Self trapping transition for a nonlinear impurity within a linear chain

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In the present work we revisit the issue of the self-trapping dynamical transition at a nonlinear impurity embedded in an otherwise linear lattice. For our Schrödinger chain example, we present rigorous arguments that establish necessary conditions and corresponding parametric bounds for the transition between linear decay and nonlinear persistence of a defect mode. The proofs combine a contraction mapping approach together with global existence results for the Schrödinger chain and invariance arguments on an appropriately defined nonlinear integral map, which governs the evolution of the defect mode. The results are relevant for both power law nonlinearities and saturable ones. The analytical results are corroborated by numerical computations.

I. INTRODUCTION

The theme of discrete linear chains with embedded nonlinear impurity nodes is one of considerable interest within condensed matter physics. It emerges, for instance, within tight-binding descriptions of electron transport, where the nonlinear terms describe local interactions with vibrations at the impurity node [5]. It also arises in the study of tunneling through a magnetic impurity connected to two perfect leads in the presence of a magnetic field [2]. It is also fairly widespread in the realm of nonlinear optics, where waveguides with practically linear and ones with essentially nonlinear characteristics can be constructed. This was proposed e.g. in [5]; however, notice that in that context linear and nonlinear waveguides were proposed to be interlaced in binary arrays. Here, instead, we have in mind a single nonlinear waveguide embedded in an otherwise linear array. Given this diverse array of physical setups, this subject was numerically examined in a wide array of studies [4–7], not only for the case of one but also for that of more embedded impurities. This topic has also recently seen a surge of renewed interest, due in part to the examination of eigenvalue and symmetry-breaking features in the presence of multiple nonlinear sites, and also due to the examination of gain/loss variants thereof [8–10].

While numerically the relevant dynamics is rather straightforward and directly tractable, on the analytical side, unfortunately, developments have been considerably less advanced. While it is possible to characterize the stationary states of the problem via the Green’s function techniques [2], and even (for specially constructed potentials) to capture symmetry-breaking effects via the demonstration of emergence of asymmetric states [8], little has been rigorously established about the dynamic problem. Assuming that initially, the excitation is placed at site \( n = 0 \) of the chain, that is, \( C_n(0) = \delta_{n,0} \), the work of [7] was intriguing in that it established a particular diagnostic

\[
\langle P \rangle \equiv \lim_{t \to \infty} \frac{1}{t} \int_0^t |C_0(s)|^2 \, ds, \quad (1.1)
\]

with a clearly distinct behavior for different parameters (i.e., nonlinearity strengths \( \chi \)) of the system. The numerical (or physical) experiment at hand is as follows. Suppose we initialize the nonlinear site at unit intensity (the relevant amplitude can always be rescaled so that there is one parameter, either the strength of the nonlinearity or interchangeably the magnitude of the compactly supported – on a single site – initial data). We then monitor \( \langle P \rangle \) [in fact, in our case, we will not compute the relevant integral numerically starting from \( t = 0 \) but rather from \( t = 25 \) to exclude short term transient dynamics]. We then observe that for \( \chi < \chi_c \) (which for the cubic nonlinear case is \( \chi_c \approx 3.2 \)), our diagnostic quantity tends to 0. On the contrary, for \( \chi > \chi_c \), the quantity remains finite and demonstrates an increasing trend as \( \chi \) increases [7].

Our aim in the present work is to establish the existence of such a behavior from a rigorous perspective and to examine (both analytically and numerically) how the behavior is modified for different types of nonlinearities. In particular, we will focus on power law nonlinearities, as well as on saturable ones. Using a contraction mapping approach, we will prove the existence of a \( \chi_\sigma \) (for the power law nonlinearity – for the saturable one, this will be called \( \chi_s \)), such that if \( \chi < \chi_\sigma \), then \( \langle P \rangle = 0 \).

It is important to note that our \( \chi_\sigma \) will naturally be a lower bound for the numerically identified \( \chi_c \). Nevertheless, it is a strong rigorous indication of the presence of the numerically identified dynamical transition. Interestingly, the obtained \( \chi_\sigma \) will provide a numerical dependence which is decreasing with the nonlinearity exponent \( \sigma \), while in the accompanying numerics we will observe that the relevant critical point will be found to monotonically increase as the exponent \( \sigma \) increases. Although the decreasing behavior of the theoretical \( \chi_\sigma \) is justified mathematically by the requirements for contractive dynamics, by using an approximation near the linear regime of the system, we will rationalize the increasing behavior of the true critical point \( \chi_c \) as well as unify our critical point estimates for the cubic and saturable case. Next, by combining fundamental properties of solutions of the nonlinear lattice dynamical system involved, together with the existence of an asymptotically in time
After solving for \( \tilde{\eta} \) property of the Laplace transform, and identifying the in-
noted by tilde) yields

\[
F(z) = |z|^{2\sigma} z, \quad (1.3)
\]

and the saturable nonlinearity

\[
F(z) = \frac{z}{1 + |z|^2}, \quad (1.4)
\]

with the single site, unit intensity initial condition indicated above. The Fourier transform of (1.2) gives

\[
i\frac{dC_k}{dt} = 2V \cos(k)C_k - \chi F(C_0). \quad (1.5)
\]

