A lower bound for the power of periodic solutions of the defocusing Discrete Nonlinear Schrödinger equation*

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Abstract

We derive lower bounds on the *power* of breather solutions $\psi_n(t) = e^{-i\Omega t}\phi_n$, $\Omega > 0$ of a Discrete Nonlinear Schrödinger Equation with cubic or higher order nonlinearity and site-dependent anharmonic parameter, supplemented with Dirichlet boundary conditions. For the case of a *defocusing* DNLS, one of the lower bounds depends not only on the dimension of the lattice, the lattice spacing, and the frequency of the periodic solution, but also on the excitation threshold of time periodic and spatially localized solutions of the *focusing* DNLS, proved by M. Weinstein in Nonlinearity **12**, 673–691, 1999. Our simple proof via a direct variational method, makes use of the interpolation inequality proved by Weinstein, and its optimal constant related to the excitation threshold. We also provide existence results (via the mountain pass theorem) and lower bounds on the power of breather solutions for DNLS lattices with *sign-changing* anharmonic parameter. Numerical studies considering the classical defocusing DNLS, the case of a single nonlinear impurity, as well as a random DNLS lattice are performed, to test the efficiency of the lower bounds.

1 Introduction

In this paper, we study solutions of a generalized DNLS equation, supplemented with Dirichlet boundary conditions

$$\mathrm{i}\dot{\psi}_n + \epsilon(\Delta_d\psi)_n - \Lambda_n|\psi_n|^{2\sigma}\psi_n = 0, \quad ||n|| \leq K, \tag{1.1}$$

$$\psi_n = 0, \quad ||n|| > K, \tag{1.2}$$

where $||n|| = \max_{1\leq i\leq N}|n_i|$ for $n = (n_1, n_2, \ldots, n_N) \in \mathbb{Z}^N$. In other words we consider the DNLS equation (1.1) in the *finite* lattice $\mathbb{Z}^N_K = \mathbb{Z}^N \cap \{-K \leq n_1, n_2, \ldots, n_N \leq K\}$. In (1.1), $\epsilon > 0$ is a discretization parameter $\epsilon \sim h^{-2}$ with h being the lattice spacing, and $(\Delta_d\psi)_n$ stands for the N-dimensional discrete Laplacian

$$(\Delta_d\psi)_{n\in\mathbb{Z}^N} = \sum_{m\in\mathcal{N}_n}\psi_m - 2N\psi_n, \tag{1.3}$$

where $\mathcal{N}_n$ denotes the set of $2N$ nearest neighbours of the point in $\mathbb{Z}^N$ with label n.

Note especially that we take the nonlinearity parameter $\Lambda := (\Lambda_n)_{||n||\leq K} \in \mathbb{R}^{(2K+1)^N}$ in Equation (1.1) to be *site-dependent.* We consider three possible alternative cases for Λ:

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(F) (*Focusing case*) $\Lambda_n \leq 0,\ \ n \in \mathbb{Z}_K^N$ and $\Lambda \neq 0$ ($\Lambda \in \mathbb{R}^{(2K+1)^N}$ is not identically the zero vector having at least one negative coordinate).

(D) (*Defocusing case*) $\Lambda_n \geq 0,\ \ n \in \mathbb{Z}_K^N$ and $\Lambda \neq 0$ ($\Lambda \in \mathbb{R}^{(2K+1)^N}$ is not identically the zero vector having at least one non-negative coordinate).

(SC) (*Sign-changing case*) In some $\mathcal{S}_+ \subset \mathbb{Z}_K^N$, $\{\Lambda_n\}_{n\in\mathcal{S}_+} > 0$ and in $\mathcal{S}_- := \mathbb{Z}_K^N \setminus \mathcal{S}_+$, $\{\Lambda_n\}_{n\in\mathcal{S}_-} \leq 0$, where $\{\Lambda_n\}_{n\in\mathcal{S}_-} \neq 0$ (not identically the zero vector in $\mathcal{S}_-$).

The solutions we consider to (1.1) are restricted to time-periodic solutions of the form

$$\psi_n(t) = e^{-\mathrm{i}\Omega t}\phi_n,\ \ \Omega > 0, \tag{1.4}$$

where the sign of Ω is crucial to our study.

