

Lower and upper estimates on the excitation threshold for breathers in DNLS lattices

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We propose analytical lower and upper estimates on the excitation threshold for breathers (in the form of spatially localized and time periodic solutions) in DNLS lattices with power nonlinearity. The estimation depending explicitly on the lattice parameters, is derived by a combination of a comparison argument on appropriate lower bounds depending on the frequency of each solution with a simple and justified heuristic argument. The numerical studies verify that the analytical estimates can be of particular usefulness, as a simple analytical detection of the activation energy for breathers in DNLS lattices.

I. INTRODUCTION

A great deal of attention has been paid to the study of localization phenomena in nonlinear discrete systems in recent years, interest which has been summarized in a number of recent reviews [1–3]. This growth has been motivated not only by its intrinsic theoretical interest, but also by numerous applications in areas as the nonlinear optics of waveguide arrays [4, 5], Bose-Einstein condensates [6–8], micro-mechanical models of cantilever arrays [9], or some models of the complex dynamics of the DNA [10].

In this framework, perhaps one of the most prototypical model is the so-called discrete nonlinear Schrödinger equation (DNLS) [11, 12]. DNLS may arise as a direct model, as a tight binding approximation, or even as an envelope wave expansion and, it could be possible to say that the DNLS is one of the most ubiquitous models in the nonlinear physics of dispersive, discrete systems [13].

Our aim in the present paper is to determine analytical lower and upper bounds for the formation of spatially localized and time periodic modes in focusing DNLS lattices, called discrete breathers or also DNLS solitons [14], with power nonlinearity.

S. Flach, K. Kladko and R. MacKay in [19], were the first who addressed the existence of energy thresholds for the formation of discrete breathers in one-, two and three-dimensional lattices. The *energy thresholds are the positive lower energy levels possessed by discrete breathers (DB)*. Their numerical and heuristic arguments apply to a generic class of Hamiltonian systems and show that the energy of a DB has a positive lower level for lattice dimension N greater than or equal to some critical dimension N_c , whereas for $N < N_c$ the energy goes to zero as the amplitude goes to zero.

For the focusing DNLS equation in the infinite lattice \mathbb{Z}^N ,

$$i\dot{\psi}_n + \epsilon(\Delta_d\psi)_n + \Lambda|\psi_n|^{2\sigma}\psi_n = 0, \quad \Lambda > 0, \quad \sigma > 0, \quad (1.1)$$

where $n = (n_1, n_2, \dots, n_N) \in \mathbb{Z}^N$, the hypothesis suggested by Flach Kladko & MacKay was resolved by M. I. Weinstein in [21]. In (1.1), $(\Delta_d\psi)_n$ stands for the N -dimensional discrete Laplacian

$$(\Delta_d\psi)_{n \in \mathbb{Z}^N} = \sum_{m \in \mathcal{N}_n} \psi_m - 2N\psi_n. \quad (1.2)$$

Here \mathcal{N}_n denotes the set of $2N$ nearest neighbors of the point in \mathbb{Z}^N with label n . The parameter $\epsilon > 0$ is a discretization parameter $\epsilon \sim h^{-2}$ with h being the lattice spacing and $\Lambda > 0$ is the parameter of anharmonicity.

The hypothesis of [19] was resolved in [21] for breathers in the form of standing waves

$$\psi_n(t) = e^{i\Omega t}\phi_n, \quad \Omega > 0, \quad (1.3)$$

spatially localized in the sense

$$|\psi_n| \rightarrow 0, \quad \text{as } |n| \rightarrow \infty,$$

(here $|n| = \max_{1 \leq i \leq N} |n_i|$ for $n = (n_1, n_2, \dots, n_N) \in \mathbb{Z}^N$). Actually, solutions of the form (1.3) correspond to the so called “rotating wave approximation”, based on the assumption of solutions with only one harmonic. It is important to stress that there can also exist solutions with infinite harmonics, $\psi_n(t) = \sum_{k=1}^{\infty} \phi_n^k \exp(ik\omega t)$.

Solutions (1.3) of (1.1) satisfy the infinite system of transcendent equations

$$-\epsilon(\Delta_d \phi)_n + \Omega \phi_n - \Lambda |\phi_n|^{2\sigma} \phi_n = 0, \quad n \in \mathbb{Z}^N. \quad (1.4)$$

We recall that the *power* of any solution of the form (1.3) is the quantity

$$\mathcal{R}[\phi] = \sum_{n \in \mathbb{Z}^N} |\phi_n|^2. \quad (1.5)$$

The power (1.5) together with the Hamiltonian

$$\mathcal{H}[\phi] = \epsilon(-\Delta_d \phi, \phi)_2 - \frac{1}{\sigma+1} \sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}, \quad (1.6)$$

are the fundamental conserved quantities for (1.1).