Subsequent application of the Laplace transform (denoted by tilde) yields

\[
i [ \omega \tilde{C}_k - 1] = 2V \cos(k)\tilde{C}_k - \chi \tilde{F}(\omega). \quad (1.6)
\]

After solving for \( \tilde{C}_k \) one obtains

\[
\tilde{C}_k = \frac{i - \chi \tilde{F}(\omega)}{i\omega - 2V \cos(k)}. \quad (1.7)
\]

The final step consists of taking the inverse Fourier and Laplace transforms, and using the convolution prop-
erty of the Laplace transform, and identifying the in-
tegral representation of the Bessel function \( J_n(z) = (1/2\pi) \int_{-\infty}^{\infty} \exp(iz\cos(\theta) - i\theta), \) to obtain

\[
C_n(t) = J_n(2Vt) + i\chi \int_0^t J_n[2V(t-s)]F(C_0(s)ds. \quad (1.8)
\]

In particular, for \( n = 0 \) we find the nonlinear integral equation for \( C_0(t) \):

\[
C_0(t) = J_0(2Vt) + i\chi \int_0^t J_0[2V(t-s)]F(C_0(s)ds. \quad (1.9)
\]

We are interested in determining the presence or absence of a self-trapping transition, i.e., to determine if there is a critical value \( \chi_c \) for which

\[
\langle \chi \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t |C_0(s)|^2 ds = \begin{cases} 0, & \text{if } \chi < \chi_c, \\ \neq 0, & \text{if } \chi > \chi_c. \end{cases} \quad (1.10)
\]

The structure of our presentation will be as follows. In section II, first we will present our contraction mapping dynamics to illustrate that \( \langle \chi \rangle \) equals to 0 for suitably small \( \chi \). We will present our estimate for \( \chi_c \) and argue about how the picture is modified once the evolution is in the near linear regime. Then, global existence and invariance arguments will illustrate that \( \langle \chi \rangle > 0 \), for suitably large \( \chi \). In section III we will present a brief set of numerical computations regarding the nonlinearities of interest. Finally, in section IV, we will summarize our findings and present our conclusions, as well as suggest some potential directions for future work.

II. FROM CONTRACTIVE DYNAMICS TO THE SELF-TRAPPING TRANSITION

It is well known that the solutions of the DNLS problem (1.2) exist globally in time (e.g. are of class \( C([0, \infty), \ell^2) \)), where \( \ell^2 \) denotes the space of square summable sequences. One of the two principal conserved quantities is the power or norm \( P = \sum_{n=-\infty}^{\infty} |C_n(t)|^2 \), and for all \( t \geq 0 \),

\[
\sum_{n=-\infty}^{+\infty} |C_n(t)|^2 = \sum_{n=-\infty}^{+\infty} |C_n(0)|^2. \quad (2.11)
\]

Then for the initial condition considered herein, the corresponding unique solution of the DNLS equation (1.2) satisfies

\[
\sum_{n=-\infty}^{+\infty} |C_n(t)|^2 = 1, \quad \text{for all } t \geq 0. \quad (2.12)
\]

The norm conservation (2.12) implies that \( C_0(t) \) satisfies the uniform in time estimate

\[
|C_0(t)| \leq 1, \quad \text{for all } t \geq 0. \quad (2.13)
\]

It is evident from (2.13) that

\[
\langle \chi \rangle \leq 1. \quad (2.14)
\]

Due to (2.13), we have \( \frac{1}{t} \int_0^t |C_0(s)|^2 ds \leq \frac{1}{t} \int_0^t ds = 1 \), for all \( t \geq 0 \). Then, by passing to the limit as \( t \to \infty \), we get (2.14).

The observed phenomenology of the self-trapping transition as discussed in (2.1) is that in the regime \( \chi \geq \chi_c \), there is a sudden increase of the time-averaged prob-
ability \( \langle \chi \rangle \), while in the regime \( \chi < \chi_c \), the average \( \langle \chi \rangle = 0 \). This phenomenology suggests to investi-
gate for contracting dynamics of the integral equation (1.9) in an appropriate regime for \( \chi \). Having assigned through the initial condition the initial value \( C_0(0) = 1 \) at \( t = 0 \), and since \( C_0(t) \) is uniformly bounded from (2.13), it is convenient mathematically to consider the self-trapping transition problem in the Banach space of the essentially bounded functions \( L^\infty([0, \infty)) \) endowed with the norm \( ||u||_{\infty} = \text{ess sup}_{[0, \infty)} |u(t)| \).

The integral equation (1.9) will define a nonlinear map \( T : L^\infty([0, T]) \to L^\infty([0, T]) \), for arbitrary large \( 0 < T < \)
∞, by the equation
\[ T[C_0(t)] = J_0(2Vt) + i\chi \int_0^t J_0[2V(t-s)]F(C_0(s))ds. \] (2.15)

For instance, due to (2.13) we shall consider the nonlinear map \( T \) on the closed unit ball of \( L^\infty([0,T]) \)
\[ B = \{ u \in L^\infty([0,T]) : ||u||_{\infty} \leq 1 \} . \]
Then, we will seek for the existence of a regime of the parameter \( \chi \) so that \( T : B \to B \) will be a contraction, and seek for the behavior of the unique fixed point for large times.

