, \( \psi_l^* \) their complex conjugates and \( l \) lattice site indices. The random on-site energies \( \epsilon_l \) are chosen uniformly from the interval \([-W/2, W/2]\), with \( W \) denoting the disorder strength. The equations of motion are generated by \( \dot{\psi}_l = \frac{\partial H_A}{\partial (i\psi_l^*)} \) and yield

\[ i\dot{\psi}_l = \epsilon_l |\psi_l|^2 - \psi_{l+1} - \psi_{l-1}. \] (1.2)

Using the ansatz \( \psi_l = A_l e^{i\lambda l} \) equation (1.2) is reduced to the linear eigenvalue problem

\[ \lambda A_l = \epsilon_l A_l - A_{l-1} - A_{l+1}. \] (1.3)

The normalized eigenvectors \( A_{\nu,l} \) (with \( \sum_l A_{\nu,l}^2 = 1 \)) are the normal modes and the eigenvalues \( \lambda_\nu \) are the frequencies of the normal modes. The width of the frequency spectrum \( \lambda_\nu \) is \( \Delta = W + 4 \) with \( \lambda_\nu \in [-2 - W/2, 2 + W/2] \).

The normal modes in the presence of sufficiently strong disorder are exponentially localized [Anderson, 1958], meaning that their asymptotic behaviour can be described by an exponential decay

\[ |A_{\nu,l}| \sim e^{-l \xi(\lambda_\nu)}, \] (1.4)

where \( \xi(\lambda_\nu) \) is a characteristic energy-dependent length, called the localization length and

\[ \xi(\lambda_\nu) \approx \frac{24(4 - \lambda_\nu^2)}{W^2} \] (1.5)

for weak disorder \( W \leq 4 \) [Anderson, 1958; Kramer and MacKinnon, 1993]. The normal mode participation number \( P_\nu = 1/\sum_l A_{\nu,l}^4 \) characterizes the normal mode spatial extent. An average measure of this extent is the localization volume \( V \), which is on the order of \( 3.3\xi(0) \) for weak disorder and unity in the limit of strong disorder [Krimer and Flach, 2010].

The average spacing \( d \) of eigenvalues of normal modes within the range of a localization volume is therefore of the order of \( d \approx \Delta/V \), which becomes \( d \approx \Delta W^2/300 \) for weak disorder. The two scales \( d < \Delta \) are expected to determine the wavepacket evolution in the presence of nonlinearity.
Figure 1.1: For Hamiltonian Equation (1.1) we present the spatial profiles in logarithmic scale of a few normal modes $A_{\nu,l}$ of a single disorder realization for different values of W: (a) W=2, (b) W=4 and (c) W=8.

In figure (1.1) the spatial profiles in logarithmic scale, of a sample of normal modes $A_{\nu,l}$ for a single disorder realization $\epsilon_l$ with 1000 oscillators are presented. The lattice has fixed boundary conditions. The normal modes of the system are calculated from Equation (1.3) and are sorted with respect to their center of norm. Then a sample of them is formed by taking one mode every hundred modes. Similar graphs are produced for the same realisation.
but for varying values of $W$: panel (a) $W=2$, panel (b) $W=4$ and panel (c) $W=8$. The tails of the normal mode profiles could be approximated by straight lines, indicating their exponential decay and thus confirming the results of Anderson’s theory. Also notice that, the spatial extent of each normal mode decreases with the increase of the disorder strength $W$, in agreement with the theoretical prediction of Equation (1.5).

Due to the localized character of the normal modes, any initially localized wave packet with size $L$, which is launched into the system, will stay localized for all times. If $L \ll V$, then the wave packet will initially expand into the localization volume. This expansion will take time of the order of $\tau_{\text{lin}} = \frac{2\pi}{d}$ [Flach, 2010]. If instead $L \geq V$, no substantial expansion will be observed. Anderson localization is relying on the phase coherence of waves. Wave packets which are trapped due to Anderson localization correspond to trajectories in phase space evolving on tori, i.e. quasiperiodic motion (for simulation results see also Section 3.2).

1.2 The DNLS and Klein Gordon Models

In our study two one-dimensional lattice models are considered. The first one is the disordered discrete nonlinear Schrödinger equation (DNLS) described by the Hamiltonian function

$$
H_D = \sum_l \epsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - (\psi_{l+1}\psi_l^* + \psi_{l-1}\psi_l) \quad (1.6)
$$

in which $\psi_l$ are complex variables, $l$ are the lattice site indices and $\beta > 0$ is the nonlinearity strength. Notice that for $\beta = 0$ the DNLS reduces to the Anderson model (1.1. Again, the random on-site energies $\epsilon_l$ are chosen uniformly from the interval $[-\frac{W}{2}, \frac{W}{2}]$, with $W$ denoting the disorder strength. The equations of motion are generated by $\dot{\psi}_l = \frac{\partial H_D}{\partial (i\psi_l^*)}$ and yield

$$
i\dot{\psi}_l = \epsilon_l + \beta |\psi_l|^2 \psi_l - \psi_{l+1} - \psi_{l-1}. \quad (1.7)
$$

This set of equations conserves both the energy of (1.6) and the norm $S = \sum_l |\psi_l|^2$. Equation (1.6) is derived when describing two-body interactions in ultracold atomic gases on an optical lattice within a mean-field approximation [Morsch and Oberthaler, 2006] but also when describing the propagation of
light through networks of coupled optical waveguides in Kerr media [Kivshar and Agrawal, 2003].

The second model considered is the quartic Klein-Gordon (KG) lattice, given by

\[ H_K = \sum_l \left( \frac{p_l^2}{2} + \bar{\epsilon}_l u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2 \right) \tag{1.8} \]

where \( u_l \) and \( p_l \) are, respectively, the generalized coordinates and momenta on site \( l \), and \( \bar{\epsilon}_l \) are chosen uniformly from the interval \([\frac{1}{2}, \frac{3}{2}]\). The equations of motion are

\[ \ddot{u}_l = -\bar{\epsilon}_l u_l - u^3 + \frac{1}{W} (u_{l+1} + u_{l-1} - 2u_l). \tag{1.9} \]

This set of equations only conserves the energy of Equation (1.8). The initial energy \( E \geq 0 \) serves as a control parameter of nonlinearity similar to \( \beta \) for the DNLS case. The KG lattice serves as a simple model for the dissipation-less dynamics of anharmonic optical lattice vibrations in molecular crystals [Ovchinnikov et al., 2001].

The coefficient \( \frac{1}{2W} \) in Equation (1.8) was chosen so that the linear part of the Hamiltonian would correspond to the eigenvalue problem of the Anderson model. In practise, by neglecting the nonlinear term \( (u_l^4) \) of Equation (1.8) and using the ansatz \( u_l = A_l e^{i \omega t} \) the KG Hamiltonian is reduced to the same linear eigenvalue problem of Equation (1.3), under the substitutions \( \lambda = W \omega^2 - W - 2 \) and \( \epsilon_l = W (\bar{\epsilon}_l - 1) \). The width of the squared frequency \( \omega^2 \nu \) spectrum is \( \Delta_K = \frac{W+4}{W} \) with \( \omega^2 \nu \in [\frac{1}{2}, \frac{3}{2} + \frac{4}{W}] \). Note that \( \Delta_D = W \Delta_K \). As in the case of DNLS, \( W \) determines the disorder strength. In Table 1.1 the main characteristics of the two models are summarized.