The following discrete analogue of a Sobolev-Gagliardo-Nirenberg type inequality

$$\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2} \leq C \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^\sigma (-\Delta_d \phi, \phi)_2, \quad \sigma \geq \frac{2}{N}, \quad (1.7)$$

has a prominent role in the proof of [21] of the existence of the excitation threshold, and its characterization. For instance, If C_* is the infimum over all constants C for which inequality (1.7) holds, then the excitation threshold $\mathcal{R}_{\text{thresh}}$ is defined by [21, pg. 680, Eqn. (4.2)]

$$(\sigma + 1)\epsilon(\mathcal{R}_{\text{thresh}})^{-\sigma} = C_*, \quad (1.8)$$

and the optimal constant C_* has the variational characterization

$$\frac{1}{C_*} = \inf_{\substack{\phi \in \ell^2 \\ \phi \neq 0}} \frac{\left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^\sigma (-\Delta_d \phi, \phi)_2}{\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}}.$$

Note that with the symbol ℓ^p , we denote the usual sequence spaces, i.e.,

$$\ell^p = \left\{ \phi = \{\phi_n\}_{n \in \mathbb{Z}^N} : \|\phi\|_p = \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^p \right)^{\frac{1}{p}} < \infty \right\}, \quad 1 \leq p < \infty,$$

with $\|\phi\|_\infty = \sup_{n \in \mathbb{Z}^N} |\phi_n|$ when $p = \infty$. The case $p = 2$ corresponds to the Hilbert space ℓ^2 and the symbol $(\cdot, \cdot)_2$ stands for its standard inner product.

Then, Weinstein’s result on the excitation threshold reads as follows: if $\mathcal{R} > \mathcal{R}_{\text{thresh}}$ then $\mathcal{I}_{\mathcal{R}} < 0$, and a ground state breather exists, that is, there exists a minimizer of the variational problem

$$\mathcal{I}_{\mathcal{R}} = \inf \{ \mathcal{H}[\phi] : \mathcal{R}[\phi] = \mathcal{R} \}. \quad (1.9)$$

On the other hand, if $\mathcal{R} < \mathcal{R}_{\text{thresh}}$ then $\mathcal{I}_{\mathcal{R}} = 0$, and there is no ground state minimizer for (1.9). In the light of the results of Weinstein, the critical dimension predicted by Flach, Kladko and MacKay is defined for the DNLS (1.1) as

$$N_c = \frac{2}{\sigma}. \quad (1.10)$$

In this paper we propose analytical lower and upper estimates for the excitation threshold $\mathcal{R}_{\text{thresh}}$, which depend explicitly on the lattice parameters. The derivation of these estimates in section 2, can be briefly described as follows. We first use a fixed point argument to derive a lower bound for the power of the breather solution satisfied for any $\Omega > 0$. The role of such local bounds (through their dependence on the frequency Ω) as thresholds for the existence of breather solutions has been analyzed in detail and tested numerically in [15, 16]. Then this is compared with a second local lower bound involving this time the unknown value of $\mathcal{R}_{\text{thresh}}$. Although the lower bound for $\mathcal{R}_{\text{thresh}}$ derived as above, depends on an unspecified positive integer, its appropriate value can be easily determined by a simple and

justified heuristic argument, explained in detail in section 3. The derivation of the upper bound comes out by simply examining the interpolation inequality (1.7) in comparison with the standard embedding inequality between the ℓ^p spaces.

The numerical studies performed in section 3, justify that the estimates for $\mathcal{R}_{\text{thresh}}$ can be useful (in view of their explicit dependence on the lattice parameters and the simplicity of the formulas), in “trapping” the exact value of $\mathcal{R}_{\text{thresh}}$ for the cases of nonlinearity exponent σ and dimension N which are of primary physical interest. This “trapping” is of particular interest in applications since the analytical estimation of the excitation threshold can be used for a simple calculation of the activation energy needed for the experimental detection of discrete breathers [19]. It is important to recall that the excitation threshold appears in the formal continuum limit $\epsilon \rightarrow \infty$ only in the case $\sigma = 2/N$, [21].

II. ANALYTICAL LOWER AND UPPER BOUNDS FOR $\mathcal{R}_{\text{thresh}}$.

To derive analytical bounds for the excitation threshold $\mathcal{R}_{\text{thresh}}$ we use technical lemmas involving lower bounds for the power of solutions (1.3) for all $\Omega > 0$.