**Proposition II.1** Consider the DNLS system (1.2) with the nonlinearities (1.3) or (1.4). There exists a critical value \( \chi_{\text{crit}} \) such that if \( \chi < \chi_{\text{crit}} \), then \( \lim_{t \to \infty} ||C_0||_{\infty} = 0 \).

**Proof:** We distinguish between the cases of the power (1.3) and saturable nonlinearity (1.4), respectively.

**A. Power nonlinearity.** Note that the power nonlinearity (1.3) is of the form \( F(z) = g(|z|^2)z \) with \( g(r) = r^\sigma, \sigma > 0 \). Next, we recall that for any \( F : \mathbb{C} \to \mathbb{C} \) which takes the form \( F(z) = g(|z|^2)z \), with \( g \) real and sufficiently smooth, the following relation holds
\[ F(\zeta) - F(\xi) = \int_0^1 (\zeta - \xi)(g(r) + rg'(r))d\theta + \int_0^1 (\zeta - \xi)\Phi^2g'(r)d\theta, \] (2.16)
for any \( \zeta, \xi \in \mathbb{C} \), where \( \Phi = \theta\zeta + (1 - \theta)\xi, \theta \in (0,1) \) and \( r = |\Phi|^2 \) (see (13), pg. 202)). Here, \( \overline{\zeta} \) denotes the complex conjugate of \( \zeta \in \mathbb{C} \).

Let \( C_0(t) \) and \( Q_0(t) \) be two elements of \( B \). Then, from (2.16) we observe that
\[ T[C_0(t)] - T[Q_0(t)] = i\chi \int_0^t J_0[2V(t-s)][F(C_0(s)) - F(Q_0(s))]ds. \] (2.17)

Applying (2.16) for \( \zeta = C_0(t), \xi = Q_0(t) \) one finds that
\[ F(C_0(t)) - F(Q_0(t)) = \int_0^1 [(\sigma + 1)(C_0(t) - Q_0(t))|\Phi|^{2\sigma}d\theta + \sigma \int_0^1 (\overline{C_0(t)} - \overline{Q_0(t)})\Phi^2|\Phi|^{2\sigma - 2}d\theta. \] (2.18)

Since \( ||\Phi||_{\infty} \leq 1 \), we get from (2.18), the inequality
\[ |F(C_0(t)) - F(Q_0(t))| \leq (2\sigma + 1) \int_0^1 |\Phi|^{2\sigma}||C_0(t) - Q_0(t)||d\theta \]
\[ \leq (2\sigma + 1) \int_0^1 ||\Phi||^{2\sigma}_{\infty}||C_0(t) - Q_0(t)||d\theta \]
\[ \leq (2\sigma + 1)||C_0(t) - Q_0(t)||. \] (2.19)

Inserting (2.19) into (2.17) and taking \( L^\infty \)-norms, we observe that
\[ ||T[C_0] - T[Q_0]||_{\infty} = \text{ess sup}_{t \in [0,\infty]}|i\chi \int_0^t J_0[2V(t-s)] | \times |F(C_0(s)) - F(Q_0(s))|ds| \]
\[ \leq ||A||_{\infty}(2\sigma + 1)\chi ||C_0 - Q_0||_{\infty}, \] (2.20)
where the function \( A(t) \) is defined as
\[ A(t) = \int_0^t J_0[2V(t-s)]ds = \frac{1}{2V} \int_0^{2Vt} |J_0(y)|dy. \] (2.21)

It is clear from (2.20) that the map \( T : E \to E \) is a contraction if \( ||A||_{\infty}(2\sigma + 1)\chi < 1 \), i.e., if
\[ \chi < \frac{1}{||A||_{\infty}(2\sigma + 1)} = \chi_{\text{crit}}. \] (2.22)

Note that for large times, the map (2.15) can be approximated as
\[ T[C_0(t)] \approx i\chi \int_0^t J_0[2V(t-s)]F(C_0(s))ds. \] (2.23)
Since \( T[0] \approx 0 \), for large times, it follows from (2.23)-by setting \( Q_0 = 0 \)-that the approximating map (2.23) satisfies
\[ ||T[C_0]||_{\infty} \leq ||A||_{\infty}(2\sigma + 1)\chi ||C_0||_{\infty}. \] (2.24)

Thus, when (2.22) holds, the approximating map (2.23) has the property \( T : B \to B \), i.e., \( T \) maps \( B \) to itself. Hence, it satisfies both of the assumptions of the contraction mapping theorem, and has a unique fixed point \( C_0 \in B \), e.g., \( T[C_0(t)] \approx C_0(t) \in B \). Furthermore, the fact that \( T[0] \approx 0 \), implies that when \( \chi \) belongs to the contraction regime (2.22), where the approximative map (2.23) has the unique fixed point, then \( C_0(t) \approx 0 \), should be the sole fixed point. Therefore, if \( \chi < \chi_{\text{crit}} \), then \( ||C_0||_{\infty} \to 0 \), for large times.