For small amplitudes an approximate mapping

\[ \beta S = 3W E \tag{1.10} \]

from the KG model to the DNLS model exists [Kivshar and Peyrard, 1992; Kivshar, 1993; Johansson, 2006]. Further theoretical estimations will be discussed in terms of the DNLS model, since it is now straightforward to adapt similar results for the KG model using the aforementioned mapping.

In the presence of nonlinearity an interaction between the normal modes is induced. In order to write the equations of motion of the DNLS Hamiltonian in the normal mode space, the relation \( \psi_l = \sum_\nu A_{\nu,l} \phi_\nu \) is inserted in Equation (1.7), with \( |\phi_\nu|^2 \) denoting the time-dependent amplitude of the \( \nu \)th normal
Table 1.1: Characteristic quantities of the DNLS and the KG models.

<table>
<thead>
<tr>
<th></th>
<th>DNLS</th>
<th>KG</th>
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<tbody>
<tr>
<td>On-site energies</td>
<td>$\epsilon_l \in [-\frac{W}{2}, \frac{W}{2}]$</td>
<td>$\bar{\epsilon}_l \in [\frac{1}{2}, \frac{3}{2}]$</td>
</tr>
<tr>
<td>Spectrum</td>
<td>$\lambda_\nu \in [-2 - \frac{W}{2}, 2 + \frac{W}{2}]$</td>
<td>$\omega_\nu^2 \in [\frac{1}{2}, \frac{3}{2} + \frac{4}{W}]$</td>
</tr>
<tr>
<td>Spectrum width $\Delta$</td>
<td>$\Delta_D = W + 4$</td>
<td>$\Delta_K = \frac{W+4}{W}$</td>
</tr>
<tr>
<td>Localization volume $V$</td>
<td>$\begin{cases} W \to 0 &amp; V = \frac{330}{W^2} \ W \to \infty &amp; V \sim \frac{1}{W^2} \end{cases}$</td>
<td>$d_{D} \sim W^2$</td>
</tr>
<tr>
<td>Average spacing $d$</td>
<td>$d_{D} \sim W^2$</td>
<td>$d_{K} \sim W$</td>
</tr>
<tr>
<td>Nonlinear frequency shift $\delta$</td>
<td>$\delta_D \sim \beta n$</td>
<td>$\delta_K \sim \frac{3}{2} E$</td>
</tr>
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</table>

mode. Then, using Equation (1.3) and the orthogonality of the normal modes the equations of motion read

$$i \dot{\phi}_\nu = \lambda_\nu \phi_\nu + \beta \sum_{\nu_1, \nu_2, \nu_3} I_{\nu, \nu_1, \nu_2, \nu_3} \phi_{\nu_1}^* \phi_{\nu_2} \phi_{\nu_3} \quad (1.11)$$

with the overlap integral $I_{\nu, \nu_1, \nu_2, \nu_3}$ being

$$I_{\nu, \nu_1, \nu_2, \nu_3} = \sum_l A_{\nu, l} A_{\nu_1, l} A_{\nu_2, l} A_{\nu_3, l} \quad (1.12)$$

Since all normal modes are exponentially localized in space, each one effectively couples to a finite number of neighbour modes. The nonlinear interactions are thus of finite range. However, the strength of this coupling is proportional to the norm density in DNLS and the energy density in KG. If the packet spreads far enough, two norm densities can be defined in general: one in real space $n_l = |\psi_l|^2$ and one in the normal mode space $n_\nu = |\phi_\nu|^2$. Averaging over realizations, no significant difference is seen between the two, and therefore, it can be treated as some characteristic norm density $n$. Then the frequency shift of a single-site oscillator induced by the nonlinearity is $\delta_D = \beta n$ for the DNLS model. The squared frequency shift of a single-site oscillator induced by the nonlinearity for the KG system is $\delta_K = 3E/2$ [Skokos et al., 2009; Laptyeva et al., 2010].

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For the KG model, which is used in all our simulations, during the wave packet evolution the normalized energy density distributions $E_i$ are tracked

$$E_i = \frac{h_i}{H_K}, \quad h_i = \frac{p_i^2}{2} + \frac{\bar{u}^2}{2} + \frac{u_i^4}{4} + \frac{(u_{i+1} - u_i)^2}{4W}.$$  

(1.13)

Two distribution measure are used in the real space. The first measure we use is the participation number $P$

$$P = \frac{1}{\sum_i E_i^2},$$  

(1.14)

which queries the quantity of strongest excited sites in the lattice. If all the energy is concentrated on only one oscillator, equation (1.14) gives $P = 1$. On the other hand, if the energy is equally distributed among the oscillators of a lattice with size $N$, equation (1.14) gives $P = N$. In all other cases $P$ takes values in $[1, N]$. The other measure we use in our study is the second moment $m_2$

$$m_2 = \sum_i (l - \bar{l})^2 E_i,$$  

(1.15)

which quantifies the the wave packet’s degree of spreading. The quantity $\bar{l} = \sum_i l E_i$ denotes the position of the mean value of the distribution $E_i$. The second moment is sensitive to the distance of the tails of a distribution form the center, while participation number is a measure of the inhomogeneity of the distribution, being insensitive to any spatial correlations.

### 1.3 Theoretical Estimations

In this section the different dynamical regimes of wave packet spreading are briefly presented and the universal laws of spreading are described.

Let’s consider compact wave packets at $t=0$ spanning a width $L$ in the center of the lattice, such that there is a constant norm density of $n$ and a random phase at each site (outside the volume $L$ the norm is zero). In the KG case, this corresponds to exciting each site in the width $L$ with the same energy density $\mathcal{E} = E/L$, i.e setting initial momenta to $p_l = \sqrt{2E}$ with randomly assigned signs.

If the nonlinear frequency shift is greater than the spectrum width $\delta \geq \Delta$, then a substantial part of the wave packet will be self-trapped [Kopidakis
et al., 2008; Skokos et al., 2009]. This is due to nonlinear frequency shifts, which will tune the excited sites immediately out of resonance with the nonexcited neighbourhood. As a result, discrete breather like structures will be formed, which can persist for immensely long times. While selftrapping and discrete breather formation are interesting localization phenomena at strong nonlinearity, they are very different from Anderson localization since they require the existence of gaps in the spectrum of the linear wave equations [Flach and Willis, 1998; Flach and Gorbach, 2008]. In fact, partial self-trapping will occur in the DNLS model already for \( \delta \geq 2 \) since at least some sites in the packet may be tuned out of resonance.

If now \( \delta < \Delta \), any self-trapping is avoided, and the packet can spread. The nonlinear frequency shift should be now compared with the average spacing between the normal modes \( d \). If \( \delta > d \), all normal modes in the packet are resonantly interacting with each other. This regime is referred as the ‘strong chaos’ regime. If \( \delta < d \), normal modes are weakly interacting with each other. This regime is referred as ‘weak chaos’ regime [Laptyeva et al., 2010]. Note that a spreading wave packet that is launched in the regime of strong chaos will increase in size, drop its norm density, and therefore a crossover into the asymptotic weak chaos regime must occur at later times.