Lemma II.1 *The power of a nontrivial breather solution (1.3) of (1.1), satisfies the lower bound*

$$\mathcal{R}_{\min,1}(\Omega) := \mathcal{R}_{\text{thresh}} \cdot \left[\frac{\Omega}{4\epsilon\Lambda N(\sigma+1)} \right]^{\frac{1}{\sigma}} < \mathcal{R}[\phi] \text{ for all } \Omega > 0. \quad (2.1)$$

Proof: Multiplying (1.4) by ϕ in the ℓ^2 -scalar product we infer that ϕ satisfies the energy equation

$$\epsilon(-\Delta_d\phi, \phi)_2 + \Omega \sum_{n \in \mathbb{Z}^N} |\phi_n|^2 = \Lambda \sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}, \text{ for all } \Omega > 0. \quad (2.2)$$

Now inserting the inequality (1.7) in the right-hand side of (2.2), and noting that

$$(-\Delta_d\phi, \phi)_2 \leq 4N \sum_{n \in \mathbb{Z}^N} |\phi_n|^2, \quad (2.3)$$

we deduce that

$$\begin{aligned} \epsilon(-\Delta_d\phi, \phi)_2 + \Omega \sum_{n \in \mathbb{Z}^N} |\phi_n|^2 &\leq \Lambda C_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^\sigma (-\Delta_d\phi, \phi)_2 \\ &\leq 4\epsilon\Lambda N C_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}. \end{aligned}$$

Since $(-\Delta_d\phi, \phi)_2 \geq 0$ we infer that

$$\Omega \sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \leq 4\Lambda N C_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}. \quad (2.4)$$

By substitution of (1.7) into (2.4), we derive the lower bound (2.1). \diamond

Remark II.1 *According to the results of [21], the excitation threshold $\mathcal{R}_{\text{thresh}}$ is attained at a frequency Ω_{thresh} which is the Lagrange multiplier in the constrained minimization problem. The excitation threshold $\mathcal{R}_{\text{thresh}}$ is the power of the nontrivial breather solution*

$$\psi_n^*(t) = e^{i\Omega_{\text{thresh}}t} \phi_n^*, \quad \Omega_{\text{thresh}} > 0,$$

where ϕ^* is the nontrivial minimizer. Since (2.1) is satisfied by the power of any nontrivial solution (1.3) for any $\Omega > 0$, it also holds that

$$\mathcal{R}_{\min,1}(\Omega_{\text{thresh}}) < \mathcal{R}_{\text{thresh}}(\Omega_{\text{thresh}}).$$

This implies an upper estimate for the frequency of the breather Ω_{thresh}

$$\Omega_{\text{thresh}} < 4\epsilon\Lambda N(\sigma+1),$$

on which the excitation threshold is attained.

Lemma II.2 *Let $\kappa \in \mathbb{R}^+$, $\kappa > \frac{1}{2}$ be arbitrary. Then every non-trivial breather solution (1.3) of (1.1) has the power satisfying*

$$\mathcal{R}_{\min,2}(\kappa, \Omega) := \left[\frac{\sqrt{2\kappa - 1}}{\kappa} \cdot \frac{\Omega}{\Lambda(2\sigma + 1)} \right]^{\frac{1}{\sigma}} < \mathcal{R}[\phi] \text{ for all } \Omega > 0. \quad (2.5)$$

Proof: We use a modified fixed point argument of [15, 20]. We consider the operator

$$-\epsilon \Delta_d + \Omega : \ell^2 \rightarrow \ell^2. \quad (2.6)$$

which is linear and continuous. It also satisfies the assumptions of Lax-Milgram Theorem [22, Theorem 18.E, pg. 68]: Note that

$$\epsilon(-\Delta_d \phi, \phi)_2 + \Omega \|\phi\|_2^2 \geq \Omega \|\phi\|_2^2 \text{ for all } \phi \in \ell^2. \quad (2.7)$$

Then according to Lax-Milgram theorem, *given* $z \in \ell^2$, the linear operator equation

$$-\epsilon \Delta_d \phi_n + \Omega \phi_n = \Lambda |z_n|^{2\sigma} z_n, \quad \Lambda > 0, \quad (2.8)$$

has a unique solution $\phi \in \ell^2$, since

$$\| |z|^{2\sigma} z \|_2^2 \leq \sum_{n \in \mathbb{Z}^N} |z_n|^{4\sigma+2} \leq \|z\|_2^{4\sigma+2}. \quad (2.9)$$

Note that (2.9) comes out by using

$$\sum_{n \in \mathbb{Z}^N} |\phi_n|^p \leq \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^q \right)^{\frac{p}{q}}, \text{ for all } 1 \leq q \leq p \leq \infty, \quad (2.10)$$

for $p = 4\sigma + 2$ and $q = 2$.

