UNDERGRADUATE DIPLOMA THESIS

DNLS in Complex Networks

Author:
Fivos PERAKIS

Supervisor:
Dr. G. P. TSIRONIS

UNIVERSITY OF CRETE
DEPARTMENT OF PHYSICS

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Abstract

We investigate numerically dynamic aspects of the discrete nonlinear Scrödinger equation (DNLS). We begin from a finite chain with periodic boundary conditions, where all the sites of the system are connected only to their nearest neighbors (NN). Then we insert complexity to that system, via the small-world networks concept, in the form of "distant connections", until we reach mean field limit (MF), where each site is connected to all the other sites of the system. The initial condition used is that which places the particle on one lattice site and the main quantity studied is the time averaged probability for the particle to remain in that site. We observe the in the NN limit the probability remains at the initial site above some values of the nonlinear parameter of DNLS (self-trapping), while in the MF limit the probability localizes again, this time because of the system's structure (symmetric lattice).

Contents

Chapter 1

Introduction

Up to the mid-1970s, models of physical phenomena were usually assumed to be linear, or nearly so, allowing advantage to be taken of the convenient but often unrealistic property that complicated causes can be resolved into more simple components, the effect of which are treated separately. Over the past three decades, however, it has become increasingly evident that the assumption of linearity leads the theorist to miss qualitatively significant phenomena.

A striking difference between linear and nonlinear laws is whether the property of superposition holds or breaks down. In a linear system the ultimate effect of the combined action of two different causes is merely the superposition of the effects of each cause taken individually. But in a nonlinear system adding two elementary actions to one another can induce dramatic new effects reflecting the onset of cooperativity between the constituent elements. This can give rise to unexpected structures and events whose properties can be quite different from those of the underlying elementary laws, in the form of abrupt transitions, multiplicity of states, pattern formation, or an irregular markedly unpredictable evolution in space and time reffered to as deterministic chaos. Nonlinear science is therefore, the science of evolution and complexity.

An exciting development in nonlinear science during the 1970s was the gradual realization that certain nonlinear partial differential equations display a variety of exact solutions. One of the most important is the *Nonlinear Scrödinger (NLS) equation*. In normalised form this equation can be written as:

$$i\frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial x^2} + 2|\psi|^2\psi = 0, \tag{1.1}$$

which arose as a model for packets of hydrodynamic waves on deep water [3]. It takes its name from the fact that the small amplitude approximation is the equation that Erwin Scrödinger proposed in 1926 for the propagation of a quantum wave packet in free space. NLS is a generic equation, arising whenever one studies undirectional propagation of wave packets in a dispersive energy conserving medium at the lowest order of nonlinearity. Perhaps the most widely applicable form of a lattice NLS equation is

the *Discrete Nonlinear Schrödinger (DNLS) equation*.

But single lattice models are often insufficient to describe more complex systems encountered in nature. In general such systems are characterised by graphs whose bonds connect sites with a wide distribution of mutual distances. Examples can be found in various fields, ranging from physics or biology to social science and computers. Because of this structural complexity arise some interesting statistical properties. These systems are known as *small-world networks*, i.e. networks whose bonds posses a high degree of local clustering, and at the same time a short average path length connecting the nodes of the system [10; 12; 13].

In this report we investigate mostly numerically the dynamic properties of DNLS in a system with complexity, which has been incorporated by the notion of small-world networks. This is an attempt to investigate a small-world network with a wave-like propagation, unlike the common approaches which focused on a particle-like. However we go beyond the small-world regime, as we reach the limit where the system is fully connected, which is known as the *Mean Field limit*.

Part I

The Theory

Chapter 2

Why DNLS

One of the well studied sets of discrete equations is the Discrete nonlinear Scrödinger equation (DNLS) which arises in a variety of instances in condensed matter [2; 4; 6], in optics [5] and recently in Bose-Einstein condensates [9].

The DNLS equation is given by:

$$i\frac{dC_n}{dt} = V(C_{n-1} + C_{n+1}) - \chi|C_n|^2 C_n \tag{2.1}$$

where the parameters χ and V respectively introduce anharmonicity and dispersion. The $C_n(t)$ are complex amplitudes with $|C_n|^2$ being the probability of finding the excitation at site n at time t. The total probability is normalized to unity $\sum |C_n|^2 = 1$.

One of the most striking features of DNLS is that it leads to *self-trapping*. Self-trapping is now widely recognized as a generic mechanism in the physics of condensed matter. In broad terms self-trapping involves the complementary interaction of two cause and effect relationships: i) the localization of some conserved quantity influences its surrounding structure and ii) this structural change reduces the energy of the conserved quantity preventing its dispersion. In this way one obtains a localized "lump" of the conserved quantity that is dynamically stable and often mobile [6]. The self-trapping properties of solutions to DNLS for finite chains of different sizes has been studied extensively in Ref. [8]

The Discrete nonlinear Schrödinger equation arises in two instances connected to our problem: The semi-classical case and the classical case.

2.1 The Semi-classical Case

The semi-classical case is when we have wave propagation in an Einstein-type oscillator lattice.

DNLS in this context was first used by Holstein for his study of polarons[1] on molecular crystals [2]. Holstein's wave is a electron moving in a one-dimensional lattice while interacting with the lattice ions.

Subsequently Davydov [4] derived DNLS in its time-dependent form during his studies of energy storage and transfer in proteins and other biological materials. Davydov referring to the atomic structure of the alpha-helix region of a protein, which is perceived as a chain:

$$\cdots H-N-C=O\cdots H-N-C=O\cdots H-N-C=O\cdots H-N-C=O\cdots$$

where the residues, or side chains which distinguish individual amino acids are not shown, proposed a polaron-like mechanism for the localization and transport of CO vibrational energy (1500 cm^{-1}). In particular he suggested that vibrational energy of the CO stretching (or Amide-I) oscillators that is localized on the helix acts through a phonon coupling effect to distort the structure of the helix by stretching the adjacent hydrogen bonds. The distortion reacts again through phonon coupling, to trap the Amide-I energy, thereby preventing its dispersion. More details in the subject can be seen on reference [14]

In both fore mentioned models an excitation is moving in a one dimensional lattice while interacting with Einstein-type oscillators. To derive DNLS in this context we begin with the Hamiltonian operator:

$$\hat{H}=\sum_n\left[\varepsilon_n\alpha_n^\dagger\alpha_n-J\left(\alpha_n^\dagger\alpha_{n+1}+\alpha_{n-1}^\dagger\alpha_n\right)\right]+\sum_n\left[\frac{\hat{p}_n^2}{2M}+\frac{1}{2}M\omega_o^2\hat{q}_n^2\right]+g\sum_n q_n\alpha_n^\dagger\alpha_n \tag{2.2}$$

where:

ε_n is the energy of site n
J is the magnitude of the wavefunction overlap of neighboring sites
$\alpha_n^\dagger$ and α_n are the boson raising and lowering operators
$\hat{p}_n$ and $\hat{q}_n$ are the momentum and position operators
M, ω_o are the mass and the frequency of the Einstein-type oscillator
g is the coupling constant of the exciton-phonon interaction

As an approximation we consider that we have classical local phonons with $p_n \approx 0$, thus neglecting the kinetic term. By performing the following ansatz at the wavefunction:

[1] A polaron is a quasiparticle composed of an electron plus its surrounding polarization field

$$|\psi>=\sum_n C_n(t)\alpha_n^\dagger|0> \tag{2.3}$$

with $<\psi|\psi>=1$, we evaluate the average value of the operator $H=<\psi|\hat{H}|\psi>$ by evaluating:

$$\begin{aligned}
<\psi|\alpha_n^\dagger a_n|\psi> &= \sum_{k,l} C_k C_l^*{}_k<0|\alpha_k\alpha_n^\dagger\alpha_n\alpha_l^\dagger|0>_l \\
&= \sum_{k,l} C_k C_l^*{}_k<0|\alpha_k(1-\alpha_n\alpha_n^\dagger)\alpha_l^\dagger|0>_l \\
&= \sum_{k,l} C_k C_l^*{}_k<0|\alpha_k\alpha_l^\dagger|0>_l \\
&= \sum_{k,l} C_k C_l^*{}_k<\psi|\psi>_l \\
&= \sum_n |C_n|^2
\end{aligned} \tag{2.4}$$

and likewise:

$$<\psi|\alpha_n^\dagger a_{n+1}|\psi> = \sum_n C_n^* C_{n+1} \tag{2.5}$$

Thus the Hamiltonian becomes:

$$H=\sum_n\left[\varepsilon_n|C_n|^2-J\left(C_n^*C_{n+1}+C_{n+1}^*C_n\right)+\frac{1}{2}M\omega_o^2q_n^2+gq_n|C_n|^2\right] \tag{2.6}$$