For a single site excitation \( L = 1 \) the strong chaos regime is not present and one is left only with either weak chaos or selftrapping [Pikovsky and Shepelyansky, 2008; Flach et al., 2009; Skokos et al., 2009]. To summarize, the expected spreading regimes for \( L \geq V \) are:

- \( \delta > \Delta \) : selftrapping regime
- \( \delta < \Delta \) : spreading in the following regimes
  - \( \delta > d \) : strong chaos regime
  - \( \delta < d \) : weak chaos regime

Figure (1.2) sketches the predicted regimes in a parametric space for the case \( L = V \) for both the DNLS and KG case. \( \mathcal{E} \) is the energy density for the initial excitation in the KG model and it equivalent to the nonlinear frequency shift \( \delta \sim \beta n \) in the DNLS model. For the DNLS model the lines represent the regime boundaries \( \delta = d \) and \( \delta = 2 \). The lower boundary is analytically found, via \( d = \Delta/(3.3\xi(0)) \) with \( \xi(0) = 96W^{-2} \) being the weak-disorder estimate. The KG analog is obtained by the small-amplitude mapping of
Equation (1.10). It should also be noted that the regime boundaries are not sharp, rather there is some transitional width between the regimes.

Interior modes of the packet interact in a nonintegrable way, leading to chaotic dynamics [Flach et al., 2009; Skokos et al., 2009]. Exterior modes close to a wavepacket boundaries may also be heated. There are two candidate mechanisms of wave packet spreading. A normal mode on the cold exterior, which borders the packet, is either incoherently heated by the packet, or resonantly excited by some particular normal mode inside the packet.

From the equation of motion in normal mode space (1.11) it is conjectured [Laptyeva et al., 2010; Flach, 2010] that an exterior mode is excited according to

\[ i\dot{\phi}_\mu \approx \lambda_\mu \phi_\mu + \beta n^{3/2} P(\beta n) f(t) \]  

(1.16)

where \( P(\beta n) \approx 1 - e^{\beta n/d} \) is the probability of a mode resonance [Flach, 2010; Krimer and Flach, 2010] and \( f(t) \) is a stochastic force. Under such conjecture, the time-dependent norm is given by

\[ |\phi(t)|^2 \sim \beta^2 n^3 (P(\beta n))^2 t \]  

(1.17)

and it will reach the level of the wavepacket norm density \( n \) at a time \( T \sim \beta^{-2} n^{-2} (P(\beta n))^{-2} \). At time \( T \) the mode becomes a part of the wavepacket. Therefore its inverse \( D = T^{-1} \sim \beta^2 n^2 (P(\beta n))^2 \) characterizes the rate of norm diffusion, which still depends on time, since \( n \) is decreasing with further spreading. Thus, it is the resonance probability that largely dictates whether
the chaos is strong or weak. From $m_2 \sim 1/n^2$ and the diffusion equation $m_2 \sim Dt$, one obtains

$$ \frac{1}{n^2} \sim \beta (1 - e^{-\beta n/d}) t^{1/2} \quad (1.18) $$

which further determines the subdiffusive spreading crossover from the regime of strong chaos to that of weak chaos

$$ m_2 \sim \begin{cases} \beta t^{1/2}, & \beta n/d > 1 \quad \text{(strong chaos)} \\ d^{-2/3}\beta^{4/3} t^{1/3}, & \beta n/d < 1 \quad \text{(weak chaos)} \end{cases} \quad (1.19) $$

Equation (1.19) yields that there are different spreading laws for the weak and strong chaos regimes. In the ‘weak chaos’ regime, the second moment of the energy distribution increases as $m_2 \sim t^{1/3}$. In the ‘strong chaos’ regime, diffusion is faster with $m_2 \sim t^{1/2}$. This results has been confirmed by extensive numerical simulations in [Skokos et al., 2009; Laptyeva et al., 2010].

### 1.4 Open Questions

From a mathematical perspective, a linear wave equation is integrable, with each normal mode evolving independently in time. A localized wave packet in the presence of Anderson localization will therefore stay localized as time evolves. Nonlinearity will usually destroy the integrability of a system and induce mode-mode interactions. It was observed numerically that wave packets in such nonlinear disordered wave equations delocalize in time without respecting Anderson localization limitations [Pikovsky and Shepelyansky, 2008; Flach et al., 2009; Skokos et al., 2009]. Thus, there are several intriguing questions which have attracted much attention during the last few years:

- Will wave packet spreading, if observed, last forever or will it stop at certain (though probably very large) time?

- Will Anderson localization be destroyed by arbitrary small strength of nonlinearity or is there a threshold below which the localization is restored?

- Is the shape of the initial wave packet crucial for the details of spreading?
The above questions, and especially the first one, give motivation for the work performed in this thesis.
Chapter 2

Numerical Techniques

This chapter is devoted to the presentation of the numerical techniques implemented in this thesis. In the first section the numerical integration schemes used to perform our simulations are discussed. After a short introduction in the symplectic integrators theory, the recently introduced tangent map method is described. In section 2.2 the basic concepts of Lyapunov Characteristic Exponents will be presented. Finally, in section 2.3 the technique used to calculate the slopes of various curves is explained.

2.1 Numerical Integration

The main way to study the dynamical evolution of nonintegrable Hamiltonian systems is through numerical integration of the equations of motion. There is a variety of method for the numerical integration of ordinary differential equations (ODEs). However there is a class of integrators which is perfectly suited for our study, namely the symplectic integrator. The main advantage of symplectic is that the relative energy error remains bounded, while common ODE integrators exhibit a constant energy drift. This feature is essential in long term simulation, like those performed in this thesis.

Symplectic Integrators

The philosophy of the symplectic integrator can be explained as follows. The time evolution map of a Hamiltonian system is obtainable from a canonical transformation. One can also say that any given canonical transforma-
tion generates the time evolution for some Hamiltonian system. A symplectic integrator is one which approximates the canonical transformation for the desired system to some order of the time step. But this approximate canonical transformation that the numerical integrator then implements is the phase flow for a Hamiltonian system that is nearby the desired one. That is, the integrator computes exactly (assuming infinite precision arithmetic) the evolution for a nearby Hamiltonian. This nearby Hamiltonian system \( \tilde{H} \) has a phase space structure that is close to that of the desired Hamiltonian system. The nature of the algorithm therefore allows for conservation of the integrals of the motion of the nearby Hamiltonian \( \tilde{H} \).

The replacement of the Hamiltonian with another may seem worrisome. However observe that this is a far better philosophy in general than common ODE integrators. The latter do not respect any global phase space structures. For example, a symplectic integrator will approximate the Hamiltonian system with another and use slightly the wrong energy manifold. However, the particle will then stay permanently on the nearby manifold. A normal ODE integrator will cause the particle to drift across the energy manifold since it has no knowledge of the phase space structures.

There are two main types of symplectic integrators: implicit and explicit. Although explicit schemes usually more computationally efficient and easier to implement, they cannot be applied in any problem. Fortunately for our models explicit schemes can be used. For Hamiltonian systems of the form

\[
H = T(p) + V(q)
\]

the simplest symplectic scheme available is a modification of the common Euler method for ODEs

\[
\begin{align*}
q' &= q + \tau \left( \frac{\partial T}{\partial p} \right)_{p=p}, \\
p' &= p - \tau \left( \frac{\partial V}{\partial q} \right)_{q=q'}.
\end{align*}
\]  

(2.2)

This mapping is symplectic because it is composed of two symplectic mappings \((q, p) \rightarrow (q', p)\) and \((q', p) \rightarrow (q', p')\).