**B. Saturable nonlinearity.** Applying (2.16) in the case of the saturable nonlinearity (1.4) where \( g(r) = \frac{1}{1+r} \), we have that
\[ F(C_0(t)) - F(Q_0(t)) = \int_0^1 \left\{ \frac{C_0(t) - Q_0(t)}{(1 + |\Phi|^2)^2} - \frac{\Phi^2(C_0(t) - Q_0(t))}{(1 + |\Phi|^2)^2} \right\}d\theta, \] (2.25)
from which the inequality
\[ |F(C_0(t)) - F(Q_0(t))| \leq \int_0^1 \frac{1 + |\Phi|^2}{(1 + |\Phi|^2)^2}|C_0(t) - Q_0(t)|d\theta \]
\[ \leq ||C_0(t) - Q_0(t)||, \] (2.26)
follows. Then from (2.17) and (2.26) we get that
\[ ||T[C_0] - T[Q_0]||_\infty \leq ||A||_\infty \chi ||C_0 - Q_0||_\infty. \]  
(2.27)

Hence, in the case of saturable nonlinearity, the map \( T : B \to B \) will be a contraction if \( ||A||_\infty \chi < 1 \), i.e., if
\[ \chi < \frac{1}{||A||_\infty} = \chi_s := \chi_{\text{crit}}. \]  
(2.28)

Considering then the analogue of the approximating nonlinear map (2.23) in the case of the saturable nonlinearity, we establish that \( ||C_0||_\infty \to 0 \) for large times, if \( \chi < \chi_s \). \( \square \)

Proposition II.1 directly implies

**Theorem II.1** If \( \chi < \chi_{\text{crit}} \), then \( \langle P \rangle = 0 \).

**Proof:** For arbitrary \( 0 < t < \infty \), it holds that
\[ \int_0^t |C_0(s)|^2 ds \leq t ||C_0||^2_\infty, \]
therefore \( \frac{1}{t} \int_0^t |C_0(s)|^2 ds \leq \frac{1}{t} ||C_0||^2_\infty \). Letting \( t \to \infty \), it follows from Proposition II.1 that if \( \chi < \chi_{\text{crit}} \), then \( \langle P \rangle = 0 \). \( \square \)

**Approximating quantifications of \( \chi_{\text{crit}} \).** Further estimates of the critical value \( \chi_{\text{crit}} \) can be given based on an estimation of the function \( A(t) \) defined in (2.21) and its norm \( ||A||_\infty \). It is known (see [14, pg. 364, eq. 9.2.1]) that as \( t \to +\infty \), the function \( J_0(t) \) has the principal asymptotic form
\[ J_0(t) \approx \sqrt{\frac{2}{\pi t}} \cos \left( t - \frac{\pi}{4} \right) = \frac{1}{\sqrt{\pi t}} (\cos t + \sin t). \]  
(2.29)

Inserting this asymptotic form in (2.21), the function \( |A(t)| \) can be computed in terms of the Fresnel’s integrals \( S(t) = \int_0^t \sin \left( \frac{\sqrt{2}}{2} y^2 \right) dy \) and \( C(t) = \int_0^t \cos \left( \frac{\sqrt{2}}{2} y^2 \right) dy \), [14], pg. 300, eqns. 7.3.1 & 7.3.2. In particular, by using the auxiliary functions \( S_2(t) = \frac{1}{\sqrt{\pi}} \int_0^t \sin \left( \frac{\sqrt{2}}{2} y^2 \right) dy \), \( C_2(t) = \frac{1}{\sqrt{\pi}} \int_0^t \cos \left( \frac{\sqrt{2}}{2} y^2 \right) dy \), their inter-relations with \( S(t), C(t) \) [14], pg. 300, eqns. 7.3.3, 7.3.4 & 7.3.7, 7.3.8, as well as the fact that \( C(t) > 0, S(t) > 0 \) for all \( t \in [0, \infty) \), we find that
\[ |A(t)| \sim \frac{\sqrt{2}}{2V} \left[ C \left( \frac{2Vt}{\sqrt{\pi}} \right) + S \left( \frac{2Vt}{\sqrt{\pi}} \right) \right] \]  
(2.30)
as \( t \to +\infty \). Furthermore, it follows from the limiting relations \( \lim_{t \to +\infty} S(t) = \lim_{t \to +\infty} C(t) = \frac{1}{2}, \) [15], pg. 941, eqns. 8.257.1 & 8.257.2, that \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{2V} \). Therefore, for \( t \to +\infty \),
\[ ||A||_\infty \sim \frac{\sqrt{2}}{2V}. \]  
(2.31)

The upper panel of Figure 1 shows the approximating function \( A(t) \) together with the corresponding \( |A(t)| \) and \(-|A(t)|\) for \( V = 1 \). The bottom panel of Figure 1 shows the graphs of the approximate functions \( |A(t)| \) for \( V = 2 \) and \( V = 3 \), demonstrating their superior limits \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{2V} \). The upper (blue) curve is for \( V = 2 \) where \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{2} = 0.707 \) and the lower (green) curve is for \( V = 3 \) where \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{3} = 0.353 \).