With variational minimization:

$$\begin{aligned}
\frac{\delta H}{\delta q_n}=0 \quad &\Rightarrow \quad M\omega_o^2+g|C_n|^2=0 \\
&\Rightarrow \quad q_n=-\frac{g}{M\omega_o^2}|C_n|^2
\end{aligned} \tag{2.7}$$

we obtain the classical Hamiltonian:

$$H=\sum_n\left[\varepsilon_n|C_n|^2-J\left(C_n^*C_{n+1}+C_{n+1}^*C_n\right)-\frac{g^2}{2M\omega_0^2}|C_n|^4\right] \tag{2.8}$$

and the use of Hamilton's equations lead the DNLS:

$$\begin{aligned}
\frac{\partial H}{\partial C_n^*}=i\frac{dC_n}{dt} \quad &\Rightarrow \quad \varepsilon_nC_n-J(C_{n+1}+C_{n-1})-\frac{g^2}{2M\omega_o^2}|C_n|^2C_n=i\frac{dC_n}{dt} \\
&\Rightarrow \quad i\frac{dC_n}{dt}+J(C_{n+1}+C_{n-1})+\chi|C_n|^2C_n=0
\end{aligned} \tag{2.9}$$

where $\chi=g^2/2M\omega_o^2$ is the nonlinear parameter.

2.2 The Classical Case

DNLS in the classical context, was introduced to describe the dynamics of a set of nonlinear anharmonic oscillators and to understand the localization phenomena [6]. In particular the problem under consideration is that of classical coupled oscillators under the potential $V_n = \frac{1}{2}\omega_o^2 u_n^2 - \frac{1}{4}\beta u_n^2$, where u_n is th longtitudal displacement of the n^{th} mass from its equilibrium position.

To derive the DNLS we begin from the equations of motion (with $M = 0$) :

$$\ddot{u}_n = k(u_{n+1} + u_{n-1} - 2u_n) - \omega_o^2 u_n + \beta u_n^3 \tag{2.10}$$

Then we by writing u_n as a complex amplitude with its complex conjugate:

$$u_n = \phi_n(t)e^{-i\omega_o t} + \phi_n^*(t)e^{i\omega_o t} \tag{2.11}$$

we get:

$$\ddot{u}_n = (\ddot{\phi}_n(t) - i\omega_o\dot{\phi}_n - \omega_o^2\phi_n)e^{-i\omega_o t} + (\ddot{\phi}_n^*(t) + i\omega_o\dot{\phi}_n^* - \omega_o^2\phi_n^*)e^{i\omega_o t}$$

and

$$\beta u_n^3 = \beta(\phi_n^3 e^{-i3\omega_o t} + 3|\phi_n|^2\phi_n e^{-i\omega_o t} + 3|\phi_n|^2\phi_n^* e^{-\omega_o t} + \phi_n^{*3}e^{3i\omega_o t})$$

We now consider the following approximations:

- We consider that $\phi_n(t)$ is varying slowly compared to the main oscillator frequency ω_o, and thus:
  $\dot{\phi}_n(t) \ll \omega_o\phi_n(t) \Rightarrow \ddot{\phi}_n(t) \simeq 0$
- Rotating wave approximation: $3\omega_o \gg k$
  which allows us to keep only the resonant terms $e^{\pm i\omega_o t}$

Thus the terms proportional to $e^{-i\omega_o t}$ give:

$$\begin{aligned} -\omega_o^2\phi_n - 2i\omega_o\dot{\phi}_n &= k(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - \omega_o^2 + \beta(3\phi_n|\phi_n|^2) \\ \Rightarrow i\dot{\phi}_n + \frac{k}{2\omega_o}(\phi_{n+1} + \phi_{n-1}) - \frac{k}{\omega_o}\phi_n + \frac{3\beta}{2\omega_o}\phi_n|\phi_n|^2 &= 0 \end{aligned} \tag{2.12}$$

Then by setting $C_n = \phi_n e^{-i\frac{k}{\omega_o}t}$, $J \equiv \frac{k}{\omega_o}$ and $\chi \equiv \frac{3\beta}{2\omega_o}$ we acquire the DNLS:

$$i\frac{dC_n}{dt} + J(C_{n+1} + C_{n-1}) + \chi|C_n|^2 C_n = 0 \tag{2.13}$$

Chapter 3

Why Small-world networks

A recurrent characteristic of networks in complex systems is the small-world phenomenon, which is defined by the co-existence of two apparently incompatible conditions, (i) the number of intermediaries between any pair of nodes in the network is quite small, typically referred to as the six-degrees of separation phenomenon [15] and (ii) the large local cliquishness or redundancy of the network i.e., the large overlap of the circles of neighbors of two network neighbors. The latter property is typical of ordered lattices, while the former is typical of random graphs [7].

Recently, Watts and Strogatz [10] proposed a minimal model for the emergence of the small-world phenomenon in simple networks. In their model, small-world networks emerge as the result of randomly rewiring a fraction p of the links in a d-dimensional lattice (Fig. 3.1). The parameter p, which is referred as *rewiring probability*, enables one to continuously interpolate between the two limiting cases of a regular lattice (p = 0) and a random graph (p = 1).

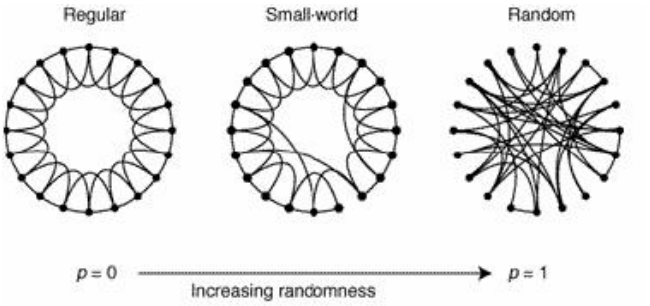

Figure 3.1: Small-world networks are a kind of networks between perfectly ordered and random.

Watts and Strogatz probed the structure of their small-world network model and of

real networks via two quantities:

- the *average path length*:

$$L = \frac{1}{N(N-1)} \sum_{i \neq j} d_{i,j} \tag{3.1}$$

  where $d_{i,j}$ is the minimal number of vertices that have to be traveled to go from the i^{th} to the j^{th} vertex of the system. Thus L measures the typical separation between two vertices in a graph, which is a global property of the system.

- the *mean clustering coefficient C* of the nodes in the network:

$$C = < c_i > = \frac{1}{N} \sum_{i} \frac{2e_i}{k_i(k_i-1)} \tag{3.2}$$

  where c_i of a vertex i with degree k_i is usually defined as the ratio of the number of existing edges e_i between the neighbors of i, to the maximum possible number of edges between neighbors of i $(k_i(k_i-1)/2)$. C measures the cliquishness of a typical neighborhood which is a local property of the system.