We can associate a *power* to any solution of the form (1.4), defined as

$$\mathcal{P}[\phi] = \sum_{n\in\mathbb{Z}^N} |\phi_n|^2 \tag{1.5}$$

Our paper is devoted to an analytic and numerical study of lower bounds on the power of solutions of the form (1.4) to (1.1) as functions of Λ and the other parameters of the problem. We concentrate on the Defocusing and the Sign-changing cases. Although historically the main interest was in the focusing case, more recently interest has grown in the other two cases, starting perhaps with the paper by Kivshar in 1993 [10].

A characteristic example of a site dependent nonlinearity parameter covered by conditions (D) or (SC), is that of a single nonlinear impurity at the origin $n = 0$, see M. I. Molina [13, 15], M. I. Molina & H. Bahlouli [14], G. P. Tsironis, M. I. Molina & D. Hennig [16]. Another recent example of work on an inhomogeneous lattice is [11].

Solutions (1.4) are usually called breathers (or sometimes solitons), from the comparison with a class of exact solutions of the sine-Gordon equation of the same name. We note that there is a growing interest in the study of such modes in discrete lattices. A number of papers have studied the stability analysis of such solutions in both cubic and saturable DNLS lattices (c.f. [1, 5, 18]).

A key work in this area on existence of solutions is the 1999 paper by Weinstein [17] on the focusing case (F) of (1.1) with *constant* Λ. Since we make extensive use of the results in [17], we briefly summarise these here to make our paper more self-contained. In this paper Weinstein considered the focusing Discrete Nonlinear Schrödinger Equation (DNLS) [4, 9]

$$\mathrm{i}\dot{\psi}_n + \epsilon(\Delta_d\psi)_n + |\psi_n|^{2\sigma}\psi_n = 0,\ \ \sigma > 0,\ n = (n_1, n_2, \ldots, n_N) \in \mathbb{Z}^N, \tag{1.6}$$

and resolved the hypothesis suggested by S. Flach, K. Kladko & R. MacKay [6] for this equation, on the existence of excitation thresholds for the existence of nonlinear localized modes for Hamiltonian dynamical systems defined on multidimensional lattices. More precisely, the numerical studies and heuristic arguments of [6], suggested that there is a lower bound on the energy of a breather (time periodic and spatially localized standing wave solutions), if the lattice dimension is greater than or equal to a certain critical value. The hypothesis of [6] was resolved by

Theorem 1.1 *(M. Weinstein [17, Theorem 3.1,pg. 678]). Let $\sigma \geq \frac{2}{N}$. Then there exists a ground state excitation threshold $\mathcal{R}_{\mathrm{thresh}} > 0$.*

A minimizer of the variational problem

$$\mathcal{I}_{\mathcal{R}} = \inf\left\{\mathcal{H}[\phi]\ :\ \mathcal{P}[\phi] = \mathcal{R}\right\}. \tag{1.7}$$

is called a *a ground state* [17, Definition, pg. 676]. Here the Hamiltonian $\mathcal{H}[\phi]$ and the power $\mathcal{P}[\phi]$ are the fundamental conserved quantities, where

$$\mathcal{H}[\phi] = \epsilon(-\Delta_d\phi, \phi)_2 - \frac{1}{\sigma+1}\sum_{n\in\mathbb{Z}^N} |\phi_n|^{2\sigma+2}. \tag{1.8}$$

Theorem 1.1, states that if $0 < \sigma < \frac{2}{N}$, then $\mathcal{I}_{\mathcal{R}} < 0$ for all $\mathcal{R} > 0$. That is, the variational problem (1.7) has a solution for all $\mathcal{R} > 0$ and there is no excitation threshold. However *when $\sigma \geq \frac{2}{N}$, there exists an excitation* *threshold* $\mathcal{R}_{\text{thresh}}$ such that *(a) if* $\mathcal{R} > \mathcal{R}_{\text{thresh}}$ *then* $\mathcal{I}_{\mathcal{R}} < 0$, *and a ground state exists* and *(b) if* $\mathcal{R} < \mathcal{R}_{\text{thresh}}$ *then* $\mathcal{I}_{\mathcal{R}} = 0$, *and there is no ground state minimizer of (1.7).*

Theorem 1.1, justifies the existence of an excitation threshold for spatially localized and time periodic solutions of the form

$$\begin{aligned} \psi_n(t) &= e^{\mathrm{i}\omega t}\phi_n,\ \omega > 0,\ \ n \in \mathbb{Z}^N,\ \ t \in \mathbb{R}, \\ \phi_n &\in \ell^2. \end{aligned} \tag{1.9}$$

The threshold value, $\mathcal{R}_{\text{thresh}}$, is related to the best constant of an interpolation inequality which is a discrete analogue of the Sobolev-Gagliardo-Nirenberg inequality.