![Figure 1](image-url)

Figure 1. (Color Online) (Upper panel) The approximation of \( A(t) \) against the approximating function (2.30) for \( A(t)- \) upper continuous (green) curve and \(-|A(t)|\)-lower dashed (red) curve, for \( V = 1 \). (Bottom panel) The graphs of the approximating function (2.30) for \( |A(t)| \) when \( V = 2 \) and \( V = 3 \), demonstrating the superior limits \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{2V} \). The upper (blue) curve is for \( V = 2 \) where \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{2} = 0.707 \) and the lower (green) curve is for \( V = 3 \) where \( \lim_{t \to +\infty} |A(t)| = \frac{\sqrt{2}}{3} = 0.353 \).

\[ \chi_{\text{crit}} = \begin{cases} \chi_\sigma = \frac{\sqrt{2V}}{2\sigma_\Omega + 1}, & \text{(power nonlinearity)}, \\ \chi_s = \sqrt{2V}, & \text{(saturable nonlinearity)}. \end{cases} \]  
(2.32)

We observe that \( \chi_\sigma < \chi_s \). However, a common threshold \( \chi_{\text{crit}} \) can be derived for both nonlinearities, if we assume that for large times the flow governing \( C_0(t) \) is asymptotically linear. This approximation is valid for the saturable nonlinearity which saturates for large amplitudes and satisfies \( F(z) \leq z \) for all \( z \in \mathbb{C} \). More precisely, since \( \langle P \rangle = 0 \) in the regime \( \chi < \chi_{\text{crit}} \), \( |C_0(t)| \) decays in an oscillatory manner, and the assumption is that in this regime, the decay is slow in amplitude, i.e. \( |C_0(t)|^2 \approx \epsilon^2 \), for large times and \( \epsilon > 0 \) sufficiently small. Thus for the nonlinearities \( F(z) = g(|z|^2)z \) the map (2.15) is linearly
approximated by the map
\[ T[C_0(t)] \approx i\chi g(\epsilon^2) \int_0^t J_0[2V(t-s)]C_0(s)ds, \]
and for (2.33), the analogue of (2.24) is
\[ ||T[0] - T[Q_0]]||_\infty \leq ||A||_\infty g(\epsilon^2)\chi||C_0 - Q_0||_\infty. \]
Note that for both types of nonlinearities, power and saturable, \( 0 < g(\epsilon^2) < 1 \), hence
\[ ||T[C_0] - T[Q_0]]||_\infty \leq ||A||_\infty \chi||C_0 - Q_0||_\infty. \]
Using (2.34), we see that the linear map (2.33) is a contraction for both types of nonlinearities, if
\[ \chi < \chi^*_\text{crit} = \sqrt{2}V. \] (2.35)
Note that \( \chi^*_\text{crit} = \chi_\text{c} \), as it was expected in the case of saturable nonlinearity.

It is also interesting that the asymptotically linear approximation may reveal different monotonicity properties of the threshold value for \( \chi \) as a function of \( \sigma \) in the case of the power nonlinearity. For instance, note from (2.32) that if \( \sigma_1 \geq \sigma_2 \), then \( \chi_\sigma_1 \leq \chi_\sigma_2 \), showing that the threshold \( \chi^*_\text{crit} \) for the contraction mapping theorem is a decreasing function of \( \sigma \). In view of the contraction mapping theorem, this monotonicity is naturally expected, since it is associated with the smallness condition for the convergence of the iteration scheme associated to the integral equation (1.9) and the corresponding approximate nonlinear map (2.23). This can be highlighted by recalling the approximating iteration scheme for (2.23)
\[ C_0^{(n+1)}(t) \approx i\chi \int_0^t J_0[2V(t-s)]|C_0^{(n)}(s)|^2\sigma C_0^{(n)}(s)ds, \]
satisfying for the convergence to the solution \( C_0(t) \approx 0 \) for large times, the error estimate
\[ ||C_0^{(n)}(t)||_\infty \leq \frac{K^n}{1-K} ||C_0^{(1)}(t) - C_0^{(0)}(t)||_\infty, \]
\[ K(\chi, \sigma) = ||A||_\infty (2\sigma + 1)\chi. \]
Increasing the strength of the nonlinearity as \( \sigma \) is increasing, the ansatz of \( K(\chi, \sigma) \) justifies that \( \chi \) should be decreasing so that \( K(\chi, \sigma) < 1 \), to guarantee convergence of the iteration scheme. This requirement for convergence, is giving rise, in turn, to the critical value \( \chi_\sigma \) of (2.34).

However, from the approximate argument of (2.31), it follows that the linearized map is a contraction if
\[ \chi < \frac{1}{||A||_\infty \epsilon^{2\sigma}} = \hat{\chi}(\epsilon), \quad 0 < \epsilon < 1. \] (2.36)
Since \( 1/\epsilon > 1 \), the threshold for the linearized map satisfies the monotonicity property
\[ \hat{\chi}(\sigma_1) > \hat{\chi}(\sigma_2), \quad \text{for} \ \sigma_1 > \sigma_2. \] (2.37)
Thus, assuming that when \( \chi < \chi_\text{c} \), the decay of \( C_0 \) is slow in amplitude, we expect that for the power nonlinearity, the true threshold \( \chi_\text{c} \) will be an increasing function of \( \sigma \).