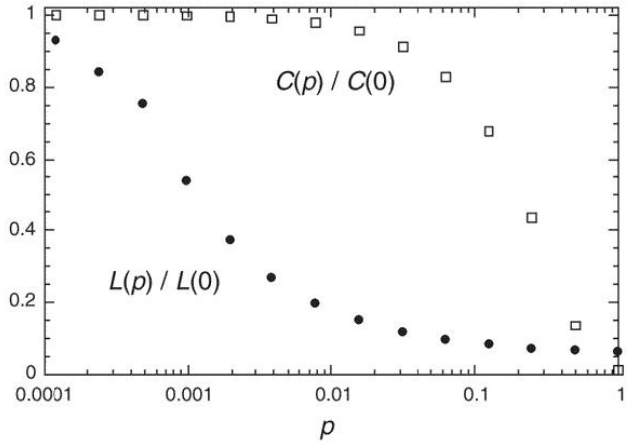

Figure 3.2: With the increase of the rewiring probability p is clear that the L drops rapidly while C remains in the ordered graph range. Between ordered and random graphs exist high-clustered small-world networks.

The emergence of the small-world regime is clear for $p > 0.01$, as L quickly converges to the random graph value, while C remains in the ordered graph range, this two characteristics defining a small-world network (Fig. 3.2). In other words between order and randomness exist high-clustered ($C \gg 1$) small worlds ($L \ll 1$). Watts and Strogatz found clear evidence of the small-world phenomenon in (a) the electric-power grid for Southern California, (b) the network of movie-actor collaborations, and (c)

the neuronal network of the worm C. elegans [16]. Recently small-world have been found suitable for describing many different kind of networks, such as social networks chemical reaction Networks, neural networks, disease spreading and epidemics, food webs, the world wide web, scientific collaborations e.t.c. For more details look in the fore mentioned references and references therein.

One specific case that is connected to our problem is seen in ref. [11] where is considered a small-world view of the protein structure, and that this specific consideration contributes to the identification of some amino-acids that play a crucial role in protein-folding. Taking this into account, and combining it with the fact that DNLS has been used, as shown in the previous chapter, to describe energy propagation in proteins, our attempt to study the dynamics of DNLS in small-world networks can also be understood as *the formulation of a more sophisticated model for energy transport in proteins*.

Part II

The Numerics

Chapter 4

The Nearest Neighbor Limit

Here is studied the case where we have an one dimensional lattice of N connected sites with periodic boundary condition. Since the system under consideration is a lattice all the site are connected only to their nearest neighbors (NN). As an initial condition we use that which places the probability initially on one site of the system. The main quantity studied throughout this report is time-averaged probability of occupation of the initially populated site:

$$\langle P_0 \rangle = \frac{1}{T} \sum P(t) \tag{4.1}$$

4.1 Linear Case

This is the trivial case where the nonlinear parameter chi of the DNLS is zero. A Because of the linear term the probability spreads from the initial and we have a wave propagating through the nearest neighbor connections. We remind here that we have a periodic boundary condition. In fig. 4.1 we see a three dimensional graph of the wave propagation for times up to $t = 100$ in a system with $N = 100$ sites. In the x-y plane we have the site number n and the time, while on the vertical z axis we have the probability of each site $P(n)$. The total probability is normalized to unity $P = \sum P(n) = \sum |C_n|^2 = 1$.

4.2 Nonlinear Case

In this section we insert nonlinearity to the problem. We observe that as we increase the nonlinear parameter the self-trapping occurs and the probability remains at the initially pertubated site. DNLS in one dimensional lattices has been studied extensively in ref [8]. We verify the results as we see that the self-trapping mechanism takes place for values between $\chi = 3$ and $\chi = 5$ of the nonlinear parameter. In fig. 4.2 we see the time averaged probability of the initially pertubated site, while in fig. 4.3 we see the 3D graphs for various values of the nonlinear parameter, where it is more clear how the self-trapping occurs.

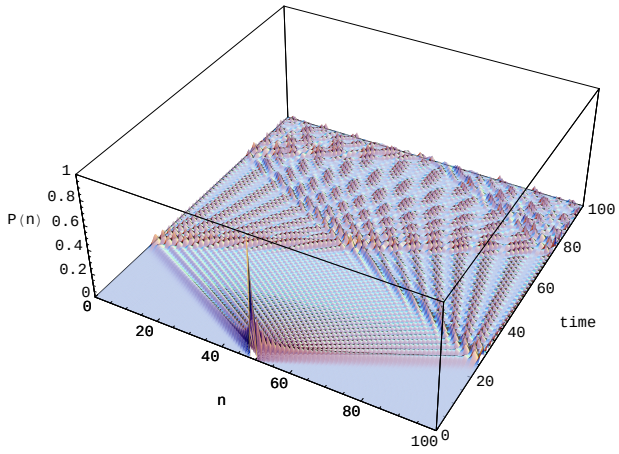

Figure 4.1: In the linear case the probability propagates throughout the system.

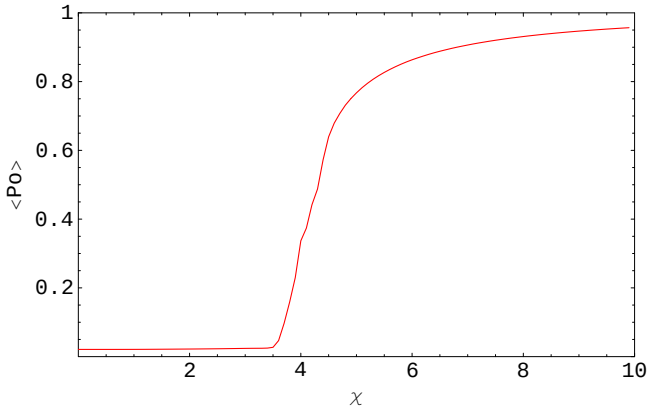

Figure 4.2: Self-trapping takes place for values between $\chi = 3$ and $\chi = 5$ of the non-linear parameter.