Theorem 1.2 *(M. Weinstein [17, Theorem 4.1,pg. 682]) Assume that* $\sigma \geq \frac{2}{N}$. *Then there exists* $C > 0$, *such that for all* $\phi \in \ell^2$, *the following interpolation inequality holds*

$$\sum_{n\in\mathbb{Z}^N} |\phi_n|^{2\sigma+2} \leq C\left(\sum_{n\in\mathbb{Z}^N} |\phi_n|^2\right)^{\sigma} (-\Delta_d\phi,\phi)_2. \tag{1.10}$$

If C_* is the infimum over all such constants for which inequality (1.10) holds, then the excitation threshold $\mathcal{R}_{\text{thresh}}$ is defined by [17, pg. 680, Eqn. (4.2)]

$$(\sigma+1)\epsilon\left(\mathcal{R}_{\text{thresh}}\right)^{-\sigma} = C_*, \tag{1.11}$$

and the optimal constant C_* has the variational characterization

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

This completes our summary of Weinstein's results.

In our paper, to establish that problem (1.1)-(1.2) admits time periodic solutions (1.4), we follow a variational approach (constrained minimization problem) as used in [17]. However, one of our claims in Section 2, is that by using the discrete interpolation inequality (1.10), a simple proof of an explicit lower bound on the power of solutions (1.4) of the DNLS (1.1)-(1.2) under condition (D), can be derived. It is shown that the lower bound exhibits an interesting relation between the parameters $N, \sigma, \Omega, \epsilon, \Lambda_n$ *as well as on the excitation threshold for the periodic solutions of the focusing DNLS (1.6)* derived by Weinstein. *A numerical comparison with an* $\mathcal{R}_{\text{thresh}}$*-independent lower bound, indicates for a derivation of an explicit upper bound on* $\mathcal{R}_{\text{thresh}}$ *depending on* σ, ϵ, N *(Section 4).*

Section 3 of our paper is devoted to the extension of the results on the existence of breathers as well on the lower bounds of their power, for the DNLS (1.1), under condition (SC). In this case, (1.1) *cannot be considered as focusing or defocusing*, and the existence of a nontrivial breather solution (1.4) is proved via the Mountain Pass Theorem (MPT) [8], as a saddle point of the functional

$$\mathcal{E}[\phi] = \frac{\epsilon}{2}(-\Delta_d\phi,\phi)_2 - \frac{\Omega}{2}\sum_{||n||\leq K}|\phi_n|^2 + \frac{1}{2\sigma+2}\sum_{||n||\leq K}\Lambda_n|\phi_n|^{2\sigma+2}.$$

We remark on an important difference of the results of this manuscript compared with those of [17]: *the threshold* $\mathcal{R}_{\text{thresh}}$ *(which is used in Theorem 2.1, to provide an optimal value for the constant* C_* *of the inequality (1.10)) is a global excitation threshold for the breathers, depending on* σ, N, *while the lower bounds derived in this paper are "local" in the sense that they depend also on the frequency* Ω *(as well as on* $\Lambda_n, \epsilon, \sigma, N$*). These bounds should not be viewed as a prediction of the excitation threshold in the case of* $\sigma \geq 2/N$ *nor as a theoretical prediction of the numerical power of periodic solutions but as prediction of the smallest power a periodic solution for any* Ω, Λ_n, ϵ,σ, N, *satisfying the assumptions for the derivation of the bounds. From this point of view, these bounds are "global" since no periodic solution has power smaller than the derived estimates. The global character of the estimates is revealed when one considers "limiting" cases of large values of* $\sigma > 2/N$*:* The numerical studies in Section 4, *verify that for large values of frequencies the estimates are not only satisfied but are also quite sharp estimates of the real power of the corresponding periodic solutions.* Thus the lower bounds derived *are of particular physical importance, since they provide a lower bound for the power of each breather of prescribed frequency* Ω, corresponding to DNLS lattices covered by the form of (1.1).

In the case of constant or constant-sign anharmonic parameters, the conditions on the existence of breather solutions with respect to the frequencies are similar to the requirement that they do not belong to the phonon band (see Remark 4.1). In the case of the indefinite sign, non trivial breathers exist for any $\Omega > 0$.