Hence, we are allowed to define the map $\mathcal{P} : \ell^2 \rightarrow \ell^2$, by $\mathcal{P}(z) := \phi$, where ϕ is a unique solution of operator equation (2.8). Clearly the map \mathcal{P} is well defined. Let ζ, ξ be in the closed ball

$$B_R := \{z \in \ell^2 : \|z\|_{\ell^2} \leq R\},$$

and $\phi = \mathcal{P}(\zeta)$, $\psi = \mathcal{P}(\xi)$. The difference $\chi := \phi - \psi$ satisfies the equation

$$-\epsilon \Delta_d \chi_n + \Omega \chi_n = \Lambda (|\zeta_n|^{2\sigma} \zeta_n - |\xi_n|^{2\sigma} \xi_n). \quad (2.11)$$

We recall that for any $F \in C(\mathbb{C}, \mathbb{C})$ which takes the form $F(z) = g(|z|^2)\zeta$, with g real and sufficiently smooth, the following relation holds

$$F(\zeta) - F(\xi) = \int_0^1 \{(\zeta - \xi)(g(r) + r g'(r)) + (\bar{\zeta} - \bar{\xi})\Phi^2 g'(r)\} d\theta, \quad (2.12)$$

for any $\zeta, \xi \in \mathbb{C}$, where $\Phi = \theta\zeta + (1-\theta)\xi$, $\theta \in (0, 1)$ and $r = |\Phi|^2$ (see [18, pg. 202]). Applying (2.12) to $F(\zeta) = |\zeta|^{2\sigma}\zeta$, one finds that

$$|\zeta|^{2\sigma}\zeta - |\xi|^{2\sigma}\xi = \int_0^1 [(\sigma + 1)(\zeta - \xi)|\Phi|^{2\sigma} + \sigma(\bar{\zeta} - \bar{\xi})\Phi^2|\Phi|^{2\sigma-2}] d\theta. \quad (2.13)$$

Assuming that $\zeta, \xi \in \mathcal{B}_R$, and noting that $\|\Phi\|_2 \leq R$, we get from (2.13) the inequality

$$\begin{aligned} \sum_{n \in \mathbb{Z}^N} \left| |\zeta_n|^{2\sigma}\zeta_n - |\xi_n|^{2\sigma}\xi_n \right|^2 &\leq (2\sigma + 1)^2 \sum_{n \in \mathbb{Z}^N} \left\{ \int_0^1 |\Phi_n|^{2\sigma} |\zeta_n - \xi_n| d\theta \right\}^2 \\ &\leq (2\sigma + 1)^2 \sum_{n \in \mathbb{Z}^N} \left\{ \int_0^1 \|\Phi\|_2^{2\sigma} |\zeta_n - \xi_n| d\theta \right\}^2 \\ &\leq (2\sigma + 1)^2 \sum_{n \in \mathbb{Z}^N} \left\{ \int_0^1 R^{2\sigma} |\zeta_n - \xi_n| d\theta \right\}^2 \\ &= (2\sigma + 1)^2 R^{4\sigma} \sum_{n \in \mathbb{Z}^N} |\zeta_n - \xi_n|^2. \end{aligned} \quad (2.14)$$

Now taking the scalar product of (2.11) with χ in ℓ^2 and using (2.14), we have

$$\begin{aligned} \epsilon(-\Delta_d \chi, \chi)_2 + \Omega \|\chi\|_2^2 &\leq \Lambda \|\chi\|_2 \|\zeta\|_2^{2\sigma} \|\zeta - \xi\|_2 - \|\xi\|_2^{2\sigma} \|\xi\|_2 \\ &\leq \Lambda(2\sigma + 1)^2 R^{2\sigma} \|\chi\|_2 \|\zeta - \xi\|_2. \end{aligned} \quad (2.15)$$

Applying Young's inequality

$$ab < \frac{\hat{\epsilon}}{p} a^p + \frac{1}{q \hat{\epsilon}^{q/p}} b^q, \quad \text{for any } \hat{\epsilon} > 0, \quad 1/p + 1/q = 1,$$

with $p = q = 2$, $a = \|\chi\|_2$, $b = \|\zeta - \xi\|_2$ and

$$\hat{\epsilon} = \frac{\omega}{\kappa}, \quad \kappa \in \mathbb{R}^+, \quad \kappa > 1/2,$$

we get that

$$\frac{(2\kappa - 1)\Omega}{2\kappa} \|\chi\|_2^2 \leq \frac{\kappa}{2\Omega} \Lambda^2 (2\sigma + 1)^2 R^{4\sigma} \|\zeta - \xi\|_2^2. \quad (2.16)$$