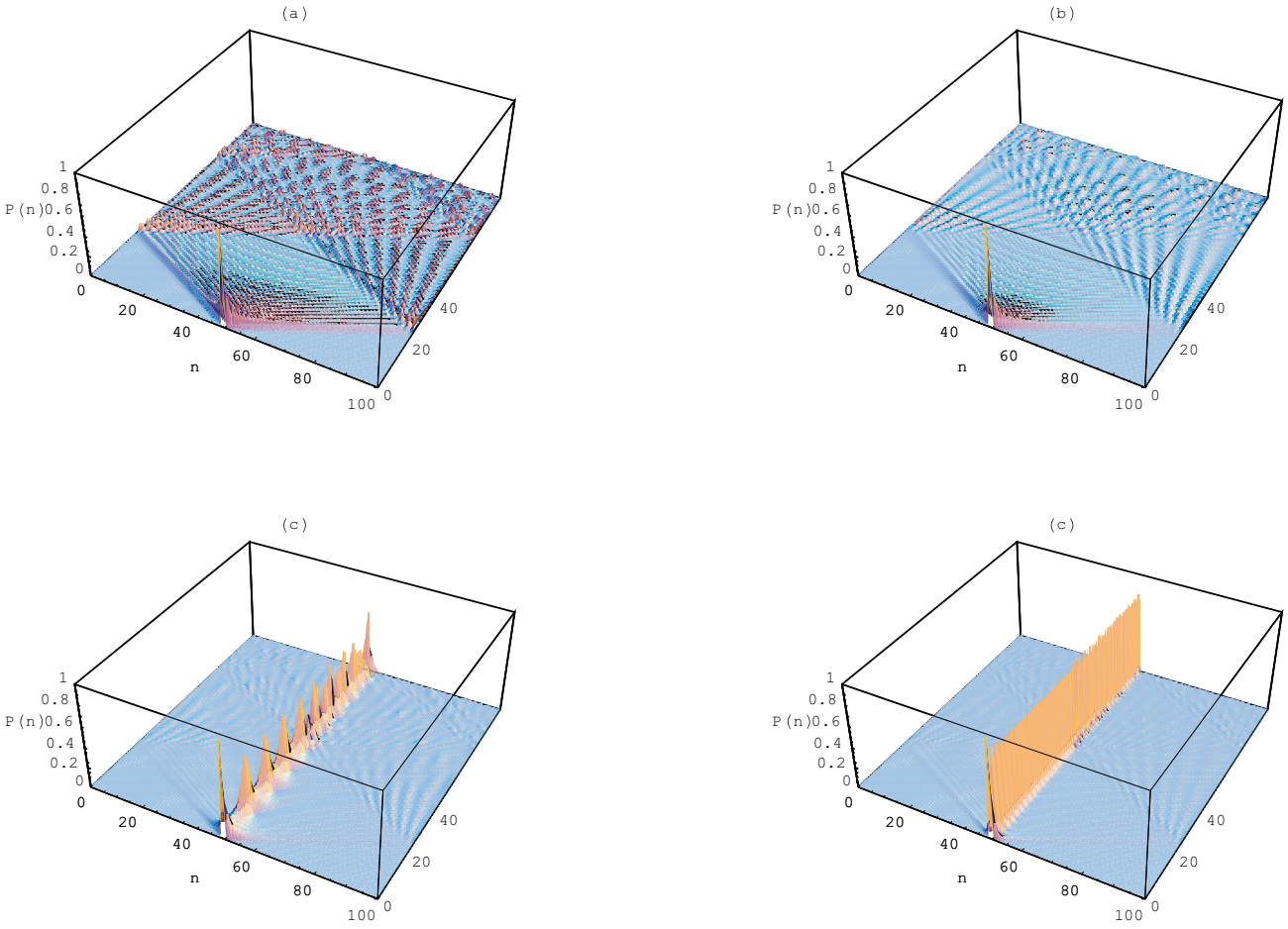

Figure 4.3: The probability 3D plot for values (a)$\chi = 0$, (b)$\chi = 3$, (c)$\chi = 4$, (d)$\chi = 5$ of the nonlinear parameter. The self-trapping initiates for values between $\chi = 3$ and $\chi = 5$.

Chapter 5

The Small-World regime

In the previous section we discussed a finite chain of N sites, confined with periodic boundary condition, which can be considered a regular one-dimensional ring. In this section we will try to insert some complexity to this model by introducing the notion of distant bonds.

To destroy the periodicity of the chain ring we randomly insert connections between distant sites, as seen on Ref [17]. To do so we consider the "vector" form of DNLS in a system of N oscillators:

$$i\dot{\mathbf{C}} = V\mathbf{C} - \chi D(|\mathbf{C}|^2)\mathbf{C} \tag{5.1}$$

where:

$\mathbf{C} = col(C_1, C_2, \ldots, C_N)$ is an N-component column vector, each component representing the complex rotating wave amplitude of a particular oscillator.

$D(|\mathbf{C}|^2) \equiv diag(|C_1, C_2, \ldots, C_N|)$ is a diagonal $N \times N$ matrix representing the nonlinear term which introduces anharmonicity.

$V = [V_{nm}]$ is a symmetric $N \times N$ matrix, the elements of which represent interactions between oscillators.

The above equation is also known as the *Discrete Self-trapping equation* (DST).

The diagonal elements of V_{nn} are the self-connections, which we forbid by keeping them 0. The periodic boundary condition is opposed by keeping the V_{N1} and V_{1N} equal to 1. The form of V for the nearest neighbor limit (NN) for N=5, as you might have guessed is:

$$\mathbf{V} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Then distant bonds are inserted to the system by adding 1 to the appropriate position of the matrix. For instance a bond between the n^{th} and the m^{th} site corresponds to inserting a 1 to the V_{nm} element of the matrix. Then we add randomly from an uniform distribution the bonds B between distant sites. The maximum number of possible distant connections is $B = N \times (N-1)/2 - N$, when the system is fully connected, to which we refer as the mean field limit (MF). The form of the interaction matrix V for the MF limit is:

$$\mathbf{V} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

As the small world region we define the case where we have the addition of distant bonds, the amount of which is analogous to the system size N. The distant bonds are added with the method described above and then we obtain results by averaging over distinct realizations R of each quantity. We focus on systems with size $N = 100$ and the ensemble averaging is done over $R = 500$ realizations.

5.1 Linear Case

A problem similar to the linear case has been studied in reference [17]. We see that with the addition of just a few distant bonds, small part of the probability remains at the initially pertubated site. In fig. 5.1 and 5.2 we see the time averaged probability of the initially perubated site as we increase the number of distant bonds. This is counter-intuitive since the addition of distant bonds would be expected to diffuse the system. However if we perceive the addition of distant bonds as some sort of disorder then we would expect what is happening, since it could be connected with the Anderson localization [1].

5.2 Nonlinear Case

Switching on nonlinearity we observe that the self trapping takes place for greater values of the nonlinear parameter(fig. 5.3). That means that the addition of distant bonds partially obstructs the self-trapping mechanism in the small world regime. Also we see that the time averaged probability of the initially pertubated site drops as we increase the number of distant bonds(fig. 5.4). For greater values of the nonlinear parameter we see that the system resists more to the delocalization as we increase the number of distant bonds added to the system. So we see that in the small-world region, the addition of distant bonds acts on the system mostly by increasing diffusion. This seems to contradict our previous observation in the linear case. But the addition of distant connections acts mostly as a diffusion mechanism of the localization because of the self-trapping, while it also acts as partially as a localizing factor because of the Anderson localization. However there is a limit of how many distant bonds we add to the system. This is called the mean field limit.

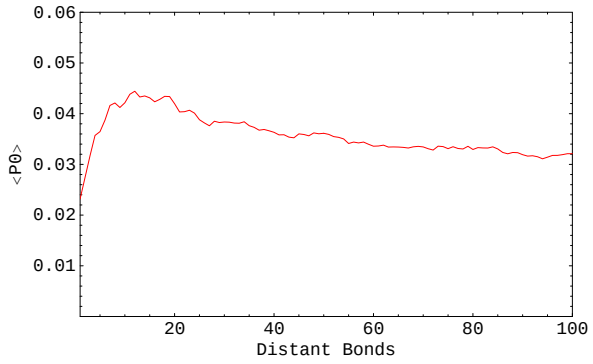

Figure 5.1: The time averaged probability as we increase the number of distant bonds B. With the addition of just a few bonds part of the probability remains at the initial site.

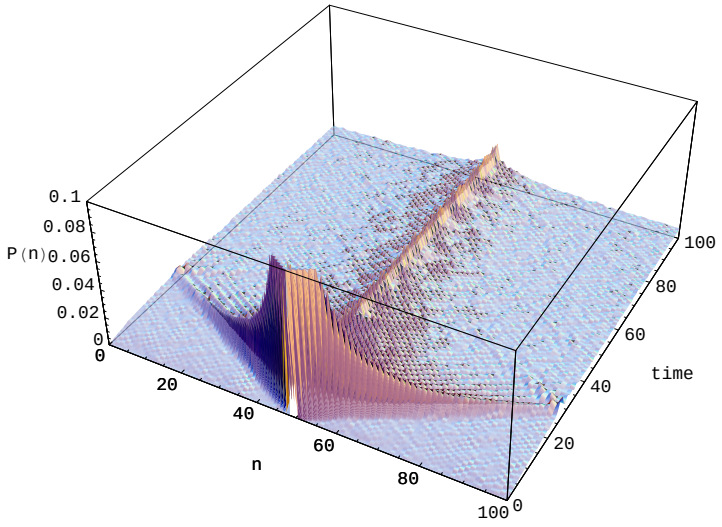

Figure 5.2: The 3D plot with the addition of $B = 5$ distant bonds. Part of the probability remains at the initial site while the rest propagates linearly throughout the system.

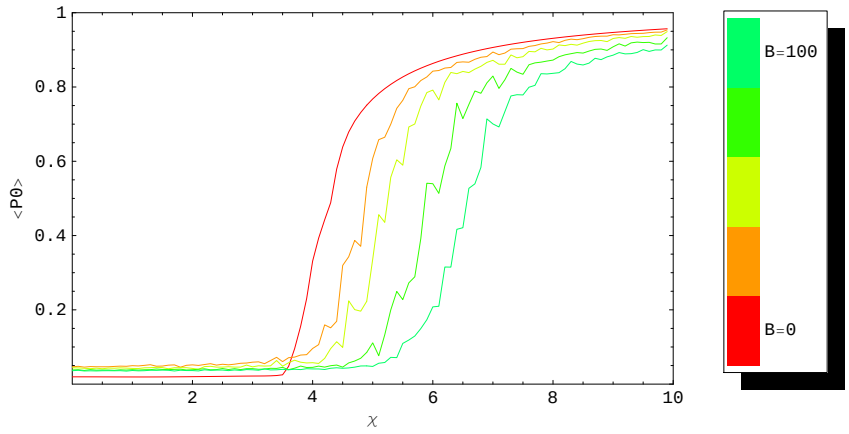

Figure 5.3: The time averaged probability of the initial site as we increase the nonlinear parameter χ. We see that the self trapping takes place for greater values of the χ as we increase the number of distant bonds. Here is shown for $B = 0, 20, 40, 60, 80, 100$ distant bonds.