Although the study is *limited to the finite dimensional lattice, this case is of importance especially for numerical simulations*: since the infinite lattice cannot be modelled numerically, numerical investigations should consider finite lattices with Dirichlet or periodic boundary conditions. The choice of boundary conditions only matters, if the pulse is moving and collides with the boundary. We expect that similar bounds can be derived for the case of periodic boundary conditions, by considering appropriate variational problems, but the details have to be checked. The numerical study performed in this paper, considers as examples, the standard defocusing DNLS, the case of a single nonlinear impurity $\Lambda_n = \delta_{n,0}$ and the case of a random DNLS where Λ_n is described by a uniform distribution of $+1$ and -1.

We mention at this point, that an analytical and numerical study, on various lower bounds of the power of time periodic solutions, of the DNLS equation with saturable and power nonlinearities in infinite and finite lattices, is considered in [3].

2 A lower bound for time periodic solutions of the defocusing DNLS in a finite lattice

In this section we discuss a lower bound for time periodic solutions of the defocusing DNLS in a finite lattice and its relation to the excitation threshold of the focusing DNLS.

Substitution of the solution (1.4) into (1.1)-(1.2) shows that ϕ_n satisfies the system of algebraic equations

$$-\epsilon(\Delta_d\phi)_n - \Omega\phi_n = -\Lambda_n|\phi_n|^{2\sigma}\phi_n, \quad \Omega > 0, \quad ||n|| \leq K, \tag{2.1}$$

$$\phi_n = 0, \ ||n|| > K. \tag{2.2}$$

The finite dimensional problem (2.1)–(2.2) will be formulated in the finite dimensional subspaces of the sequence spaces ℓ^p, $1 \leq p \leq \infty$,

$$\ell^p(\mathbb{Z}^N_K) = \{\phi \in \ell^p \ : \ \phi_n = 0 \ \text{ for } \ ||n||| > K\}. \tag{2.3}$$

Clearly $\ell^p(\mathbb{Z}^N_K) \equiv \mathbb{C}^{(2K+1)^N}$, endowed with the norm

$$||\phi||_p = \left(\sum_{||n||\leq K} |\phi_n|^p\right)^{\frac{1}{p}}.$$

Moreover, it is easy to check by using Hölder's inequality that

$$||\phi||_p \leq (2K+1)^{\frac{N(q-p)}{qp}}||\phi||_q \leq ||\phi||_p, \quad 1 \leq p \leq q < \infty. \tag{2.4}$$

The principal eigenvalue of the operator $-\Delta_d$ denoted by $\lambda_1 > 0$, can be characterized as

$$\lambda_1 = \inf_{\substack{\phi \in \ell^2(\mathbb{Z}^N_K) \\ \phi \neq 0}} \frac{(-\Delta_d\phi, \phi)_2}{\sum_{||n||\leq K}|\phi_n|^2}, \tag{2.5}$$

Hence (2.5) implies the inequality

$$\epsilon\lambda_1 \sum_{||n||\leq K} |\phi_n|^2 \leq \epsilon(-\Delta_d\phi, \phi)_2 \leq 4\epsilon N \sum_{||n||\leq K} |\phi_n|^2. \tag{2.6}$$

Thus from (2.6), we find for λ_1 the bound

$$\lambda_1 \leq 4N. \tag{2.7}$$

In the case of an $1D$-lattice $n = 1, \ldots, K$, the eigenvalues of the discrete Dirichlet problem $-\Delta_d\phi = \lambda\phi$, with ϕ real, are given explicitly by

$$\lambda_n = 4\sin^2\left(\frac{n\pi}{4(K+1)}\right), \quad n = 1, \ldots, K,$$

while for a N-dimensional problem, the eigenvalues are:

$$\lambda_{(n_1,n_2,\ldots,n_N)} = 4\left[\sin^2\left(\frac{n_1\pi}{4(K+1)}\right) + \sin^2\left(\frac{n_2\pi}{4(K+1)}\right) + \ldots + \sin^2\left(\frac{n_N\pi}{4(K+1)}\right)\right],$$
$$n_j = 1,\ldots,K \quad j = 1,\ldots,N.$$

In consequence, the principal eigenvalue of the discrete Dirichlet problem $-\Delta_d\phi = \lambda\phi$, with ϕ real, is given by

$$\lambda_1 \equiv \lambda_{(1,1,\ldots,1)} = 4N\sin^2\left(\frac{\pi}{4(K+1)}\right).$$