The problem of deriving explicit symplectic integrator schemes was formulated in terms of Lie algebraic notation [Neri, 1988]. If \( x = (p, q) \) the equations of motion for Equation (2.1) can be written in the form

\[
\frac{dx}{dt} = \{ x, H(x) \} = L_H(x)
\]

(2.3)
where \( \{ f, g \} \) is the poisson bracket defined as
\[
\{ f, g \} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}
\] (2.4)
and the differential operator \( L_a \) is defined as
\[
L_a f = \{ f, g \}.
\] (2.5)

The exact time evolution of \( x(t) \) form \( t = 0 \) to \( t = \tau \) is given by
\[
x(\tau) = [\exp(\tau L_H)] x(0)
\] (2.6)
For a Hamiltonian of form (2.1), \( L_H = L_T + L_V \) and the formal solution reads
\[
x(\tau) = [\exp(\tau (L_T + L_V))] x(0)
\] (2.7)
where the operators \( L_T \) and \( L_V \) do not commute in general. Suppose now \((c_i, d_i)\) is a set of real numbers which satisfies the equality
\[
\exp[\tau(L_T + L_V)] = \prod_{i=1}^{k} \exp(c_i \tau L_T) \exp(d_i \tau L_V) + \mathcal{O}(\tau^{n+1})
\] (2.8)
for a given integer \( n \), which corresponds to the order of integrator. Now consider a mapping from \( x(0) \) to \( x(\tau) \) given by
\[
x(\tau) = \left[ \prod_{i=1}^{k} \exp(c_i \tau L_T) \exp(d_i \tau L_V) \right] x(0).
\] (2.9)
This map is symplectic because it is just a product of elementary symplectic mappings, and approximates the exact solution Equation (2.7), up to the order of \( \tau^n \). Furthermore it is explicitly computable. In fact Equation (2.9) gives the succession of the mappings
\[
q_i = q_{i-1} + \tau c_i \left( \frac{\partial T}{\partial p} \right)_{p=p_{i-1}, q=q_i},
p_i = p_{i-1} - \tau d_i \left( \frac{\partial V}{\partial q} \right)_{q=q_i}.
\] (2.10)
In this notation, for \( c_i = 1, d_i = 1 \) the modified Euler method in Equation (2.2) can be written as
\[
\exp[\tau(L_T + L_V)] = \exp(\tau L_T) \exp(\tau L_V) + \mathcal{O}(\tau^2)
\] (2.11)
with $n=1$, which implies that it is a first order symplectic integrator. For $n=2$, the solution for the coefficients can easily be computed $c_1 = c_2 = 1/2$, $d_1 = 1$, $d_2 = 0$ which leads to the formula

$$
\exp[\tau(L_T + L_V)] = \exp(\frac{T}{2} L_T) \exp(\tau L_V) \exp(\frac{T}{2} L_T) + O(\tau^3)
$$

and implies a second order integrator, known as the leap-frog scheme. A forth order integrator $n = 4$ was obtained in a rather straightforward way [Forest and Ruth, 1990; Candy and Rozmus, 1991] with the result,

$$
c_1 = c_4 = \frac{1}{2(2-2^{1/3})}, c_2 = c_3 = \frac{1-2^{1/3}}{2(2-2^{1/3})}, d_2 = \frac{-2^{1/3}}{2-2^{1/3}}, d_4 = 0.
$$

One can notice that the forth order integrator is composed of second order ones. With the use of the notation

$$
S_2(\tau) = \exp(\frac{T}{2} L_T) \exp(\tau L_V) \exp(\frac{T}{2} L_T)
$$

the forth order integrator $S_4(\tau)$ can be written as

$$
S_4(\tau) = S_2(a_1 \tau) S_2(a_0 \tau) S_2(a_1 \tau)
$$

where

$$
a_0 = -\frac{2^{1/3}}{2 - 2^{1/3}}, a_1 = \frac{1}{2 - 2^{1/3}}.
$$

Actually the, $a_0, a_1$ are determined as the solution of the algebraic equations

$$
a_0 + 2a_1 = 1, x_0^3 + 2x_1^3 = 0
$$

and this interpretations gives the simplest derivation of the forth order integrator [Yoshida, 1990].

Another interesting class of explicit high order symplectic integrators is the SABA [Laskar and Robutel, 2001], used for Hamiltonians of the form

$$
H = A + \epsilon B
$$

whith $A, B$ both integrable and $\epsilon$ a small parameter.

The SABA integrators are symmetric and they use only positive coefficients $c_i, d_i > 0$. The use of exclusively positive time steps was introduced
because there were reports of instabilities caused by the negative ones. A second order integrator \( SABA_2 \) has the following form

\[
SABA_2 = \exp(\tau c_1 L_A)\exp(\tau d_1 L_B)\exp(\tau c_2 L_A)\exp(\tau d_1 L_B)\exp(\tau c_1 L_A)
\]

with

\[
c_2 = \frac{1}{\sqrt{3}}, c_1 = \frac{1}{2} \left( 1 - \frac{1}{\sqrt{3}} \right), d_1 = \frac{1}{2}.
\]

The accuracy of the integrator can further increase with the use of a corrector term. With \( C = \{B, \{B, A\}\} \) the \( SABA_{2C} \) integrator has the form

\[
SABA_{2C} = \exp(-\tau^3 \frac{g}{2} L_C)(SABA_2)\exp(-\tau^3 \frac{g}{2} L_C)
\]

with \( g = (2 - \sqrt{3})/24 \). The new corrected integrator \( SABA_{2C} \) is still symmetric and its accuracy is improved to fourth order.

**The Tangent Map Method**

The tangent map method [Skokos and Gerlach, 2010] is a recently introduced technique which takes advantage of the explicit symplectic integration schemes to integrate the system of the variational equation along with the equations of motion. Consider the autonomous Hamiltonian of the from

\[
H(p_i, q_i) = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + V(\vec{q})
\]

with \( V(\vec{q}) \) being the potential function. The Hamilton equations of motion become

\[
\begin{bmatrix}
\dot{\vec{q}} \\
\dot{\vec{p}}
\end{bmatrix} =
\begin{bmatrix}
-\frac{\partial V(\vec{q})}{\partial \vec{q}} \\
0
\end{bmatrix}
\]

while the variational equations of this system take the form

\[
\begin{bmatrix}
\dot{\delta q} \\
\dot{\delta p}
\end{bmatrix} =
\begin{bmatrix}
0_N & I_N \\
-D^2_V(\vec{q}(t)) & 0_N
\end{bmatrix}
\begin{bmatrix}
\delta \vec{q} \\
\delta \vec{p}
\end{bmatrix}
\]

which leads to the equations

\[
\dot{\delta q} = \delta \vec{p}, \dot{\delta p} = -D^2_V(\vec{q}(t))\delta \vec{q}
\]
with
\[ D^2_V(\vec{q}(t))_{j,k} = \frac{\partial^2 V(\vec{q})}{\partial q_j \partial q_k} |_{\vec{q}(t)}, j, k = 1, 2, \ldots, N. \]  

(2.26)

Thus the tangent dynamics of Hamiltonian Equation (2.22) are represented by the time-dependent Hamiltonian function
\[ H_V(\delta \vec{q}, \delta \vec{p}; t) = \frac{1}{2} \sum_{i=1}^{N} \delta p_i^2 + \frac{1}{2} \sum_{j,k} D^2_V(\vec{q}(t))_{j,k} \delta q_j \delta q_k \]  

(2.27)

which is called the tangent dynamic Hamiltonian and whose equations of motion are exactly the variational equations.