The discussion above, between the difference of the monotonicity properties of the critical value \( \chi^*_\text{crit} \), derived by the contraction mapping argument of Proposition II.1 and the real threshold \( \chi_\text{c} \), indicates on the one side, that \( \chi^*_\text{crit} \) can serve as a lower bound for \( \chi_\text{c} \) but cannot be sharp. On the other side, the lack of sharpness of \( \chi^*_\text{crit} \) is justified by the fact that a violation of the condition of Proposition II.1 that, assuming \( \chi > \chi^*_\text{crit} \), does not imply the non-existence of another nontrivial fixed point \( C_0 \) for the approximating map (2.23) and that \( ||C_0||_\infty = 0 \), for large times. In other words, although the smallness conditions on \( \chi \) stemming from Proposition II.1 and Theorem II.1 are sufficient for establishing \( (P) = 0 \), they are not necessary.

On account of the common threshold (2.33) for both type of nonlinearities, we may summarize on the following lower bound for the true critical value,
\[ \sqrt{2}V < \chi. \] (2.38)
A first attempt to approximate \( \chi_\text{c} \) closer to its real value is provided by noting that, according to numerical results, when \( \chi > \chi_\text{c} \), it seems that \( |C_0(t)| \) is approaching a constant value. That is, \( C_0(t) \) resembles a stationary state. Thus, after a long time, we assume that in the trapping regime \( C_0(t) \approx \alpha \exp(i\beta t) \). Replacing the stationary state in the long-time approximation
\[ C_0(t) \approx i\chi \int_0^t J_0[2V(t-s)]|C_0(s)|^2C_0(s)ds, \]
and after splitting into real and imaginary parts, one obtains:
\[ 1 = i\chi |\alpha|^2 \int_0^\infty J_0(2Vz) \sin(\beta z)dz, \]
\[ 0 = \int_0^\infty J_0(2Vz) \cos(\beta z)dz. \]
Using basic Bessel integral properties [15, pg. 731] one concludes \( 2V < \beta \) and
\[ 1 = \frac{\chi |\alpha|^2}{\sqrt{\beta^2 - (2V)^2}}. \]
This implies,
\[ \chi = \frac{\sqrt{\beta^2 - (2V)^2}}{|\alpha|^2}. \]
In particular, when \( V \rightarrow 0 \), there is complete self-trapping and \( |\alpha| \rightarrow 1 \) implying \( \chi \rightarrow \beta > 2V \). Therefore, inside the trapping regime, \( \chi > 2V \) at long times. The critical value \( 2V \) also coincides with the minimum value to create a nonlinear stationary state, and the lower bound
\[ \chi_{\text{stationary}} = 2V < \chi_\text{c}, \] (2.39)
accompanying becomes meaningful. Intuitively, the critical value \( \chi_{\text{stationary}} \) for the formation of the stationary mode, should always be smaller than the corresponding value \( \chi_c \) for the dynamical problem, since the former value stems from a variational principle.

Complementing the above considerations in a natural way, the next results will establish the existence of a sufficiently large value of \( \chi \), above which the nonlinear persistence of a defect mode takes place. First, we prove the following auxiliary proposition, showing the invariance of an annular region in the phase space of \( C_0(t) \) under the action of the approximating map \( (2.23) \), and a lower bound on \( \chi \) for this invariance.

**Proposition II.2** For any \( 0 < \delta < 1 \), consider the following subset of \( X = L^\infty([0, \infty)) \)

\[
\mathcal{M} = \{ C_0(t) : X \neq \{ |C_0(t)| \leq 1 \text{ for all } t \in [0, T_\delta] \} \}.
\]

There exists \( \hat{\chi}_{\text{crit}}(\delta) \), satisfying the \( \delta \)-independent lower bound

\[
\hat{\chi}_{\text{crit}}(\delta) > 4V^2,
\]

with the following property: If \( \chi > \hat{\chi}_{\text{crit}}(\delta) \), then for any \( C_0 \in \mathcal{M} \), the nonlinear map \( T : L^\infty([0, \infty)) \rightarrow L^\infty([0, \infty)) \) defined by \( (2.17) \) satisfies \( |T[C_0]| > \delta \) as \( t \rightarrow \infty \).

**Proof:** We shall only consider the case of the power nonlinearity \( (1.3) \) for \( \sigma > 0 \). The case of the saturable nonlinearity is \( (1.3) \) can be proved similarly. Since for large times, the approximation \( (2.23) \) holds, we may apply the reverse Holder’s inequality [12, Theorem 2.6, pg. 24], times, the approximation \( (2.23) \) holds, we may apply the bound accordingly becomes meaningful. Intuitively, the critical should always be smaller than the corresponding value \( \chi_c \) for the dynamical problem, since the former value stems from a variational principle.

for the dynamical problem, since the former value stems from a variational principle.