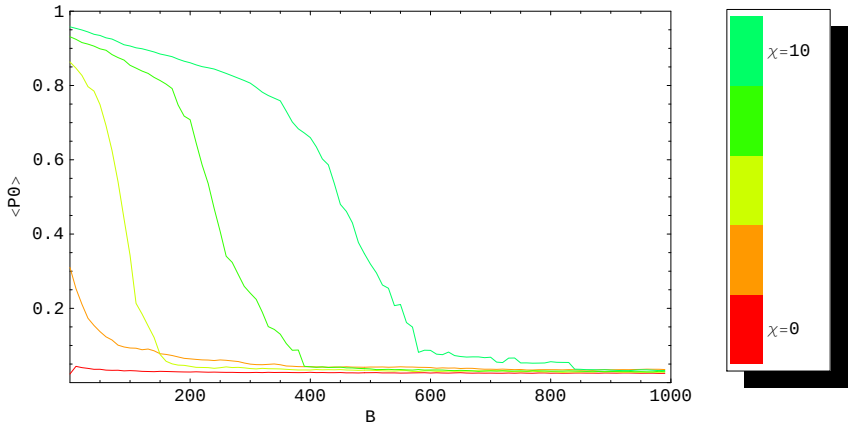

Figure 5.4: The time averaged probability of the initially pertubated site drops as we increase the number of distant bonds. Here is shown for $\chi = 0, 4, 6, 8, 10$. The addition of distant bonds acts as a diffusion mechanism, while nonlinearity seems to act as an agent of localization, since it increases the systems resistance to diffuse.

Chapter 6

Mean Field Limit

In the mean field limit (MF) we have the maximum number of distant bonds $B = N \times (N-1)/2 - N$. This is the case where each site is connected to all the other sites of the system. While exploring the MF at the linear case we observe that the probability tends to remain localized at the initially pertubated site(fig. 6.1).

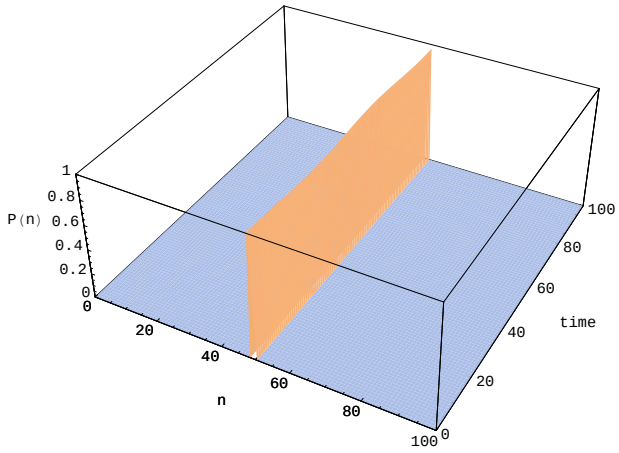

Figure 6.1: In the mean field limit the probability tends to remain localized at the initially pertubated site.

To understand the reason behind this we must look at the eigenvalues of the system. Solving numerically the linear case:

$$V\mathbf{C} = \lambda\mathbf{C} \Rightarrow det[V - \lambda I] = 0 \tag{6.1}$$

where **C** is the n-component column vector and V is the interaction matrix, we obtain $N-1$ eigenvalues with $\lambda_i = -1$, and one $\lambda_N = N-1$.

Thus we see that two possible solutions come up: one that keeps the probability localized at the initial site ($\lambda = -1$), and the $N-1$ that have the completely delocalized throughout the system ($\lambda = N-1$). Since we choose as an initial condition the case where the probability is initially localized on one site, we tend to favor the first solution. In order to obtain numerically the second type of solutions, these which the probability is delocalized, we choose as an initial condition a case where the probability is initially spread throughout the system.

To do so we consider the case where the probability is divided equally to all the sites except a small amount which varies throughout the system periodically. To be more specific, since we consider a system of size $N = 100$ and since the total probability is normalised to unity, the probability which corresponds to an equal sharing would be 0.01 to each site. Then to add some dynamics to our process, we subtract from that initial condition a periodic term $a \times cos(4\pi n/N)$, thus creating a cosinal initial pertubation throughout the system (a here is a constant that indicates the amplitude of the cosinal pertubation, we choose $a = 0.002$).

To examine the dynamics of the delocalized initial condition lets see first how it behaves in the NN limit. In the linear case (fig. 6.2) we see that the probability is exchanged throughout the system, as seen for greater times up to $t = 1000$ in fig. 6.3.

Lets look now into the linear MF limit. What we observe is that the probability is exchanged throughout the system in a similar fashion to the NN but the waves propagate much faster in the MF. (fig. 6.4 and in more detail fig. 6.5). What is happening here is not clear to us and needs to be examined in a greater extend.

It would be interesting to see the effect of nonlinearity in the fore mentioned initial condition. But to solve the nonlinear "eigenvalue" problem a different method would have to be used, beyond that of the standard methods of normal mode theory. In ref. [6] some numerical methods are presented for approaching similar problems.

The main conclusion that we keep from this section is that with the localized initial condition used in the MF we observe localization not because of nonlinearity but because of the system's structure. Lets see now how the system behaves in the area between the two extremes: between the NN and the MF limit.

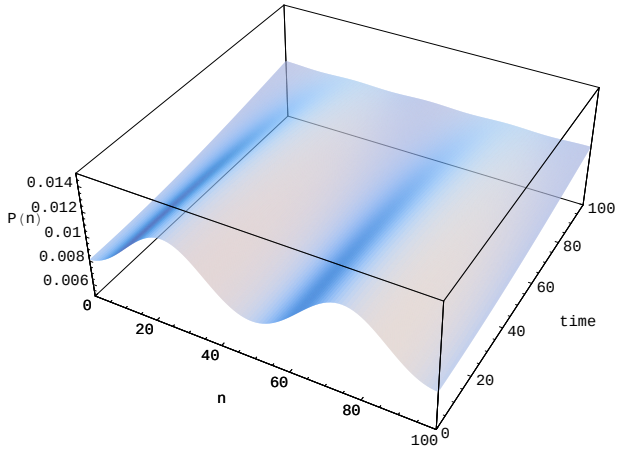

Figure 6.2: Using a delocalized initial condition to the linear NN limit.

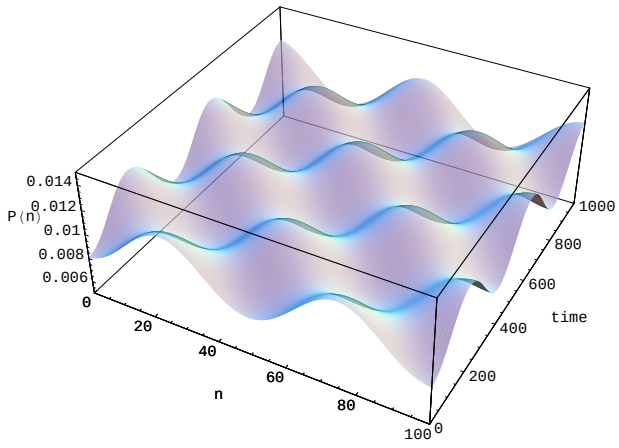

Figure 6.3: In the linear NN case the probability is exchanged throughout the system.