The set of equations (2.23) and (2.25) can be considered as a unified set of differential equations
\[
\begin{align*}
\dot{\vec{q}} &= \vec{p} \\
\dot{\vec{p}} &= -\frac{\partial V(\vec{q})}{\partial \vec{q}} \\
\dot{\delta \vec{q}} &= \dot{\delta \vec{p}} \\
\dot{\delta \vec{p}} &= -D^2_V(\vec{q}) \delta \vec{q}
\end{align*}
\]

⇒ \[ \frac{d\vec{u}}{dt} = L_{HV} \vec{u} \]  

(2.28)

where \( \vec{u} = (\vec{q}, \vec{p}, \delta \vec{q}, vec \delta \vec{p}) \) is a vector formed by the phase-space vector \((\vec{q}, \vec{p})\) and the deviation vector \((\delta \vec{q}, \delta \vec{p})\) and \(L_{HV}\) is the differential operator of the whole system.

The operator \(L_{HV}\) can be written as \(L_{HV} = L_{AV} + L_{BV}\) and the time evolution maps for \(L_{AV}, L_{BV}\) are:
\[
\begin{align*}
exp(\tau L_{AV}) = \begin{cases} \\
\dot{\vec{q}}' &= \vec{q}' + \vec{p}' \tau \\
\dot{\vec{p}}' &= \vec{p}' \\
\delta \vec{q}' &= \vec{q}' + \vec{p}' \tau \\
\delta \vec{p}' &= \delta \vec{p}
\end{cases} \\
\end{align*}
\]

(2.29)

and
\[
\begin{align*}
exp(\tau L_{BV}) = \begin{cases} \\
\dot{\vec{q}}' &= \vec{q}' \\
\dot{\vec{p}}' &= \vec{p}' - \frac{\partial V(\vec{q})}{\partial \vec{q}} \tau \\
\delta \vec{q}' &= \delta \vec{q} \\
\delta \vec{p}' &= \delta \vec{p} - D^2_V(\vec{q}) \delta \vec{q} \tau
\end{cases} \\
\end{align*}
\]

(2.30)
Now the whole set of the equations can be integrated with the explicit symplectic integrators discussed in section 2.1. For the KG model,

\[ H_K = \sum_l \frac{p_l^2}{2} + \frac{\bar{\epsilon}}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2 \]

we can split the Hamiltonian into two parts \( H_K = A + B \) with

\[ A \equiv \sum_l \frac{p_l^2}{2}, \quad B \equiv \sum_l \frac{\bar{\epsilon}}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2 \]  

(2.31)

and \( A, B \) both integrable parts. Then, the implementation of the tangent map method for the KG yields:

\[
\exp(\tau L_{AV}) = \begin{cases} 
    u'_{l} = u_l + p_l \tau \\
    p'_l = p_l \\
    \delta u'_l = \delta u_l + \delta p_l \tau \\
    \delta p'_l = \delta p_l
\end{cases}
\]  

(2.32)

and

\[
\exp(\tau L_{BV}) = \begin{cases} 
    u'_l = u_l \\
    p'_l = p_l + \left[ -u_l (\bar{\epsilon} + u_l^2) + \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_l) \right] \tau \\
    \delta u'_l = \delta u_l \\
    \delta p'_l = \delta p_l + \left[ \frac{1}{W} (\delta u_{l-1} - 2\delta u_l + \delta u_{l+1}) - \delta u_l (\bar{\epsilon} - 3u_l^2) \right] \tau
\end{cases}
\]  

(2.33)

### 2.2 Lyapunov Characteristic Exponents

The Lyapunov Characteristic Exponents (LCEs) are asymptotic measures characterizing the average rate of growth of small perturbations to the solutions of a dynamical system. Their concept was introduced by Lyapunov when studying the stability of nonstationary solutions of ordinary differential equations and has been widely employed in studying dynamical systems since then.

**The maximal Lyapunov Characteristic Exponent**

The theory of LCEs was first applied to to characterize chaotic orbits [Oseledec, 1968] and later the connection between LCEs and exponential
divergence of nearby orbits was pointed out [Benettin et al., 1976]. For a chaotic orbit at least one LCE is positive, implying exponential divergence of nearby orbits, which is a characteristic of chaotic behaviour. On the other hand, in the case of regular orbits all LCEs are zero or negative. Therefore, the computation of the maximal LCE $\lambda_1$ is sufficient for determining the nature of an orbit, because $\xi_1 > 0$ guarantees that the orbit is chaotic. A recent review of the theory of LCEs is given in [Skokos, 2010].

The mLCE is computed as the limit for $t \to \infty$ of the quantity

$$\Lambda_1(t) = \frac{1}{t} \ln \frac{||\vec{v}(t)||}{||\vec{v}(0)||}$$

(2.34)

often called finite-time mLCE, where $\vec{v}(0)$ and $\vec{w}(t)$ are deviation vectors from a given orbit at times $t = 0$ and $t > 0$ respectively, and $|| \cdot ||$ denotes the norm of a vector. In the limit $t \to \infty$

$$\lambda_1 = \lim_{t \to \infty} \Lambda_1(t)$$

(2.35)

If the energy surface defined by the Hamiltonian of the system is compact, it has been shown that this limit is finite, independent of the choice of the metric for the space, and converges to $\lambda_1$ for almost all initial deviation vectors $\vec{v}(0)$ [Oseledec, 1968; Benettin et al., 1980]. $\Lambda$ ($\Lambda$ will be used instead of $\Lambda_1$ for simplicity) tends to zero in the case of regular orbits, following a power law [Benettin et al., 1976]

$$\Lambda(t) \propto t^{-1}$$

(2.36)

while it tends to nonzero values in the case of chaotic orbits.

**The spectrum of LCEs**

An $N$-dimensional Hamiltonian system has $2N$ LCEs, which are ordered as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{2N}$. In 1978 a theorem was formulated [Benettin et al., 1978], which led directly to the development of a numerical technique for the computation of all LCEs. The technique is based on the time evolution of many deviation vectors, kept linearly independent through a Gram-Schmidt orthonormalization procedure. Two years later, a concrete theoretical framework, as well as the corresponding numerical method for the computation of all LCEs was presented [Benettin et al., 1980]. According to this method,
usually called the *standard method*, all other LCEs $\lambda_2, \lambda_3, \ldots$ are computed as limits for $t \to \infty$ of some appropriate quantities $\Lambda_2, \Lambda_3, \ldots$, which are called the finite-time LCEs.

Although the standard method is reliable and easy to program, one can use more computationally efficient methods to calculate the Lyapunov spectrum. In the calculations performed in this thesis the QR-decomposition technique [Press et al., 2002] was used instead of the classical Gram-Schmidt, which is a variation of the standard method [Skokos, 2010].

In the case of an autonomous hamiltonian flow, the set of LCEs consists of pairs of values having opposite signs [Benettin et al., 1980],

$$\lambda_i = -\lambda_{2N-i+1}, \quad i = 1, 2, \ldots, N$$

(2.37)

In addition, since the Hamiltonian function is an integral of motion, at least two LCEs vanish

$$\lambda_N = \lambda_{N+1} = 0$$

(2.38)

while the presence of any additional independent integral of motion lead to the vanishing of another pair of LCEs.