By using \( (2.44) \), we derive that

\[
|T[C_0]| > \chi \delta^{2(\sigma+m)+2} \quad (4V^2).
\]

Although \( \delta^{2(\sigma+m)+2} \) is small, we require the right-hand side of \( (2.44) \) to be significant, e.g. of size \( \delta \). This can happen if \( \chi \) is significantly large. Indeed, we observe that

\[
\chi > \hat{\chi}_{\text{crit}}(\delta) := \frac{4V^2}{\delta^{2(\sigma+m)+1}},
\]

and that \( \hat{\chi}_{\text{crit}}(\delta) > 4V^2 \) since \( \delta < 1 \). \( \square \)

Combining the invariance result of Proposition II.2 with the global existence and continuity properties of the solutions of the DNLS \( (1.2) \), we prove the transition to the nonlinear defect mode.

**Theorem II.2** Let \( 0 < \delta < 1 \), and assume that \( \chi > \hat{\chi}_{\text{crit}}(\delta) \). where \( \hat{\chi}_{\text{crit}}(\delta) \) is defined as in \( (2.40) \). Then there exists \( T^* > 0 \) sufficiently large such that for all \( t > T^* \), \( C_0(t) \in \mathcal{M} \), where the set \( \mathcal{M} \) is defined in Proposition II.2. Furthermore,

\[
\lim_{t \rightarrow \infty} \frac{1}{t - T^*} \int_{T^*}^{t} |C_0(s)|^2 ds > 0.
\]

**Proof:** We consider the DNLS system \( (1.2) \) with the initial condition of unit intensity at a single site. Recall from the beginning of Sec. III that a unique, global in time solution \( C_0(t) \in L^\infty([0, \infty), L^2) \), is defined (in fact, the unique solution is of class \( C^1([0, \infty), L^2) \)), satisfying the conservation of norm \( (2.12) \). Hence, a unique function \( C_0(t) \) is defined, satisfying \( (2.13) \). Now let \( 0 < \delta < 1 \), and \( \chi > \hat{\chi}(\delta) \) as assumed. Since \( C_0(0) = 1 \) and \( C_0(t) \) is
continuous for all \( t \in [0, \infty) \), there exists at least a small time interval \([0, T_3]\) such that
\[ \delta < |C_0(t)| \leq 1, \quad \text{for all } t \in [0, T_3]. \] (2.46)
The function \( C_0(t) \) satisfies also the integral equation \((1.9)\) and the continuity property \((2.40)\) can be also verified by a modification of the contraction mapping argument for small times. Indeed, by using the fact that \(|J_0(t)| \leq 1\) for all \( t \in [0, \infty) \) we get the variant of \((2.20)\)
\[ ||T[C_0] - T[Q_0]|| \leq \tau(t(2 + \sigma) + 1)||C_0 - Q_0||_{C^0}. \] (2.47)

Therefore the map \( T \) defined by \((2.10)\) is a contraction when \( \chi > \tilde{\chi}_{\text{crit}}(\delta) \), at least for
\[ 0 < t < \frac{1}{2(\sigma + 1)\chi} - \frac{1}{2(\sigma + 1)\tilde{\chi}_{\text{crit}}(\delta)} := T_3, \] (2.48)
On the one hand, \( C_0(t) \) is globally existing in time, as defined by the unique solution of the DNLS system \((1.2)\) and on the other hand, \( C_0(t) \) is a solution of the integral equation \((1.3)\) defined alternatively as the unique fixed point of the map \( T \). Since both solutions should coincide, we may summarize the above observations as follows:
\[ |C_0(t)| = ||T[C_0(t)]|| \leq 1, \quad \text{for all } t \in [0, \infty), \] (2.49)
due to the global existence of \( C_0(t) \) as defined from the unique global in time solution of the DNLS system \((1.2)\), and furthermore
\[ \delta < |C_0(t)| \equiv ||T[C_0(t)]|| \leq 1, \quad \text{for all } t \in [0, T_3], \] (2.50)

Hence, \( C_0(t) \in \mathcal{M} \). Then, Proposition \(1.2\) implies that \( |C_0(t)| = ||T[C_0(t)]|| > \delta \) for large times, if \( \chi > \tilde{\chi}(\delta) \). Actually, Proposition \(1.2\) guarantees the following behavior for \( C_0(t) \): even if there exists time \( T_1 > T_3 \), on which
\[ 0 < |C_0(T_1)| = \delta \quad \text{and} \quad 0 < |C_0(t)| \leq \delta \quad \text{for a finite interval} \quad [T_1, T_2], \]
a time \( T^* \) should exist, such that \( \delta > |C_0(t)| \) for all \( t > T^* \). Therefore, for large times \( t > T^* \),
\[ \int_{T^*}^{t} |C_0(s)|^2 ds > \delta^2 (t - T^*), \]
implying that \( \lim_{t \to \infty} \frac{1}{t - T^*} \int_{T^*}^{t} |C_0(t)|^2 dt > \delta^2 \), if \( \chi > \chi_{\text{crit}}(\delta) \). \( \square \)

Theorem \(1.2\) establishes the existence of an appropriate threshold value \( \chi_{\text{c}} \), such that \( \langle P \rangle > 0 \) in the slightly weaker sense of \((2.45)\) – for \( \chi > \chi_{\text{c}} \). It is convenient to summarize the results of Theorems \(1.1\) and \(1.2\) in

**Theorem II.3** Consider the DNLS system \((1.3)\) with either the power nonlinearity \((1.4)\) or the saturable nonlinearity \((1.4)\). We have the following:

A. *(Weak nonlinear regime):* Assume that \( \chi < \sqrt{2V} \)
Then \( \langle P \rangle = 0 \).

B. *(Strong nonlinear regime):* Consider \( \hat{\chi}_{\text{crit}} \) as defined by \((2.40)\). Then, there exists \( \chi^* > \hat{\chi}_{\text{crit}} > 4V^2 \), such that \( \langle P \rangle > 0 \) in the sense of \((2.47)\).

