Discrete nonlinear Schrödinger equation in complex networks

F. Perakis\textsuperscript{1} and G. P. Tsironis\textsuperscript{2}

\textsuperscript{1}Physikalisch-Chemisches Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland and 
\textsuperscript{2}Department of Physics, University of Crete and Institute of Electronic Structure and Laser, FORTH, P.O. Box 2208, Heraklion 71003, Crete, Greece.

We investigate numerically dynamical aspects of the discrete nonlinear Schrödinger equation (DNLS) in finite lattices. We start from a periodic chain with nearest neighbor interaction and insert distant links that connect random pairs of sites across the lattice. For a localized initial condition we focus on the time averaged probability at the initial site analyzed as a function of the degree of complexity of the lattice. We find that selftrapping occurs at increasingly larger values of the nonlinearity parameter as the lattice connectivity increases while close to the fully connected network localization becomes more preferred. The nonlinear network dynamical behavior is understood as a competition of two lattice limits, viz. that of pure nearest neighbor interaction as well as the mean field limit where all sites are mutually coupled.

I. INTRODUCTION

The aim of this work is to investigate what happens when two distinct aspects of complex systems coexist simultaneously. The first feature is that of selftrapping, viz. a generic dynamical property of nonlinear lattices that leads to localization in a translationally invariant system. The second is the geometrical feature that emerges from a small world network (SWN). In order to probe the former we use the Discrete nonlinear Schrödinger (DNLS) equation that is an ubiquitous equation arising in a variety of contexts in condensed matter \cite{1,2,3}, in optics \cite{4}, in Bose-Einstein condensation \cite{5}, etc. For the second feature we use Newman-Watts Small-world networks (NWSWNS) where random links are inserted linking pairs of the original nearest neighbor coupled lattice sites \cite{6,7,8}.

The DNLS equation is given by:

\begin{equation}
\frac{dC_n}{dt} = V(C_{n-1} + C_{n+1}) - \chi |C_n|^2 C_n
\end{equation}

where the parameters $\chi$ and $V$ respectively introduce anharmonicity and dispersion; hereafter we set $V = 1$. The $C_n(t)$ are complex amplitudes with $|C_n|^2$ being the probability for finding the excitation at site $n$ at time $t$. We take the total probability normalized to unity $\sum |C_n|^2 = 1$. We may express the DNLS equation also in matrix form \cite{3}:

\begin{equation}
iC = MC - \chi D(|C|^2)C
\end{equation}

where $C = \text{col}(C_1, C_2, \ldots, C_N)$ is an $N$-component column vector, each component representing the complex rotating wave amplitude of a particular oscillator, $D(|C|^2) \equiv \text{diag}(|C_1|^2, |C_2|^2, \ldots, |C_N|^2)$ is a diagonal $N \times N$ matrix representing the nonlinear term which introduces anharmonicity and $M = |M_{nm}|$ is a symmetric $N \times N$ matrix, the elements of which represent linear interactions between oscillators.

One of the most interesting features of DNLS is that it leads to self-trapping, viz. while for small values of $\chi$ the probability wave is delocalized, this does not hold for larger nonlinearity values \cite{5}. The self-trapping properties of DNLS for finite chains of sites have been studied extensively in Ref \cite{5}. But single lattice models are often insufficient to describe more complex systems encountered in nature. In general such systems are characterized by graphs with bonds connecting 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. This structural complexity gives rise to interesting statistical properties. These systems are known as small-world networks, i.e. networks whose bonds possess a high degree of local clustering, and at the same time a short average path length connecting the nodes of the system \cite{6,7,8}.

In the present paper we extend the work of Ref. \cite{9} to structurally complex networks. Specifically, we focus on the dependence of localization properties of DNLS on the degree of complexity of the network; the problem is set as follows: We begin with $N$ lattice sites that form a one dimensional ring. For relatively large values of $N$ the DNLS dynamics on this ring is not different form the one in very long one dimensional lattices \cite{9}. Subsequently, we destroy the periodicity of the lattice by randomly inserting connections between distant sites, as seen in Ref \cite{10}. As an initial condition we use that which places the probability initially on one site of the system. The main quantity studied throughout this paper is the long time-averaged probability $P_0(t)$, viz. the occupation probability of the initially populated site:

\begin{equation}
(P_0)_t = \frac{1}{T} \sum_{t=0}^{T} P_0(t)
\end{equation}

Physically, we are placing a quantum particle at a given lattice site and follow its time evolution in the semiclassical limit. This study is related to work done on DNLS in disordered lattices \cite{11,12,13}.