We also mention that the inequality (1.10) holds for any element of the finite dimensional space $\phi \in \ell^2(\mathbb{Z}_K^N)$. The result of this note is stated in the following

Theorem 2.1 *We consider the functional*

$$\mathcal{H}[\phi] = \epsilon(-\Delta_d\phi,\phi)_2 + \frac{1}{\sigma+1}\sum_{||n||\leq K}\Lambda_n|\phi_n|^{2\sigma+2}, \tag{2.8}$$

and the variational problem on $\ell^2(\mathbb{Z}_K^N)$

$$\inf\left\{\mathcal{H}[\phi] \ : \sum_{||n||\leq K}|\phi_n|^2 = R > 0\right\}, \tag{2.9}$$

Then there exists a minimizer $\hat{\phi} \in \ell^2(\mathbb{Z}_K^N)$ *for the variational problem (2.9) and* $\Omega = \Omega(R) > 0$*, such that*

$$\Omega > \epsilon\lambda_1, \tag{2.10}$$

both satisfying the Euler-Lagrange equation (2.1), and $\sum_{||n||\leq K}|\hat{\phi}_n|^2 = R^2$.

Moreover, if $\sigma \geq \frac{2}{N}$ *and*

$$\Omega > 4\epsilon N, \tag{2.11}$$

the power of the minimizer $\mathcal{P}[\hat{\phi}]$ *satisfies the lower bound*

$$\mathcal{R}_{\text{thresh}}\cdot\left[\frac{\Omega - 4N\epsilon}{4\epsilon MN(\sigma+1)}\right]^{\frac{1}{\sigma}} \leq \mathcal{P}[\hat{\phi}], \quad M = \max_{||n||\leq K}\{\Lambda_n\} \tag{2.12}$$

where $\mathcal{R}_{\text{thresh}} \equiv \mathcal{R}_{\text{thresh}}(\sigma,N,\epsilon)$ *is the excitation threshold of solutions (1.9) of the focusing DNLS (1.6).*

Proof: We consider the set

$$B = \left\{\phi \in \ell^2(\mathbb{Z}_K^N) \ : \sum_{||n||\leq K}|\phi_n|^2 = R^2\right\}. \tag{2.13}$$

Clearly $\mathcal{H} : B \to \mathbb{R}$ is a C^1-functional (see [8, Lemma 2.3, pg. 121]). Also, it is bounded from below: inequality (2.6), implies that

$$\mathcal{H}[\phi] \geq \epsilon(-\Delta_d\phi,\phi)_2 \geq \epsilon\lambda_1 R^2. \tag{2.14}$$

We are restricted to the finite dimensional space $\ell^2(\mathbb{Z}_K^N)$, and it follows that any minimizing sequence associated with the variational problem (2.9) is precompact: any minimizing sequence has a subsequence, converging to a minimizer. Thus $\mathcal{E}$ attains its infimum at a point $\hat{\phi}$ in B. Now, for the C^1-functional

$$\mathcal{L}_R[\phi] = \sum_{||n||\leq K}|\phi_n|^2 - R^2, \tag{2.15}$$

we get that for any $\phi \in B$

$$\langle\mathcal{L}'_R[\phi],\phi\rangle = 2\sum_{||n||\leq K}|\phi|^2 = 2R^2 > 0. \tag{2.16}$$

Thus the Regular Value Theorem ([2, Section 2.9], [7, Appendix A,pg. 556]) implies that the set $R^2 = \mathcal{L}_R^{-1}(0)$ is a C^1-submanifold of $\ell^2(\mathbb{Z}_K^N)$. By applying the Lagrange multiplier rule, we get the existence of a parameter $\Omega = \Omega(R) \in \mathbb{R}$, such that

$$\begin{aligned}\left\langle \mathcal{H}'[\hat{\phi}] - \Omega\mathcal{L}_R'[\hat{\phi}], \psi \right\rangle &= 2\epsilon(-\Delta_d\hat{\phi}, \psi)_2 + 2\sum_{||n||\leq K} \Lambda_n|\hat{\phi}_n|^{2\sigma}\hat{\phi}_n\overline{\psi_n} \\ &\quad -2\Omega\mathrm{Re}\sum_{||n||\leq K} \hat{\phi}_n\overline{\psi}_n = 0, \quad \text{for all } \psi \in \ell^2(\mathbb{Z}_K^N).\end{aligned} \tag{2.17}$$