Theorem \(1.3\) confirms in a rigorous fashion the existence of a self-trapping transition for a value of \( \chi \) intermediate between the interval \([\sqrt{2V}, \chi^*]\). In particular, the real threshold value \( \chi_{\text{c}} \) lies between this interval. The qualitative theoretical predictions proved and discussed in this section, will now be tested by numerical simulations.

**III. NUMERICAL RESULTS**

In this section, we briefly revisit the relevant computations of the quantities of interest such as \( \langle P \rangle \) for signaling the relevant self-trapping dynamical transition. For \( V = 1 \) and for the cases of \( \sigma = 1, 2 \) and \( 3 \), the relevant quantity is shown (past an initial transient interval) for different values of \( \chi \) in the left panel of Fig. 2. The case of \( \sigma = 1 \) was also shown in \((1)\) and in excellent agreement with the latter, we find that \( \chi_{\text{c}} \approx 3.2 \) in this case. In the quintic case of \( \sigma = 2 \), the corresponding value becomes \( \chi_{\text{c}} = 5.48 \), while for the septic case of \( \sigma = 3 \), the relevant critical point shifts to \( \chi_{\text{c}} = 7.05 \). It is also interesting to point out that the relevant curves become progressively steeper, as we increase \( \sigma \). By necessity, the real \( \chi_{\text{c}} \) lies between the interval \([\sqrt{2V}, \chi^*]\) as established in Theorem \(1.3\) and in particular, we note that in the cases \( \sigma = 2, 3 \), the real threshold \( \chi_{\text{c}} > 4V^2 = 4 \). Moreover, in accordance with our expectation in the comment associated with the monotonicity properties of \( \chi \) with respect to its dependence on \( \sigma \) discussed in Section II, the relevant critical point is, in fact, increasing as a function of \( \sigma \), as \((2.37)\) suggested.

The right panel of Fig. 2 shows a similar comparison but now with the saturable nonlinearity. Remarkably the latter also appears to possess a higher value of \( \chi_{\text{c}} \approx 4.4 \), in comparison to the cubic case. However, in consonance to the expectation of a more proximal case to the linear one, the increase in the relevant dependence of \( \chi \) is less steep and occurs over a wider interval of nonlinearity strengths.

It is also interesting to note that the decay dynamics follows a very typical pattern similar to the one shown in the upper panel of Fig. 1. The corresponding log-log plot inset indicates that the central site amplitude decreases according to a \( t^{-1} \) power law (in terms of its envelope). It is important to point out that we have confirmed that this decay is present for different values of the nonlinearity (with the same exponent). Essentially, in accordance with our arguments in Sec. II (recall \((2.45)\) and the relevant discussion above), once the linear regime sets in the nonlinearity is irrelevant and plays a negligible role in the ensuing dynamics, which is governed by the linear decay. On the other hand, as illustrated in the right panel, past the relevant real critical point \( \chi_{\text{c}} \), only a transient decay is observed, past which the amplitude settles to a constant value and to the corresponding defect mode.

**IV. CONCLUSIONS AND FUTURE CHALLENGES**

In the present paper, we have revisited the widely relevant theme of a single nonlinear defect embedded in an otherwise linear lattice.

We have addressed this problem from an up to now missing rigorous dynamical perspective enabling the characterization of a weak nonlinearity regime, via a
suitable contraction mapping argument. This enabled us (for different intervals of nonlinearity strength and for different nonlinearities –power law and saturable–) to come up with a proof of the fact that $\langle P \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t |C_0(s)|^2 ds = 0$ for a sufficiently weak nonlinearity. On the other hand, by combining the fundamental global existence, conservation and continuity properties of the solutions of the involved DNLS equation, together with an asymptotic invariance argument on the nonlinear map governing $C_0(t)$, we have proved that $\langle P \rangle > 0$ for a sufficiently strong nonlinearity, in the slightly weaker sense of (2.45).

In both regimes established in Theorem II.3, we have provided conditions that guarantee the two distinct dynamical behaviors straddling the self-trapping transition. In the weakly nonlinear regime, upon suitable further assumptions (which, however, are less straightforward to justify rigorously), our critical point can be pushed closer to the ones observed in the numerical experiments that we performed.

Naturally, there are numerous open questions that are still in need of rigorous analysis. An important one concerns an improved estimation of the true threshold separating the weak from the nonlinear regime. However, clearly the techniques to address the latter issue should be of a fundamentally different kind than the ones used herein, and could be possibly based on analytical bifurcation theory for nonlinear integral equations. On a related note, generalization of either the former (contraction mapping and invariance arguments) or the latter (analytical bifurcation theory) considerations to higher-dimensional or multi-defect settings would also be of particular interest. These themes are presently under consideration and will be reported in future publications.

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