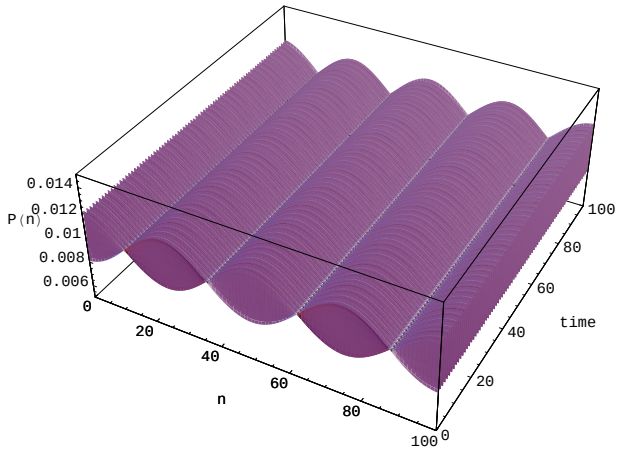

Figure 6.4: The MF limit with a delocalized initial condition. We see that the oscillation frequency increases.

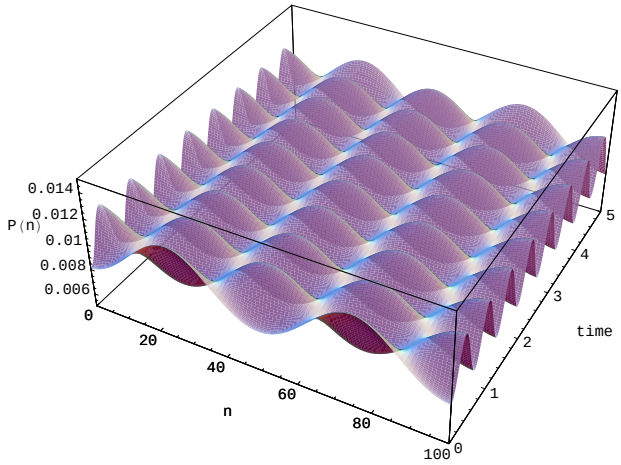

Figure 6.5: The MF limit with a delocalized initial condition for lesser times to observe in more detail what si happening.

Chapter 7

From the NN to MF limit

We consider two ways of approaching the mean field limit:

7.1 By increasing distant bond intensity

First we gradually increase the intensity Is of all the distant bonds of the system. The process is seen in Fir. 7.1. We begin from $Is = 0$, which is the nearest neighbor limit, and we reach $Is = 1$ where all the sites are fully connected. Throughout this process the nearest neighbor bond intensity is 1.

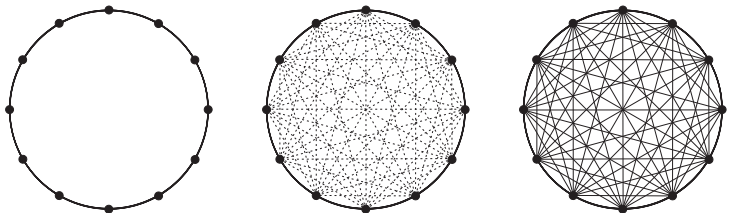

Figure 7.1: Increasing the distant bonds intensity Is.

We see that despite the addition of distant connections the wave propagates only through the nearest neighbor connections and that the distant connections act as some sort of disorder that prevents the wave from propagating. We also notice that as we gradually increase the Is that the probability of the initially pertubated site mark a rapid change for values very close to 1.

Repeating the process for different values of the nonlinear parameter chi we see that as we increase nonlinearity probability becomes self-trapped for earlier values of Is(fig. 7.2). We also note here that for the phase transitional values near $\chi = 4$ we notice some *anomalous behavior* as seen in more detail in fig. 7.3.

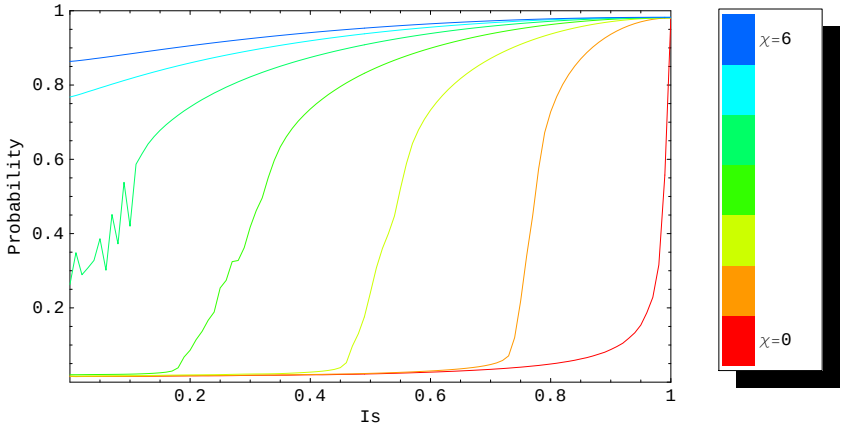

Figure 7.2: Time averaged probability of the initial site as we increase the distant bond intensity Is for various values of the nonlinear parameter.

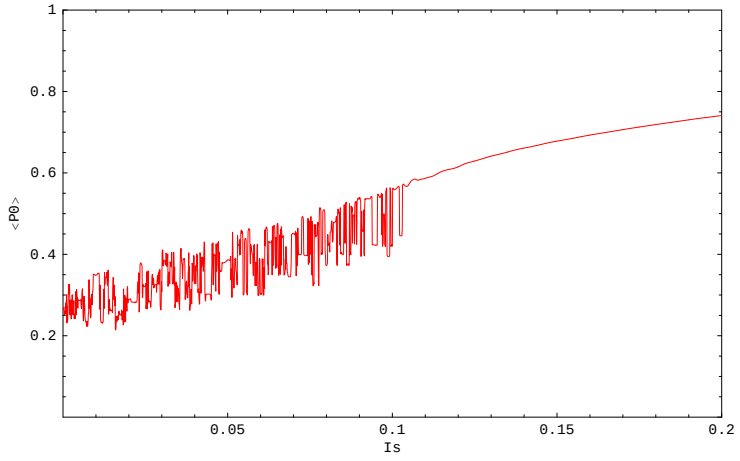

Figure 7.3: We observe some interesting behavior for early Is and for chi=4.

7.2 By increasing the number of distant bonds

The other method used to approach the mean field limit is by increasing the number of distant bonds B (fig. 7.4). Starting from the first neighbor limit where $B = 0$, we randomly add bonds with the method described above, until we reach the mean field limit where the maximum number of distant bonds has been reached, which is $B = N \times (N-1)/2 - N$. Since we observe a chain of $N = 100$ sites, the MF occurs for $B = 4895$.

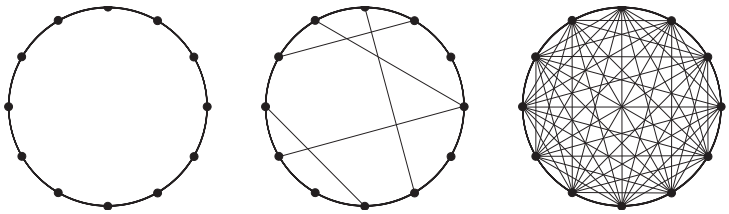

Figure 7.4: Increasing the number of distant bonds B.

In the linear case we observe that as we approach the MF limit (fig. 7.5), a rapid transition occurs for values very close to the MF. The probability which remains delocalized throughout the whole process, suddenly for values very close to the MF becomes localized. This is counter-intuitive since one would expect that the localized solution would emerge gradually, since the addition of distant connections are understood as some sort of disorder. So as the degree of disorder increases, so would the tendency to localize. On the contrary we see that the localized property of the MF limit arises rather suddenly. A similar conclusion is drawn from the previous case, where we approached the MF by increasing the distant bond intensity.