By $\langle\cdot,\cdot\rangle$ we denote the duality bracket between $\ell^2(\mathbb{Z}_K^N)$ and its isomorphic dual $\mathbb{C}^{(2K+1)^N}$ (hence this bracket actually coincides with the scalar product $(\cdot,\cdot)_2$). Setting $\psi = \hat{\phi}$ in (2.17), we find that

$$2\epsilon(-\Delta_d\hat{\phi}, \hat{\phi})_2 + 2\sum_{||n||\leq K} \Lambda_n|\hat{\phi}|^{2\sigma+2} = 2\Omega\sum_{||n||\leq K} |\hat{\phi}_n|^2. \tag{2.18}$$

By using inequality (2.6) and (2.17) we get the inequality

$$2\epsilon\lambda_1 \sum_{||n||\leq K} |\hat{\phi}_n|^2 \leq 2\epsilon(-\Delta_d\hat{\phi}, \hat{\phi})_2 + 2\sum_{||n||\leq K} \Lambda_n|\hat{\phi}|^{2\sigma+2} = 2\Omega\sum_{||n||\leq K} |\hat{\phi}_n|^2, \tag{2.19}$$

implying that

$$\Omega > \epsilon\lambda_1,$$

that is, (2.10). Lastly, we shall use (1.10), with the optimal constant (1.11), to estimate the second term on the rhs of (2.18): we have

$$2\epsilon(-\Delta_d\hat{\phi}, \hat{\phi})_2 + 2\max_{||n||\leq K}\{\Lambda_n\}C_*\left(\sum_{||n||\leq K} |\hat{\phi}_n|^2\right)^{\sigma}(-\Delta_d\hat{\phi}, \hat{\phi})_2 \geq 2\Omega\sum_{||n||\leq K} |\hat{\phi}_n|^2. \tag{2.20}$$

Since from (2.6)

$$\sum_{||n||\leq K} |\hat{\phi}_n|^2 \geq \frac{1}{4N}(-\Delta_d\hat{\phi}, \hat{\phi})_2,$$

inequality (2.20) becomes

$$\begin{aligned}2\epsilon(-\Delta_d\hat{\phi}, \hat{\phi})_2 &+ 2MC_*\left(\sum_{||n||\leq K} |\hat{\phi}_n|^2\right)^{\sigma}(-\Delta_d\hat{\phi}, \hat{\phi})_2 \\ &\geq \frac{2\Omega}{4N}(-\Delta_d\hat{\phi}, \hat{\phi})_2.\end{aligned} \tag{2.21}$$

Thus, from (2.21), we get

$$\epsilon + MC_*R^{2\sigma} \geq \frac{\Omega}{4N}. \tag{2.22}$$

Now from (2.22) we may infer the the lower bound

$$\left[\frac{\Omega - 4N\epsilon}{4MNC_*}\right]^{\frac{1}{\sigma}} < R^2. \tag{2.23}$$

Replacing the value C_*, given by (1.2), in inequality (2.23), we find

$$\mathcal{R}_{\mathrm{thresh}} \cdot \left[\frac{\Omega - 4N\epsilon}{4\epsilon MN(\sigma+1)}\right]^{\frac{1}{\sigma}} \leq R^2, \quad M = \max_{||n||\leq K}\{\Lambda_n\},$$

which is the lower bound (2.12). Note that (2.10) implies (2.20), due to (2.7). $\diamond$

Remark 2.1 *The lower bound (2.12) has the following implementation, through Theorem 2.1. There exists a frequency* $\Omega > \epsilon\lambda_1$ *and a nontrivial minimizer* $\hat{\phi} \in \ell^2(\mathbb{Z}_K^N)$ *of the problem (2.9), such that* $\psi_n(t) = e^{-i\Omega t}\hat{\phi}_n$*, is a solution of (1.1)-(1.2). Furthermore if* Ω *satisfies (2.11), its power satisfies the lower bound (2.12).*

A lower bound for the minimizer $\hat{\phi}$ *without using the interpolation inequality (1.10), can be derived directly by (2.18), by using (2.6) instead. We find from (2.18) that*

$$4\epsilon N R^2 + M R^{2\sigma+2} \geq \Omega R^{2\sigma+2}. \tag{2.24}$$

From (2.24) we find the estimate

$$\left[\frac{\Omega - 4N\epsilon}{M}\right]^{\frac{1}{\sigma}} \leq R^2, \quad \sigma > 0. \tag{2.25}$$

It is our aim in Section 4, to examine by a numerical study if the lower bounds (2.12) and (2.25) can serve as estimates for the threshold on the power of breather solutions (1.4) of (1.1)-(1.2), as well as a comparison with respect to their possible optimal behaviour.