II. SELFTRAPPING IN A COMPLEX LATTICE

Before we address the dynamics of the DNLS equation in a small world network we need first to establish two specific limits. In order to form a small world network, we start from a periodic ring of sites and add randomly (using a uniform distribution) $B$ bonds linking distant sites. For $B = 0$ only first neighbors are connected; this is the nearest neighbor limit.
(NN). On the other hand, the system is fully connected for the maximum number of possible distant connections, viz. for $B_{\text{max}} = N \times (N-1)/2 - N$; we refer to this as the mean field (MF) limit. In the NN limit we have the DNLS equation on a regular lattice with periodic boundary conditions. In this case, when nonlinearity is zero, an initially localized state spreads throughout the lattice and after long times the probability to find it at a given site will be of the order of $1/N$. Increasing of the nonlinearity parameter $\chi$ leads to breather formation signaled by selftrapping for values in the range $\chi \approx 3 - 5 \ [9]$. In the MF limit, on the other hand, the network is fully connected and this has ramifications for the DNLS selftrapping properties. We note that the pure linear chain on a small world network has been investigated in Ref [10]. It was found that for $B$ small partial localization of the probability at the initial site occurs.

In order to study the general case of the DNLS on a SWN we use the following numerical procedures: We start from the chain with nearest neighbor couplings and add randomly bonds to distant sites. We place initially all probability at a given site (referred to as the “zeroth” site) and for each lattice we follow the evolution of the probability amplitudes as a function of time. We evaluate $P_0(t)$, viz. the probability at the initial site, for long times ($T_{\text{max}} = 10^5$) and time-average this probability in order to obtain $\langle P_0 \rangle$. This numerical experiment is repeated for $R$ distinct lattice realizations and, finally, we obtain the averaged self-probability $\bar{P}$ over these realizations. We present results for $N = 100$ while the ensemble averaging is done over $R = 500$ realizations. Repeating the above procedures for different values of the nonlinearity parameter $\chi$ results in the behavior seen in Fig. 1. We observe that the well known selftrapping transition of the finite, extended lattice ($B = 0$) occurring for $\chi \approx 3.5 \ [9]$ shifts to larger values of the nonlinearity parameter as we increase the distant bond value $B$. In other words, the onset for the breather regime close to the NN limit becomes delayed by the presence of a small number of distant bonds. This behavior is understood since, in this limit, the addition of few distant bonds, even though adds disorder to the system, nevertheless, increases the connectivity of the lattice and, as a result, the amount of nonlinearity necessary for selftrapping is higher.

III. FROM THE NEAREST NEIGHBOR TO THE MEAN FIELD LIMIT

In order to explore the whole range of complex lattices from $B = 0$ to $B = B_{\text{max}}$ we need to focus first on the dynamics at the fully coupled MF limit where each site is connect to every other site. In the purely linear case ($\chi = 0$) the nonlinear eigenvalue problem of Eq. (2) reduces to

$$MC = \lambda C \Rightarrow \det[M - \lambda I] = 0$$

where $C$ is the n-component column vector and $V$ is the interaction matrix. This system is solved easily leading to $N - 1$ degenerate localized eigenvalues with $\lambda_{\text{loc}} = -1$ and a single, delocalized (Perron-Frobenius) eigenvalue for $\lambda_{\text{del}} = N - 1$.

FIG. 1: Time and realization averaged probability $\bar{P}$ as a function of the nonlinearity parameter $\chi$ for different dilute SWN lattices. Selftrapping occurs at increasingly larger values of $\chi$ as a function of $B$.

In the large-$N$ limit thus, initial conditions remain fully localized except for the special case where the particle is placed equally on all sites; in the latter case it remains delocalized. We thus find that in the linear case while the NN limit favors delocalization the MF limit promotes localization! This feature will thus dominate the behavior of DNLS in the large-$B$ limit.

In order to study the dynamics of DNLS towards the MF limit we employ two distinct approaches. In the first we simply change the number of bonds $B$ to $B_{\text{max}}$ while in second we add all $B_{\text{max}}$ bonds in the system from the beginning while assigning to each one a given strength $W_b$. Subsequently we change $W_b$ from zero (no small world links) to one (MF limit).