From (2.16), we conclude with

$$\|\chi\|_2^2 = \|\mathcal{P}(z) - \mathcal{P}(\xi)\|_2^2 \leq \frac{\kappa^2}{\Omega^2 (2\kappa - 1)} \Lambda^2 (2\sigma + 1)^2 R^{4\sigma} \|\zeta - \xi\|_2^2,$$

and hence, the map $\mathcal{P} : B_R \rightarrow B_R$ is Lipschitz continuous with the Lipschitz constant

$$L = \frac{\kappa}{\Omega \sqrt{2\kappa - 1}} \Lambda (2\sigma + 1) R^{2\sigma}.$$

The map \mathcal{P} is a contraction, and hence, has a unique fixed point if $L < 1$. This unique fixed point is the trivial one, since $\mathcal{P}(0) = 0$. Hence, for

$$R^2 < \left[\frac{\sqrt{2\kappa - 1}}{\kappa} \cdot \frac{\Omega}{\Lambda(2\sigma + 1)} \right]^{\frac{1}{\sigma}}$$

the only breather solution is the trivial one. Therefore, a non-trivial breather solution (1.3) should have power $\mathcal{R}[\phi] \geq \mathcal{P}_{\min,2}$. \diamond

Both $\mathcal{R}_{\min,2}(\kappa, \Omega)$ and $\mathcal{R}_{\min,1}(\Omega)$ are Ω -dependent and $\mathcal{R}_{\min,1}$ contains the unknown $\mathcal{R}_{\text{thresh}}$. Due to the same order of dependence of $\mathcal{R}_{\min,2}(\kappa)$, $\mathcal{R}_{\min,1}$ on Ω , an explicit Ω -independent estimation for $\mathcal{R}_{\text{thresh}}$ will be derived immediately by an ordering of $\mathcal{R}_{\min,2}(\kappa)$, $\mathcal{R}_{\min,1}$ which will eliminate Ω .

Note that the maximum value $\mathcal{R}_{\min,2}(1)$ for $\kappa = 1$ can't be used a-priori for a rigorous derivation of an ordering since $\mathcal{R}_{\text{thresh}}$ is unknown. This ordering is rigorously valid only for some "sufficiently large $\kappa > 1/2$ ", as it will be proved in the next proposition. However the numerical simulations, together with justified arguments on the behavior of $\mathcal{R}_{\text{thresh}}$ for large σ will reveal that for practical purposes, the constant κ can be easily determined. It will be shown in section 3 that even $\kappa = 1$, is a satisfactory and sharp choice to insert in the Ω -independent lower bound which will be derived in the proposition, for values of σ which are of physical significance.

Proposition II.1 *Let $\sigma \geq 2/N$. There exist $\kappa_{\text{crit}} > 1/2$ such that*

$$\left[\frac{\sqrt{2\kappa_{\text{crit}} - 1}}{\kappa_{\text{crit}}} \cdot \frac{4N\epsilon(\sigma + 1)}{2\sigma + 1} \right]^{\frac{1}{\sigma}} < R_{\text{thresh}} < [4\epsilon N(\sigma + 1)]^{\frac{1}{\sigma}}. \quad (2.17)$$

Proof: Due to (2.5) which holds for any $\Omega > 0$, and on the account of the remark II.1, we have

$$\mathcal{R}_{\text{thresh}}(\Omega_{\text{thresh}}) > \max\{\mathcal{R}_{\min,1}(\Omega_{\text{thresh}}), \mathcal{R}_{\min,2}(\kappa, \Omega_{\text{thresh}})\}.$$

Since $\mathcal{R}_{\text{thresh}}$ is attained on the fixed value Ω_{thresh} , it follows from Lemma II.2 that

$$\lim_{\kappa \rightarrow \infty} \mathcal{R}_{\min,2}(\kappa, \Omega_{\text{thresh}}) = 0.$$

Therefore, we can make $\mathcal{R}_{\min,2}(\kappa, \Omega_{\text{thresh}}) > 0$ as small as we want by taking κ large enough. More precisely, for every $\hat{\epsilon} > 0$, there exists $K(\hat{\epsilon}) > 1/2$ such that for all $\kappa > K(\hat{\epsilon})$,

$$\mathcal{R}_{\min,2}(\kappa, \Omega_{\text{thresh}}) < \hat{\epsilon}.$$

Consequently, by setting $\hat{\epsilon} = \mathcal{R}_{\min,1}(\Omega_{\text{thresh}})$ there exists a $\kappa_{\text{crit}} > K(\hat{\epsilon})$ such that

$$\mathcal{R}_{\min,2}(\kappa_{\text{crit}}, \Omega_{\text{thresh}}) < \mathcal{R}_{\min,1}(\Omega_{\text{thresh}}),$$

implying the first inequality in (2.17).

Note also that $\mathcal{R}_{\min,2}(\kappa, \Omega_{\text{thresh}}) < \mathcal{R}_{\min,1}(\Omega_{\text{thresh}})$ for all $\kappa \geq \kappa_{\text{crit}} > K(\hat{\epsilon})$.