**Deviation Vector Distributions**

In the models used in our work, i.e. 1-dimensional hamiltonian systems with a large number of degrees of freedom, it is interesting to also monitor the regions of the lattice where the chaoticity is stronger. A good way to do that, is by computing the Deviation Vector Distribution (DVD):

$$w_l = \frac{\delta u_l^2 + \delta p_l^2}{\delta u_l^2 + \delta p_l^2}$$

(2.39)

$l$ is the site index and $\delta u_l, \delta p_l$ the components of the deviation vector. The deviation vector aligns with the most unstable direction of the phase space. Thus, computing the DVD gives us an indication of the position of the chaotic hot spots in our lattice.

**2.3 Slope Calculation**

In general, the calculation of the slope of noisy data curves is an ill-posed problem. The methods used to numerically calculate derivatives are very
sensitive to noise. However, our averaged data include a significant level of noise. A way to tackle this problem, proposed in [Laptyeva et al., 2010], is the following: first a smoothed curve is produced from the actual data using a locally weighted regression algorithm [Cleveland and Devlin, 1988]. Then a central finite difference formula is applied to calculate the local derivative

$$\alpha(x) = \frac{dy}{dx}$$

where x is usually the control parameter e.g. time and y are the data.

![Figure 2.1: The function $y = |x|$ with noise (a) and its slope calculation (b).](image)

A simple way to test our method is to check if it can compute the actual slopes out of noisy data. The function

$$y(x) = |x|, x \in [-10, 10]$$

is considered with slope $-1, x \in [-10, 0)$ and $1, x \in (0, 10]$. In order to create noise, we add a normally distributed random number (with $\mu = 0$ and $\sigma = 0.25$) to each function value. Then, the data is analysed using the method described above. The results are satisfying, shown in Figure (2.1), suggesting also that this method could be used to extract slope information from real datasets.
Chapter 3

Results

In this chapter the results of our numerical simulations are reported. The chapter is structured in the following way: In the first section some preliminary but crucial details for the computations are discussed. It may seem unnecessary to discuss about which compiler to use or what initial deviation vector to select, but when planning to do hundreds and hundreds of simulations, it is crucial to examine every detail. Also some tests for the linear disordered model are also presented. Then the main results are presented, divided into sections by the dynamical behaviour of the wavepacket evolution.

The first to explore is the weak chaos regime (section 3.3). Different sets of initial conditions, which all lead to sub-diffusive spreading in the weak chaos regime, are considered. For each one of them, the time evolution of the mLCE, averaged over disorder realisations is presented. Also the evolution of the energy and deviation vector distributions are reported for a representative realisation of this regime.

Next the similar results are presented also for the strong chaos (section 3.4) and the self-trapping regime (section 3.5. Finally the special case of the crossover from strong to weak chaos regime is discussed (section 3.6).

At his point it should be also mentioned, that for all the simulations presented in this chapter the KG model is used.

3.1 Practical Considerations

Before every extensive numerical work is performed, there are a few things that should be decided. For our study the following issues are of particular
importance:

- the selection of compiler
- the selection of the numerical integration scheme
- the selection of the initial deviation vector
- whether the whole Lyapunov spectrum should be calculated or only \( \Lambda \)

For the benchmarks, a homogeneous cluster of the HellasGrid infrastructure was used. In this kind of cluster all the computer nodes have the same technical specifications, enabling the direct comparison of the results.

The Compiler

The code used to produce our numerical simulations was written in C. So one of the first decisions to be made was which compiler to use. In HellasGrid, which runs under Scientific Linux, the two main options were the GNU Compiler Collection (GCC) or the Intel C/C++ Compiler Suite (ICC). Various optimization levels were tested before we settle at optimization level 3 (-O3) for both compilers. The executable produced by the ICC compiler consistently performed 10-20% faster than the one obtained by the compiler GCC. Thus the ICC compiler was the one we choose for our simulations.

The Numerical Integrator

Another concern was, which numerical integration scheme to use. It was clear that a symplectic integrator should be used, but there were still some options. The two main competitors were the 4th order Yoshida and the \( SABA_{2C} \). Although it was mentioned in [Skokos et al., 2009] that the \( SABA_{2C} \) integrator performs better with the specific problem, we decided to verify this for our model. After a set of simulations with both integrators and various step-sizes, the \( SABA_{2C} \) was selected with step-size \( t = 0.2 \) time units. This set-up provided a fast and reliable framework for our simulations. The relative error of the integration was fluctuating around \( 10^{-5} \) with maximum value in all cases smaller than \( 5 \cdot 10^{-4} \).
The Initial Deviation Vector

Another concern was whether our Λ calculations are affected by the choice of the initial deviation vector. In order to tackle this question, a set of four different initial deviation vector was considered to test the robustness of our results.

- DV1: a single site deviation vector
- DV2: a random deviation vector
- DV3: a center placed block site deviation vector
- DV4: a deviation vector with components only in the cold exterior of the lattice, i.e. the edges of the lattice

Figure 3.1: In panel (a) the initial DVDs for each deviation vector DV1 (blue), DV2 (red), DV3 (green) and DV4 (orange) are presented. Then the time evolution of Λ is computed for each case using a single site excitation (panel (b)).

The initial distributions $w_i = (\delta p_i^2 + \delta u_i^2)/\sum_i (\delta p_i^2 + \delta u_i^2)$ for deviation vectors DV1 (blue), DV2 (red), DV3 (green) and DV4 (orange) are presented in Figure 3.1a. There is an offset of 16 units in the vertical axis separating each initial DVD. In order to test the influence of the initial deviation vector distribution on the computation of the mLCE (Λ), a simulation of a single site
excitation with $E=0.4$ was used for a 1000 site lattice with $W=4$. In Figure (3.1b) the time evolution of the $\Lambda$ is reported for each initial deviation vector. The straight lines guide the eye for slopes $-1/4$ (solid) and $-1$ (dashed). In Figure (3.2) the time evolution of each DVD is presented. The colour bar corresponds to the values of the logarithm of $w_i$.

Figure 3.2: The time evolution of the DVD for the initial deviation vectors (a) DV1, (b) DV2, (c) DV3 and (d) DV4.

It is clear that, after a transient time, the value of $\Lambda$ is independent of the choice of the initial deviation vector. This is in agreement with the theory of finite time Lyapunov exponents. However, for a practical point of view there are good and bad choices of the initial deviation vector. For instance an initial deviation vector with components only in the edges of the
lattice (DV4), is not a good choice for calculating $\Lambda$ in a simulation with the excitation happening in the center of the lattice. Overall a center placed block site initial deviation vector (DV3) seemed like a good choice for our general purpose and it was the one used in almost all our simulations.

The Spectrum of Lyapunov Exponents

Our final consideration during the benchmark phase of our work was, whether only the mLCE should be computed or also a part of the Lyapunov spectrum. In order to decide that, the first ten components of the Lyapunov spectrum were computed along with the mLCE for a single site excitation with $W=4$ and $E=0.4$. The results are presented in Fig 3.3. The lines guide the eye for slopes $-1/4$ (solid) and $-1$ (dashed). One can notice that the $\Lambda_i, i > 2$ (cyan lines) have similar time evolutions to the one of the $\Lambda$. In conclusion, at this stage of the research where the study of the dynamics behind the spreading process is primarily in question, the evolution of the spectrum of LCEs do not provide any further information than the evolution of mLCE itself. Thus in what follows we restrict our study to the computation of the mLCE $\Lambda$.