A. Variable distant bond number

We construct our lattice by starting from the NN limit where $B = 0$ and add randomly bonds until we reach the MF limit where $B = B_{\text{max}}$ (Fig. 2). We use $N = 100$ and thus $B_{\text{max}} = 4850$. The linear case ($\chi = 0$) for relatively small $B$ has been addressed by Blumen et al. [10] where is noted that the addition of a few distant bonds, while primarily delocalizes the probability, it nevertheless causes small, partial localization, a phenomenon that could be connected with Anderson localization [14]. We also observe this behavior, viz. that approximately 5% of the total probability remains at the initial site (fig 3) in the small-$B$ limit, while the majority of the probability wave spreads in the network. However, as the number of bonds increases and upon approaching the MF limit a relatively sharp transition occurs for values of $B$ very close to the MF, as can be seen in Fig. 3. The averaged probability, while being essentially delocalized for all intermediate $B$ values, it now collapses back to the initially populated site. As a result, when the linear network is close to the MF limit it tends to trap the probability in the initially populated site.
We now turn the nonlinear term on and observe in the regime from $B = 0$ to $B$ close to $B_{\text{max}}$ two competing tendencies, viz. delocalization due to bond addition as well as localization due to nonlinearity. For small number of bonds nonlinearity induces localization that nevertheless occurs for larger values of $\chi$ as the bond number increases. In the intermediate $B$ regime we observe delocalization unless the nonlinearity parameter values become very large. In this range nonlinearity competes strongly with the delocalization induced from the distant bonds and a minimum is reached where the system acquires its most delocalized form. Finally, in the large bond number regime the MF regime augments the localization in complex lattices in the form of small world networks. The nonlinearity parameter $\chi$ and the number of small world connections $B$ (or their strength $W_b$) are the two variables that induce localization and delocalization respectively.

We saw that in the fully linear regime ($\chi = 0$) the increase of the small world link number leads essentially to delocalization due to the effective increase of the lattice dimensionality. This trend is true except very close to the mean field limit; in the latter, exact solution shows that the lattice has complete localization tendency (except in the case of a totally delocalized initial condition). We note, however, that in the very small $B$

\[ W_b = \text{depending on the nonlinearity parameter values. As the value of nonlinearity increases the onset of localization occurs at smaller values of } W_b \text{ as expected. If we follow a curve for specific } \chi \text{ we note that first we enter in the selftrapping regime while for larger values of } W_b \text{ we get an additional "transition" stemming from the MF attractor. This further localization occurs for smaller } W_b \text{ values as the nonlinearity parameter increases.}

![Figure 2](image2.png)

FIG. 2: Starting from the NN limit where $B = 0$ and we add randomly bonds until we reach the MF limit where $B = B_{\text{max}}$.

We notice that as we gradually increase the $W_b$’s that the probability of the initially pertubated site mark a rapid change for values very close to one.

![Figure 3](image3.png)

FIG. 3: Time and realization averaged probability of occupation of the initial site as a function of the bond number $B$ for different nonlinearity values. (a) Full bond number range, (b) detail of the nearest neighbor regime and (c) detail of the mean field regime.

**B. Variable distant bond strength**

We employ additionally a second approach whereby we start from the full SWN system assigning however a certain weight $W_b$ to all the distant bonds ranging from $W_b = 0$ (NN regime) to $W_b = 1$ (MF limit) as seen in Fig. 4. We find qualitatively similar results as in the previous case as shown in Fig. 5; the selftrapping transition occurs at distinct values of $W_b$ depending on the nonlinearity parameter values.

![Figure 4](image4.png)

FIG. 4: Starting from the fully connected SWN system assigning however a certain weight $W_b$ to all the distant bonds ranging from $W_b = 0$ (NN regime) to $W_b = 1$ (MF limit) with $V = 1$.

![Figure 5](image5.png)

FIG. 5: Time and realization averaged probability of occupation of the initially populated site as a function of the bond strength $W_b$ for different nonlinearity parameter values.

**IV. CONCLUSIONS**

We investigated dynamical properties of the DNLS equation related to selftrapping and the onset of nonlinear localization in complex lattices in the form of small world networks. The nonlinearity parameter $\chi$ and the number of small world connections $B$ (or their strength $W_b$) are the two variables that induce localization and delocalization respectively.

We saw that in the fully linear regime ($\chi = 0$) the increase of the small world link number leads essentially to delocalization due to the effective increase of the lattice dimensionality. This trend is true except very close to the mean field limit; in the latter, exact solution shows that the lattice has complete localization tendency (except in the case of a totally delocalized initial condition). We note, however, that in the very small $B$
regime, while the system is delocalized, some partial localization is observed [10]. When the nonlinearity parameter is non zero we observe a competition between localization induced by the latter and delocalization induced by the small world connections. This competition makes selftrapping occur at larger $\chi$-values compared to the translationally invariant lattice case while for very large nonlinearities the probability becomes to a large extent selftrapped. An interesting feature appears from the linear MF behavior, viz. close to the large $B$ regime the nonlinear localization tendency is augmented by the linear MF localization behavior. These features are also seen in the fully linked lattice with variable bond strength. The DNLS properties on the SWN may have some applications in energy propagation and storage in complex networks.

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