To prove the second inequality in (2.17), we apply first the inequality (2.10) for $p = 2\sigma + 2$ and $q = 2$ and we get that

$$\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2} \leq \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}, \quad \text{for all } \sigma \geq 0, \phi \in \ell^2. \quad (2.18)$$

From (2.18) we have

$$\sup_{\substack{\phi \in \ell^2 \\ \phi \neq 0}} \frac{\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}}{\left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}} \leq 1, \quad \text{for all } \sigma \geq 0.$$

Since the above inequality holds for all $\sigma \geq 0$ and all $\phi \in \ell^2$, taking as ϕ in (2.18) any element of the standard orthonormal basis of ℓ^2 , we get that

$$\sup_{\substack{\phi \in \ell^2 \\ \phi \neq 0}} \frac{\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}}{\left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}} = 1, \quad \text{for all } \sigma \geq 0. \quad (2.19)$$

On the other hand, it follows from (1.7) and (2.3) that

$$\begin{aligned} \sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2} &\leq C_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^\sigma (-\Delta_d \phi, \phi)_2 \leq 4NC_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^\sigma \sum_{n \in \mathbb{Z}^N} |\phi_n|^2. \\ &= 4NC_* \left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}, \quad \sigma \geq 2/N, \end{aligned}$$

which implies that

$$\frac{\sum_{n \in \mathbb{Z}^N} |\phi_n|^{2\sigma+2}}{\left(\sum_{n \in \mathbb{Z}^N} |\phi_n|^2 \right)^{\sigma+1}} \leq 4NC_*, \quad \text{for all } \sigma \geq 2/N, \phi \in \ell^2. \quad (2.20)$$

Then a comparison of (2.19) which holds for all $\sigma > 0$, with (2.20) implies that

$$1 < 4NC_* = 4\epsilon N(\sigma + 1)R_{\text{thresh}}^{-\sigma}, \quad (2.21)$$

from which we conclude the right-hand side of (2.17). \diamond

III. NUMERICAL STUDY

Since the upper bound on (2.17) depends explicitly on known parameters of the lattice, the estimates would have a full strength in applications if the undetermined constant κ_{crit} could be easily determined, at least by a simple heuristic argument. For such a simple heuristic determination of the constant κ_{crit} , it looks natural to restrict to