Repeating the above calculation for the nonlinear case we observe that nonlinearity acts as an agent of localization. For small values of the distant bonds B, we observe that the greater the the values of the nonlinear parameter χ, the greater the resistance of the system to delocalize. Then somewhere in the middle of the range of B we observe a minimum. This is the area between the NN and the MF regimes. In the NN we observe localization because of the self-trapping mechanism due to nonlinearity, while in the MF limit we observe localization which arises as a solution to the eigenvalue problem of the MF. So between these two limits lyes the area where nonlinearity competes with the delocalization because of the distant bonds, and the minimum is the area where the system reaches its most delocalized form. Then beyond this area and as we approach the MF limit, nonlinearity contributes the the localization of the probability. It is worth mentioning here that, as we see on fig. 7.5, for great values of the nonlinear parameter χ the system never delocalizes completely.

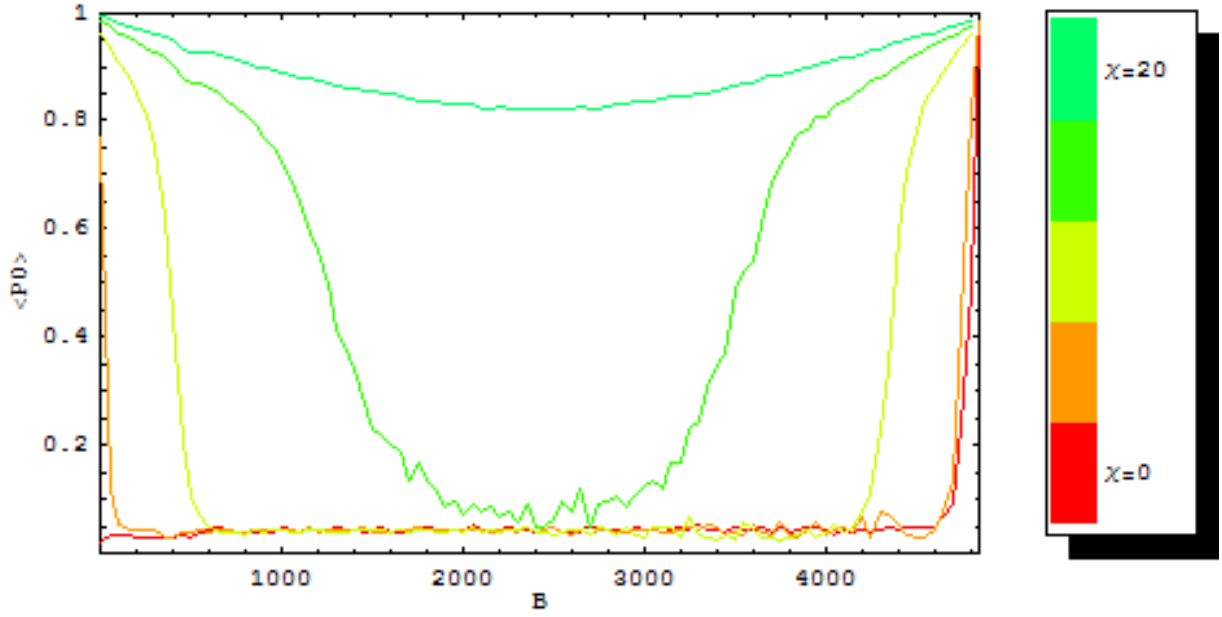

Figure 7.5: This is our main conclusion: we observe the change of the time averaged probability of the initial site as we increase the number of distant bonds, ranging from the NN to the MF, for different values of χ. The localization noticed in the NN is because of the self-trapping mechanism, while that in the MF limit is because of the systems structure. Here are shown the cases where the nonlinearity parameter is $\chi = 0, 5, 10, 15, 20$.

Chapter 8

Conclusions

We investigated the dynamic properties of DNLS between the nearest neighbor (NN) and the mean field (MF) limit.

Nearest Neighbor Limit:
We began from the NN limit, where we investigated the self-trapping properties of DNLS in a ring lattice, verifying the values of the nonlinear parameter for which the self-trapping occurs.

Mean Field Limit:
Solving the linear eigenvalue problem for the MF limit, we obtained 1 solution with $\lambda = N - 1$, and N-1 degenerate solutions with $\lambda = -1$. With initial condition that places the particle on one site we obtained the localized solution, while with a periodic delocalized initial condition we obtained the degenerate solutions in the form of stationary waves. What needs further investigation is the "nonlinear eigenvalue problem" in the NN and the MF, as well as in the range between the two limits, where a statistical approach must be considered.

From NN to MF: Increasing Distant Bond Intensity I
We begin the investigation between the two limits by considering the system fully connected and by gradually increasing the intensity I of the distant bonds. In the linear case we note that the system remains delocalized until late values of I, when it converges to the localized state. Switching on nonlinearity we observe that for greater values of χ the system localizes more easily (meaning for earlier values of I). What might be interesting to explore is the anomalous behavior exhibited for values $\chi = 4$ of the nonlinear parameter.

From NN to MF: Increasing the Number of Distant Bonds B
Another way to approach the mean field limit is by increasing the number of distant bonds B. In the linear case we observe that we observe that with the addition of just a few bonds a small fraction of of the probability tends to localize, a phenomenon which could be connected with the Anderson localization, since the above process can be also

interpreted as the addition of some kind of disorder to the system. In the nonlinear case we observe that the addition of distant bonds tend to initially diffuse the system, while nonlinear obstructs to that diffusion. However as we approach the MF limit the system converges tho a localized state, and once again nonlinearity enhance that tendency.

So what we observe is two kinds of localization: one that is connected with nonlinearity (self-trapping) and another that has to do with the systems structure (MF limit). What needs to be investigated is how the system behaves under both, i.e. when the system is in the MF limit with nonlinearity.

Appendix A

The program code

In this appendix we appose the program code in Fortran g77. The program is divided in parts and some explanatory comments have been added. In the same folder as the program a DNLS.txt file must be included from which the problem will read the parameters used.

The main program. This version is for the creation of 3D data graphs.

```
! program dnls.f
C
C Discrete Nonlinear Schroedinger equation
C       with the addition of Small World connections.
C       Maximum ns:500
C
C July 08

        implicit none
        real*8 time,z(500,2),zt(500,2),chi,v
        real*8 sum,U(1:500,1:500),p
        real*8 dt,tmax,t
        integer runge,ns,bonds,rcount,m,nsnaps
integer Repeat,k,i,j,tcount,InitCond
        integer*4 today(3), now(3),seed
        integer R_index,Rmax,R(1:250000)

common /block1/ z,zt,dt
common /block2/ chi,v
        common /block3/ time
        common /block4/ sum
        common /block5/ ns,bonds
        common /block6/ U
```

```
        common /block7/ p
        common /block8/ R_index,R,Rmax
        common /block9/ seed
        common /block10/ InitCond
        common m

open(1,file='Prob.txt')

        open(4,file='dnls.txt')
read(4,*)ns !The number of sites
read(4,*)chi !The nonlinear parameter
        read(4,*)v !The linear parameter
read(4,*)dt,tmax,nsnaps !time step, max, and nsnaps=tmax/dt
        read(4,*)bonds   !Bonds is the number of SW connections
read(4,*)Repeat  !Number of realizations
        read(4,*)InitCond  !0 for delocalised, 1 for localised
        close(4)

        i=0
        j=0

        !Initializing z,zt
        do i=1,500
           z(i,1)=0.0d0
           z(i,2)=0.0d0
           zt(i,1)=0.0d0
           zt(i,2)=0.0d0
        enddo

        !Initializing U
        i=0
        j=0
        do i=1,500
           do j=1,500
              U(i,j)=0.d0
           enddo
        enddo

      do rcount=1,Repeat
            print*, '----------------r=',rcount,'-----------------'

            t=0.0d0
            time=t
            call incond

    t=0.0d0
```

```
            Do while (t.lt.tmax)
                k=1!Here k is a constant used by RK to show when it is completed(k=0)
                do while(k.eq.1)
                   k=runge(t)
                   call eqmot
                enddo
                time=t
                call crfile
            enddo!the t-loop
      enddo!The r-loop

 close(1)

 stop
         end
```