Figure 3.3: The time evolution of the mLCE $\Lambda$ (blue) and the 10 first LCEs $\Lambda_i, i = 2, \ldots 10$ (cyan) for a single site excitation.
3.2 The Linear Case

In this section the results for the linear case of the disordered lattice will be presented. The Klein-Gordon Hamiltonian (1.8) is used by eliminating the nonlinear term \( u^4 \). As expected from the theory, Anderson localization prevails in this case, and diffusion is absent. The second moment \( m_2 \) and participation number \( P \) of the energy distribution remain practically constant, fluctuating around constant values. The motion is expected to be regular and so the mLCE vanishes as \( \Lambda \sim t^{-1} \).

All these are shown in figure (3.4) where a simulation of a single site excitation with \( W=4 \) and \( E=0.4 \) for the linear case is presented. In panel (a) the evolution of \( m_2 \) (red) and \( P \) (green) is reported. Straight lines guide the eye for slope 0. In panel (b) the evolution of the mLCE \( \Lambda \) is presented. The straight line denotes the slope -1. As expected the results are in agreement with the theoretical predictions. In figure (3.5) the energy and deviation vector distributions are presented. Given the fact that the initial condition is a single site excitation in real space (\( p_l = \sqrt{2E} \) for \( l = N/2 \) and \( u_l = p_l = 0 \) for all other \( l \)), there is a finite number of excited normal modes. The wavepacket expands until it reaches the localization length of the excited modes. The time needed is of order \( \tau_{lin} = 2\pi/d \) (for theoretical details see also Section 1.1). Then the distribution does not spread any further,
suggesting as expected an absence of diffusion.

Figure 3.5: The time evolution of the energy and deviation vector distributions for the linear KG model.

### 3.3 Weak Chaos Regime

In this section the weak chaos regime is explored. As already mentioned in chapter 1, in this regime the Anderson Localization is destroyed by the weak nonlinear interaction between the normal modes. Subsequently, an initial localized wavepacket spreads with the second moment increasing as $m_2 \sim t^{1/3}$ and the participation number as $P \sim t^{1/6}$. Three different sets of initial condition where considered

- **Case W-I**: a single site excitation with $W=4$ and $E=0.4$
- **Case W-II**: a central block site excitation of $L=21$ sites with $W=4$ and energy per site $E = 0.01$
- **Case W-III**: a central block site excitation of $L=37$ sites with $W=3$ and energy per site $E = 0.01$

The lattice sizes were $N = 1000$ sites for cases W-I and W-II and $N = 1500$ sites for W-III. It has already been reported in the literature that for all of
these cases a weak chaos behaviour is expected [Skokos et al., 2009; Laptyeva et al., 2010].

First a representative case of this regime is presented. Then an ensemble of 50 disorder realisations is considered for each case in order to obtain averaged data for the time evolution of the mLCE Λ.

**Single Realisation**

Here the evolution for a single realisation of Case W-I is presented. The results are also similar for individual realisations in Cases W-II and W-III. In figure (3.6) the time evolution of $m_2$, $P$ and $Λ$ is presented. In panel (a) straight lines guide the eye for slopes 1/3 (solid) and 1/6 (dashed). In panel (b) the straight lines denote the slopes -1/4 (solid) and -1 (dashed).

![Figure 3.6](image)

Figure 3.6: The time evolution of $m_2$ (red), $P$ (green) and $Λ$ (blue) for a single realisation in the weak chaos regime.

The results for the evolution of the energy and deviation vector evolution are reported in (Figure 3.7). The position of the distribution’s mean value is traced by a thick white curve. Notice that the DVD mean position is observed to perform fluctuations whose amplitude increases with time. The importance of this result will be discussed later.
Figure 3.7: The time evolution of the energy and deviation vector distributions in the weak chaos regime.

**Averaged Data**

In order to reliably estimate the slope of the time evolution of mLCE, ensembles of 50 realisation were considered for each case. In panel (a) of (Fig 3.8), the time evolution of the averaged $\Lambda$ for the weak chaos cases W-I (red), W-II (blue) and W-III (green) is reported. Straight lines guide the eye for slopes -1 and -1/4. In panel (b) the numerically computed slopes $a_\Lambda$ of the three curves of panel (a) are presented. The horizontal dotted line denotes the value -1/4.
3.4 Strong Chaos Regime

In this section the results for the strong chaos regime are presented. In this regime the diffusion is faster, yielding a $m_2 \sim t^{1/2}$ and $P \sim t^{1/4}$. As the wavepacket spreads a subsequent slow crossover to the asymptotic weak chaos regime is expected. Three different sets of initial condition were considered:

- Case S-I: a central block site excitation of $L=83$ sites with $W=3$ and energy per site $E = 0.1$
- Case S-II: a central block site excitation of $L=37$ sites with $W=3$ and energy per site $E = 0.2$
- Case S-III: a central block site excitation of $L=330$ sites with $W=1$ and energy per site $E = 0.1$

The lattice size was 2000 sites for the S-I case, 1500 sites for the S-II case and 5000 sites for the S-III case. It is known that all cases belong to the strong chaos regime [Laptyeva et al., 2010].

Single Realization

Here the evolution for a single disorder realisation belonging to the S-I set is presented. The results are also similar for almost all the disorder
realisations of S-II. In (Figure 3.9) the time evolution of $m_2$, $P$ and $\Lambda$ is presented. In panel (a) straight lines guide the eye for slopes $1/2$ (solid) and $1/4$ (dashed). In panel (b) the straight lines denote the slopes $-1/3$ (solid), $-1/4$ (dashed) and $-1$ (dash-dotted).

![Figure 3.9: The time evolution of $m_2$ (red), $P$ (green) and $\Lambda$ (blue) for a single realisation in the strong chaos regime.](image1)

![Figure 3.10: The time evolution of the energy and deviation vector distributions in the strong chaos regime.](image2)
The results for the evolution of the energy and deviation vector evolution are reported in (Figure 3.10). The position of the position of the distribution’s mean value is traced by a thick white curve.

Averaged Data

In order to determine the decrease rate of the mLCE Λ ensembles of approximately 50 disorder realisations were used for each case. In panel (a) of figure (3.11), the time evolution of the averaged Λ for the strong chaos cases S-I (red), S-II (blue) and S-III (green) is reported. Straight lines guide the eye for slopes 1 (dash-dotted), -1/4 (dashed) and -1/3 (solid). In panel (b) the numerically computed slopes $a_{\Lambda}$ of the two curves of panel (a) are presented. The horizontal lines denote the values -1/4(dash-dotted) and -1/3 (dotted).

![Figure 3.11: The time evolution of $<\Lambda>$ and its slope for cases S-I (red) and S-II (blue).](image)

3.5 Self-trapping regime

In this section the self-trapping regime will be explored. In this regime it has been proven for the DNLS model, that a single site excitation can not uniformly spread over the entire lattice [Kopidakis et al., 2008]. Therefore, at
least a part of the wave packet will not spread and will stay localized. Similar results hold also for the KG model we study here [Kopidakis et al., 2008; Skokos et al., 2009]. On the other hand there is a part of the wavepacket which sub-diffusively spreads. For a single site excitation it has been confirmed that $m_2$ grows as $t^{1/3}$. The participation number $P$, however, does not grow [Skokos et al., 2009]. The following parameter values that lead to the self-trapping behaviour of the KG model are used in our study:

- Case SF-I : single site excitation with $E=1.5$ and $W=4$

The lattice size used was 1000 sites. In the next paragraph, a representative case of this regime is presented. Then an ensemble of 20 disorder realisations is considered in order to obtain averaged data for the time evolution of $\Lambda$.