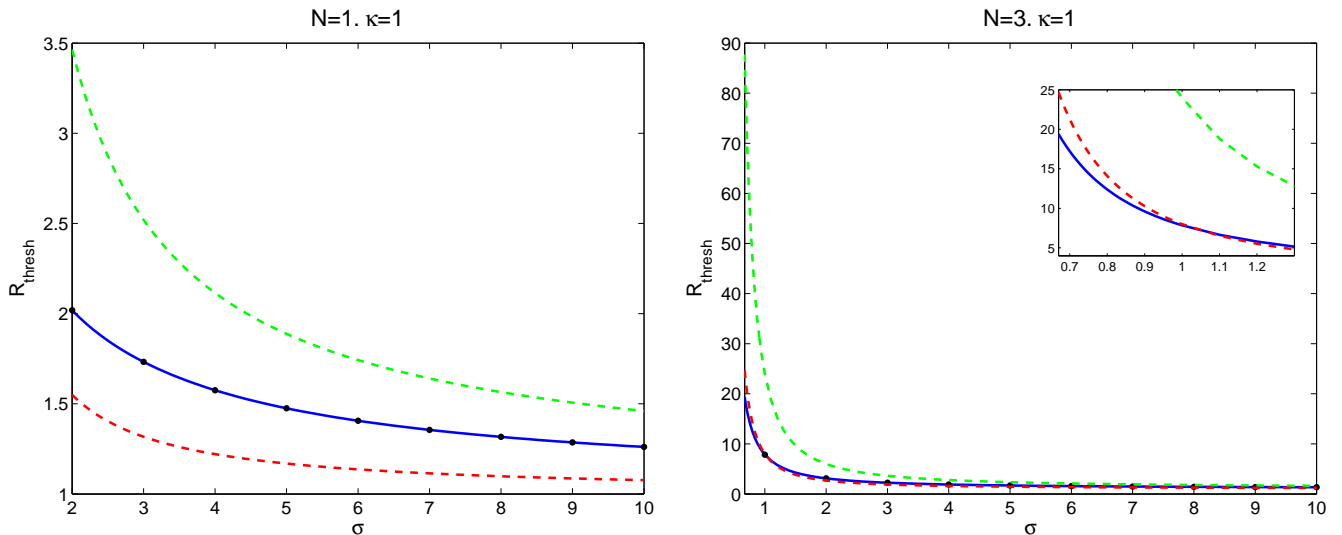


Figure 1: Numerical values for $\mathcal{R}_{\text{thresh}}$ as a function of $\sigma \geq 2/N$ against its lower and upper estimation (2.17) for $\kappa_{\text{crit}} = 1$ (formula (3.2)). (a) $N = 1$, $\sigma \geq 2$, (b) $N = 3$, $\sigma \geq 2/3$. In both cases $\epsilon = 1$. Green dashed line corresponds to the upper estimate, blue full line to the numerical $\mathcal{R}_{\text{thresh}}$ and red dashed line to the lower estimate. The inset in (b) magnifies the discrepancy observed for the prediction of the lower estimate of (3.2) in the interval $\sigma \in (2/3, 1)$. Black dots correspond to integer values of the nonlinearity exponent σ .

the case $\kappa \in \mathbb{Z}^+$, $\kappa \geq 1$. Then, the simplicity of the formula (2.17) suggests that the appropriate value of κ can be determined by considering successive choices of κ . Setting

$$\mathcal{R}_{lb} = \left[\frac{\sqrt{2\kappa_{\text{crit}} - 1}}{\kappa_{\text{crit}}} \cdot \frac{4N\epsilon(\sigma + 1)}{2\sigma + 1} \right]^{\frac{1}{\sigma}},$$

and rewriting (1.8) as

$$\mathcal{R}_{\text{thresh}} = \left[\frac{(\sigma + 1)\epsilon}{C_*} \right]^{\frac{1}{\sigma}},$$

we observe that

$$\lim_{\sigma \rightarrow \infty} \mathcal{R}_{lb} = \lim_{\sigma \rightarrow \infty} \mathcal{R}_{\text{thresh}} = 1. \quad (3.1)$$

independently of the choice of κ, ϵ, N . This behavior completely justifies that even the first choice $\kappa_{\text{crit}} = 1$ is valid for “sufficiently large” σ . The first numerical study whose results are demonstrated in Figure 1, examines the range of $\sigma > 0$ on which this simplest choice $\kappa_{\text{crit}} = 1$ is valid, i.e. the validity of the formula

$$\left[\frac{4N\epsilon(\sigma + 1)}{2\sigma + 1} \right]^{\frac{1}{\sigma}} < \mathcal{R}_{\text{thresh}} < [4\epsilon N(\sigma + 1)]^{\frac{1}{\sigma}}. \quad (3.2)$$

The green dashed line represents the theoretical upper estimate $\mathcal{R}_{ub} := [4\epsilon N(\sigma + 1)]^{\frac{1}{\sigma}}$, the blue full line corresponds to the numerical $\mathcal{R}_{\text{thresh}}$ as a function of $\sigma \geq 2/N$ and the red dashed line represents the theoretical lower estimate \mathcal{R}_{lb} . The first numerical study, not only reveals that the formula (3.2) is valid for the case $N = 1, 2$ but also of very good accuracy for $N = 2$ and excellent for $N = 3$ for $\sigma \geq 1$ with a discrepancy regarding the prediction of the lower bound \mathcal{R}_{lb} appearing in the interval $\sigma \in (2/3, 1)$. In the light of the behavior (3.1), the choice $\kappa_{\text{crit}} = 1$ is satisfied for all $\sigma \geq 1$. Motivated by the recent work of J. Dorniac, J. Zhou and D.K. Campbell [17] which considers integer values of $\sigma \geq 2/N$ (represented by the black dots in the figures) it seems fair to state that the prediction of (3.2) is of particular usefulness for such nonlinearity exponents and lattice dimensions which are of main physical interest.

Seeking for the value of κ_{crit} which would remove the small discrepancy of (3.2) for $N = 3$ and real values of $\sigma \geq 2/N$, our numerical investigations verified that in the choice $\kappa_{\text{crit}} = 2$ this discrepancy is reduced to the interval