The subroutine used to initialise the program:

```
        subroutine incond

        implicit none

        Real*8 z(500,2),zt(500,2),dt,chi,v,U(1:500,1:500)
        Real*8 x,y,pi
        Integer ns,bonds,k,l,ins,i,j,MeanField
        Integer R_index,R(1:250000),Rmax,seed,InitCond

common /block1/ z,zt,dt
common /block2/ chi,v
common /block5/ ns,bonds
common /block6/ U
common /block8/ R_index,R,Rmax
common /block9/ seed
common /block10/ InitCond

        pi = 4.d0*datan(1.d0)

        k=1
do k=1,ns
   z(k,1)=0.0d0
   z(k,2)=0.0d0
        enddo

C     Initial Condition
        ins=ns/2
        if(InitCond.eq.1)then
```

```
     z(ins,1)=1.0d0 !Localised initial condition
        elseif(InitCond.eq.0)then
             do i=1,ns
                z(i,1)=0.1d0 - 0.001*Cos(100*pi*float(i)/float(ns))!Delocalised
             enddo
        else
             print*,'Invalid Initial Condition. '
             print*,'InCond=1 for localised'
             print*,'Incond=0 for delocalised'
             stop
        endif

C     Initializing U(k,l)
        k=0
        l=0
        do k=1,ns
           do l=1,ns
              U(k,l)=0.d0
           enddo
        enddo

C     First Neighbor Interactions
        k=0
        do k=1,ns-1
           l=k+1
           U(l,k)=1.d0
           U(k,l)=1.d0
        enddo

C     Boundary Condition
        U(1,ns)=1.d0
        U(ns,1)=1.d0

C     Initializing R(ns*ns)
      i=1
      j=1
      k=1
      l=1
      Do i=1,ns
         Do j=1,ns
            if(j.gt.(i+1))then
               R(k)=l
               k=k+1
            endif
            l=l+1
         Enddo
```

```
      Enddo

      Rmax = k-1
      !Maximum number of small world connections are:
      ! Rmax = ns*(ns-1)/2 - ns
      !In the last term we substract the first neighbor interactions

      !Remove from R(i) because of periodic boundary condition
      R_index=ns-2
      call Recalibrate

      !The mean Field limit for this size
      MeanField=Rmax

C CREATION OF RANDOM SW CONNECTIONS

      i=1
      if((bonds.ge.0).and.(bonds.lt.MeanField))then
          do i=1,bonds
              seed = i*i*seed
              call RandomBondCreate
              call Recalibrate
          enddo
      elseif(bonds.gt.MeanField)then
          print*,'Too many bonds.'
          print*,'The meanfield limit is:',MeanField
          stop
      elseif(bonds.eq.MeanField)then
          print*, '...Mean Field Limit...'
          i=1
          j=1
          do i=1,ns
             do j=1,ns
                If((i.ne.j).and.(i.ne.(j+1)).and.(i.ne.(j-1)))then
                    U(i,j)=1.0d0
                endif
             enddo
          enddo
      endif

      call crfile

      return
      end
```

The subroutine used to write the results in a file:

```
         subroutine crfile

        implicit none
        Real*8 z(500,2),zt(500,2),dt,chi,v,time
        Real*8 U(1:500,1:500),p,cmin
        Integer ns,bonds,i,tcount

        common /block1/ z,zt,dt
common /block2/ chi,v
        common /block3/ time
        common /block5/ ns,bonds
common /block6/ U
        common /block7/ p

        i=1
cmin=1.0d-10
tcount=IDNint(time/dt)
if((mod(tcount,10)).eq.0)then !shrinks the por.txt
   do i=1,ns
       p= z(i,1)*z(i,1)+z(i,2)*z(i,2)
       print*, 't = ',tcount
       if(p.le.cmin)then
           write(1,*) 0.d0
       else
           write(1,*) p
       endif
           enddo
        endif
        return
        end
```

The DNLS equations:

```
        subroutine eqmot

        implicit none
        real*8 z(500,2),zt(500,2),chi,v
        real*8 sum,U(1:500,1:500)
        real*8 d1,d2,an1,an2,dsum,dt,time
        integer m,ns,i,bonds,tcount

common /block1/ z,zt,dt
common /block2/ chi,v
common /block3/ time
        common /block4/ sum
```

```
        common /block5/ ns,bonds
        common /block6/ U


sum=0.0d0

        m=0
        do m=1,ns
           d1=0.d0
           d2=0.d0
           i=0
           do  i=1,ns
   d1=d1+U(m,i)*z(i,1)
   d2=d2+U(m,i) *z(i,2)
           enddo

   an1=chi*(z(m,1)*z(m,1)+z(m,2)*z(m,2))*z(m,1)
   an2=chi*(z(m,1)*z(m,1)+z(m,2)*z(m,2))*z(m,2)

   zt(m,1)=v*d2-an2
   zt(m,2)=-v*d1+an1
enddo

        m=0
        do m=1,ns
   sum=sum+z(m,1)*z(m,1)+z(m,2)*z(m,2)
        enddo

dsum=0.001d0
if(abs(sum-1.0d0).gt.dsum) write(*,*)' ERROR ','sum = ',sum

return
        end
```

The Runge-Kutta 4 function:

```
        function runge(t)

        implicit none
        Real*8 phi(500,2),savey(500,2),z(500,2),zt(500,2)
        Real*8 t,dt
        Integer ns,bonds,i,j
        integer runge, m
        common /block1/ z,zt,dt
        common /block5/ ns,bonds
        common m
```

```
        m=m+1
        go to (1,2,3,4,5),m
1       runge=1
        return
2       do 21 j=1,2
        do 22 i=1,ns
        savey(i,j)=z(i,j)
        phi(i,j)=zt(i,j)
22      z(i,j)=savey(i,j)+0.50*dt*zt(i,j)
21      continue
        t=t+0.50*dt
        runge=1
        return
3       do 32 j=1,2
        do 33 i=1,ns
        phi(i,j)=phi(i,j)+2.00*zt(i,j)
33      z(i,j)=savey(i,j)+0.50*dt*zt(i,j)
32      continue
        runge=1
        return
4       do 43 j=1,2
        do 44 i=1,ns
        phi(i,j)=phi(i,j)+2.00*zt(i,j)
44      z(i,j)=savey(i,j)+dt*zt(i,j)
43      continue
        t=t+0.50*dt
        runge=1
        return
5       do 54 j=1,2
        do 55 i=1,ns
55      z(i,j)=savey(i,j)+(phi(i,j)+zt(i,j))*dt/6.0
54      continue
        m=0
        runge=0
        return
        end
```

The Subroutine used to create random bonds

```
      Subroutine RandomBondCreate

      implicit none
      integer seed,R_index,R(1:250000),b,ns,x,y,Rmax,bonds
      real*8 a,U(1:500,1:500)
      integer*4 today(3),now(3)

      common /block8/ R_index,R,Rmax
```

```
      common /block5/ ns,bonds
      common /block6/ U
      common /block9/ seed

      if(Rmax.le.0)then
           print*,'Matrix Full!!!'
           return
      endif

      call idate(today)   ! today(1)=day, (2)=month, (3)=year
      call itime(now)     ! now(1)=hour, (2)=minute, (3)=second

69    seed = abs(seed*now(3)-seed*now(2)+6985748)

      call srand(seed)
      a=rand(seed)
      R_index = IDNint(a*Rmax)
      If (R_index.eq.0) then
         goto 69
      endif

      b = R(R_index)
      x=mod(b,ns)
      y= b/ns +1
      if(x.eq.0)then
         x = ns
         y=y-1
      endif

      if(U(x,y).ne.(1.d0))then
          U(x,y)=1.d0
          U(y,x)=1.d0
      else
          print*,'ERROR..............(',x,',',y,')...R(',R_index,')=',b
      endif


      return
      end
```

The subroutine used to recalibrate the matrix R, which is a matrix of the free connections (i.e. not used) connections of the system

```
      Subroutine Recalibrate

      implicit none
```

```
integer R_index,Rmax,i,R(1:250000)

common /block8/ R_index,R,Rmax

i=R_index
do i=R_index,Rmax
   R(i)=R(i+1)
enddo

R(Rmax) = 0
Rmax = Rmax - 1

return
end
```

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