**Single realisation**

Here the evolution for a single realisation of case SF-I is presented. The results are also similar for all the other realisations. In (Figure 3.12) the time evolution of $m_2$, $P$ and $\Lambda$ is presented. In panel (a) straight lines guide the eye for slopes $1/3$ (solid) and $0$ (dashed). In panel (b) the straight lines denote the slopes $-1/4$ (solid) and -1 (dashed).

![Figure 3.12: Time evolution of $m_2$ (red), $P$ (green) and $\Lambda$ (blue) for a single realisation in the self-trapping regime.](image)
Figure 3.13: Time evolution of the energy and deviation vector distributions in the self-trapping regime.

The results for the evolution of the energy and deviation vector evolution are reported in (Figure 3.13). In panel (b) the position of the position of the distribution’s mean value is traced by a thick white curve. Under the white curve, there is a dark-blue line in the center of the lattice, corresponding to the self-trapped part of the wavepacket.

**Averaged Results**

In order to confirm the slopes for the \( \Lambda \) time evolution, an ensemble of 20 realisations was used. In panel (a) of (Figure 3.14), the time evolution of the averaged \( \Lambda \) for the self-trapping regime is reported. Straight lines guide the eye for slopes -1 (dashed) and -1/4 (solid). In panel (b) the numerically computed slope \( a_\Lambda \) of curve of panel (a) is presented. The horizontal dotted line denotes the values 1/4.
3.6 Crossover

As already discussed, a realisation in the strong chaos regime will slowly crossover to the asymptotic weak-chaos regime. The crossover was observed for the first time in [Laptyeva et al., 2010]. The initial conditions used for this purpose was:

- Case CO-I: a central block site excitation of L=21 sites with W=4 and energy per site $E = 0.2$

In this section the same initial conditions will be used for a lattice of 1300 sites. Although expected during the simulation to observe the crossover, this is not the case for all the disorder realisations. Actually, in a total of 30 realizations only half of them exhibited crossover indications. The remaining ones evolved as in the strong chaos regime. Thereafter, a representative crossover realisation is presented. Then averaged data are reported, taking into account only the realization with crossover.

**Single realisation**

Here the evolution for a single realisation of case SF-I is presented. The results are also similar for all the other realisations. In (Figure 3.15) the time evolution of $m_2$, $P$ and $\Lambda$ is presented. In panel (a) straight lines guide the
Figure 3.15: Time evolution of $m_2$ (red), $P$ (green) and $\Lambda$ (blue) for a single realisation which crossover from the strong to the weak chaos regime.

eye for slopes of the strong chaos (1/2 & 1/4 - solid lines) and weak chaos (1/3 & 1/6 - dashed lines) regime. In panel (b) the straight lines denote the slopes -1/3 (solid) and -1/4 (dashed).

Figure 3.16: Time evolution of the energy and deviation vector distributions for the crossover.

The results for the evolution of the energy and deviation vector evolution
are reported in (Figure 3.16). The position of the position of the distribution’s mean value is traced by a thick white curve.

**Averaged Results**

In order to confirm the slopes for the Λ time evolution, an ensemble of 14 realisations was used. The averaged \( m_2 \) is reported in panel (a) of (Figure 3.17). Straight line guide the eye for slopes 1/2 (solid) and 1/3 (dashed). In panel (b), the time evolution of the averaged Λ for the self-trapping regime is reported. Straight lines guide the eye for slope -1/3 (solid) and -1/4 (dashed). In panel (b) the numerically computed slope \( a_Λ \) of curve of panel (b) is presented. The horizontal lines denote the values -1/3 (dotted) and -1/4 (dash-dotted).

![Graphs showing time evolution of \( m_2 \), \( \langle Λ \rangle \), and slope of \( \langle Λ \rangle \).](image)

Figure 3.17: Time evolution of \( m_2, \langle Λ \rangle \) and the slope of \( \langle Λ \rangle \) for the realizations of case CO-I with crossover.
Summary

In the present work, for the first time systematic numerical calculations of finite Lyapunov exponents are reported for disordered nonlinear lattices. The results yield that the dynamics inside the spreading wave packet remains chaotic up to the largest simulation times. The mLCE follows $\Lambda \sim t^{1/4}$ in the 'weak chaos' regime and $\Lambda \sim t^{1/3}$ in the 'strong chaos' regime. In all our simulations, we do not observe any tendency towards ordered motion $\Lambda \neq t^{-1}$.

An important assumption needed for subdiffusive spreading theories is that the spreading wavepacket, first thermalizes and then another oscillator joins the wavepacket. In order to provide numerical evidence about this assumption we will compare the chaotic with the spreading timescales of the system. The Lyapunov time $T_L$

$$T_L = \frac{1}{L} \sim t^{1/4}$$

indicates the time needed for the system to become chaotic. A spreading time scale can be defined from the inverse of the diffusion coefficient. Then in the 'weak chaos' regime it is $m_2 = Dt \Rightarrow D \sim t^{-2/3}$ because $m_2 \sim t^{1/3}$ and the spreading timescale is [Laptyeva et al., 2012]

$$T_S = \frac{1}{D} \sim t^{2/3}.$$ 

The comparison between the two timescales

$$\frac{T_S}{T_L} \sim t^{5/12}$$

proves that the choaticity timescale is always shorter that the spreading time scale, and their ratio diverges as a power law. We are able to confirm for the
Figure 3.18: The dynamics of an individual trajectory of case W-I. Normalized (a) energy ($\epsilon_l$) and (b) deviation vector ($w_l$) distributions at $t = 4 \times 10^6$, $t = 3 \times 10^7$, $t = 4 \times 10^8$ [(r) red; (g) green; (bl) black]. Time evolution of (c) the energy distribution and (d) the DVD for the realization of panel (a) in $\log_{10}$ scale.

First time the assumption about persistent and fast enough chaoticity needed for subdiffusive theories.

Another very important assumption for these theories is that the chaotic seed move randomly into the wavepacket, resulting to its thermalization. A way to visually the motion of these chaotic seeds is to follow the spatial evolution of the deviation vector used for the computation of the mLCE.
In figure (3.18a) the energy density distribution for an individual trajectory of case I at three different times $t \approx 10^6$, $10^7$, $10^8$ is plotted and in figure (3.18b) the corresponding DVD. We obtain that the energy densities spread more evenly over the lattice the more the wave packet grows. At the same time the DVD stays localized, but the peak positions clearly meander in time, covering distances of the order of the wave packet width. The full time evolution of the energy density and the DVD is shown in figures (3.18c,3.18d) together with the track of the distribution’s mean position (central white curve). While the energy density distribution shows a modest time dependence of the position of its mean, the DVD mean position is observed to perform fluctuations whose amplitude increases with time.

All these findings clearly show that nonlinear wave packets spread in random potentials due to deterministic chaos and dephasing. Moreover, wave packets first thermalize, and only later perform subdiffusive spreading. That is a basic prerequisite for the existing theoretical description of energy spreading in disordered nonlinear lattices, and the applicability of nonlinear diffusion equations [Laptyeva et al., 2012; Mulansky and Pikovsky, 2010, 2013; Lucioni et al., 2013].
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Bibliography