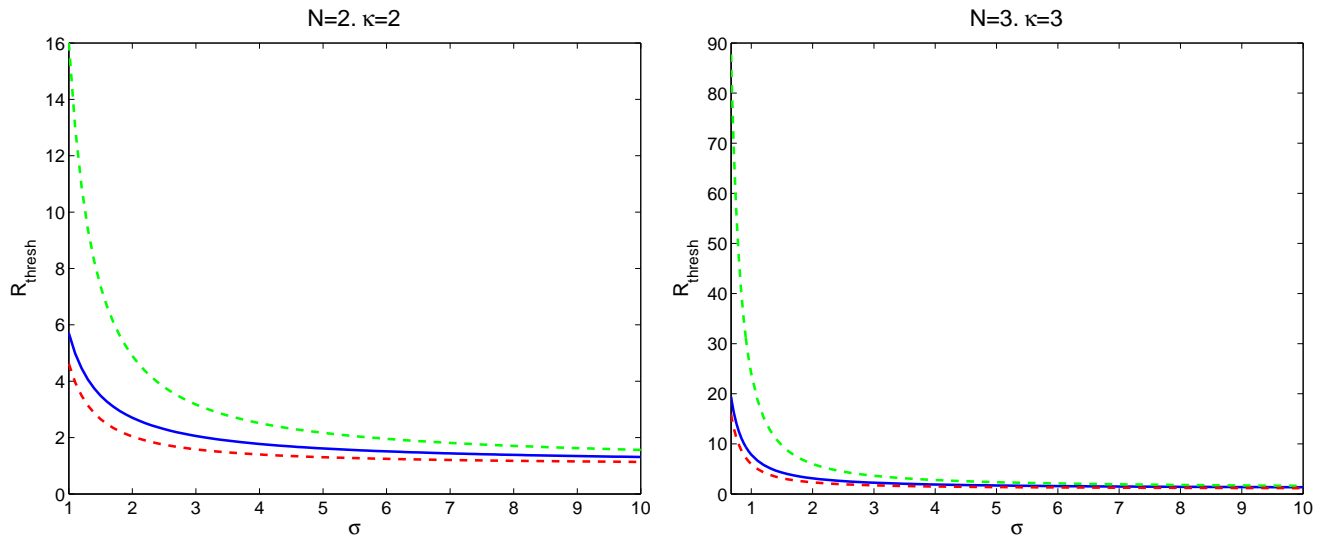


Figure 2: Numerical values for $\mathcal{R}_{\text{thresh}}$ as a function of $\sigma \geq 2/N$ against its lower and upper estimation (2.17). (a) $N = 2$, $\sigma \geq 2$, $\kappa_{\text{crit}} = 2$, (b) $N = 3$, $\sigma \geq 2/3$, $\kappa_{\text{crit}} = 3$. The choice of $\kappa_{\text{crit}} = 3$ removes the discrepancies observed in the cases $N = 3$, $\kappa_{\text{crit}} = 1, 2$ (see Figure 1 (b)), suggesting the generalized formula (3.4) for the estimation of $\mathcal{R}_{\text{thresh}}$.

$\sigma \in (2/3, 0.72)$, and it is completely removed for the choice of $\kappa_{\text{crit}} = 3$, as it is shown in Figure 2 (b). A summary of our findings for the cases $N = 1, 2, 3$, suggests to restate Proposition II.1 taking into account the dependence of κ_{crit} on the dimension of the lattice: Letting $\kappa \in \mathbb{Z}^+$ and N being fixed, we observe that since $\lim_{\kappa \rightarrow \infty} \mathcal{R}_{\text{min},2}(\kappa) = 0$, we can always find $\kappa_{\text{crit}}(N) \geq N$ such that

$$\left[\frac{\sqrt{2\kappa_{\text{crit}}(N) - 1}}{\kappa_{\text{crit}}(N)} \cdot \frac{4N\epsilon(\sigma + 1)}{2\sigma + 1} \right]^{\frac{1}{\sigma}} < R_{\text{thresh}} < [4\epsilon N(\sigma + 1)]^{\frac{1}{\sigma}}, \text{ for all } 1 \leq N \leq \kappa_{\text{crit}}(N). \quad (3.3)$$

With the rigorously valid estimates (3.3) at hand, the numerical study for the cases $N = 1, 2, 3$ suggest that it is justified to consider $\kappa_{\text{crit}}(N) = N$ and that

$$\left[\frac{\sqrt{2N - 1}}{N} \cdot \frac{4N\epsilon(\sigma + 1)}{2\sigma + 1} \right]^{\frac{1}{\sigma}} < R_{\text{thresh}} < [4\epsilon N(\sigma + 1)]^{\frac{1}{\sigma}}, \text{ for all } 1 \leq N \leq 3, \quad (3.4)$$

which is of valuable accuracy for $N = 2, 3$. The estimates (3.4) have the advantage of removing the small discrepancy of (3.2) observed in the case $N = 3$, for real $\sigma \geq 2/N$. However we believe that the above formulas derived by a simple heuristic implementation of Proposition II.1, serve as a very satisfactory analytical estimation of the excitation threshold in the cases of σ, N which are of physical significance.

IV. CONCLUSIONS

In this work, we have determined analytical upper and lower estimates on the excitation threshold for breathers in N -dimensional DNLS lattices. Numerical calculations show that, in cases studied, the theoretical bound is close to the true threshold providing useful analytical expressions to determine analytical energy activation of breathers in these systems. On the other hand, extensions of previous results to more general situations, as DNLS systems with impurities, are currently under investigation and will be reported in future publications.

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