3 Lower bounds for periodic solutions in the the case of sign-changing anharmonic parameters.

We shall extend the results of the previous section to the case of (1.1)-(1.2) with sign-changing anharmonic parameter. Under condition (SG), the DNLS equation (1.1) cannot be considered as focusing or defocusing. The method based on the Mountain Pass Theorem (MPT) [2, Theorem 6.1, pg. 140] will be used also here (see [8]), to establish that there exist nontrivial breathers (1.4).

Theorem 3.1 *We consider the DNLS equation (1.1) assuming that* (SG) *is satisfied. For* $\Omega > 0$ *given, there exists nontrivial* $\phi \in \ell^2(\mathbb{Z}_K^N)$ *such that* $\psi_n(t) = e^{-i\Omega t}\phi_n$*, is a solution of the DNLS equation (1.1). Moreover the power of the nontrivial periodic solution satisfies the lower bounds*

$$\left[\frac{\epsilon\lambda_1 - \Omega}{-\min_{n\in\mathcal{S}_-}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} < R^2, \quad 0 < \Omega < \epsilon\lambda_1 \;\; \sigma > 0, \tag{3.1}$$

$$\left[\frac{\Omega - 4N\epsilon}{\max_{n\in\mathcal{S}_+}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} < R^2, \quad \Omega > 4\epsilon N, \;\; \sigma > 0. \tag{3.2}$$

Proof: As in [8], we shall seek for non-trivial breathers as critical points of C^1-functional $\mathcal{E} : \ell^2 \to \mathbb{R}$ defined as

$$\mathcal{E}(\phi) = \frac{\epsilon}{2}(-\Delta_d\phi, \phi)_2 - \frac{\Omega}{2}\sum_{||n||\leq K}|\phi_n|^2 + \frac{1}{2\sigma+2}\sum_{||n||\leq K}\Lambda_n|\phi_n|^{2\sigma+2}. \tag{3.3}$$

By the differentiability of $\mathcal{E}$, it can be easily checked that any critical point of $\mathcal{E}$ is a solution of

$$(-\Delta_d\phi, \psi)_2 - \Omega(\phi, \psi)_2 = (-\Lambda|\phi|^{2\sigma}\phi, \psi)_2, \;\; \text{for all} \;\; \psi \in \ell^2, \;\; \Lambda = (\Lambda_n)_{||n||\leq K}, \tag{3.4}$$

which in turns, is equivalently, a solution of (1.1).

Clearly $\mathcal{E}[0] = 0$. Next, we shall verify the existence of $z \in \ell^2(\mathbb{Z}_K^N)$, such that $||z||_2^2 = \theta^2 > 0$ satisfying $\mathcal{E}[z] > 0$, which is the first assumption of MPT. We consider

$$\{z_n\}_{n\in\mathbb{Z}_K^N} = \{z_n\}_{n\in\mathcal{S}_+} + \{z_n\}_{n\in\mathcal{S}_-}, \;\; \text{such that} \;\; \left\{\begin{array}{ll} \{z_n\}_{n\in\mathcal{S}_+} & > 0, \\ \{z_n\}_{n\in\mathcal{S}_-} & = 0. \end{array}\right. \tag{3.5}$$

We observe that

$$\begin{aligned} \mathcal{E}[z] &= \frac{\epsilon}{2}(-\Delta_d z, z)_2 - \frac{\Omega}{2}\sum_{n\in\mathcal{S}_+}|z_n|^2 + \frac{1}{2\sigma+2}\sum_{n\in\mathcal{S}_+}\Lambda_n|z_n|^{2\sigma+2} \\ &\geq \frac{\epsilon}{2}(-\Delta_d z, z)_2 - \frac{\Omega}{2}\sum_{n\in\mathcal{S}_+}|z_n|^2 + \frac{\min_{n\in\mathcal{S}_+}\{\Lambda_n\}}{2\sigma+2}\sum_{n\in\mathcal{S}_+}|z_n|^{2\sigma+2} \\ &\geq -\frac{\Omega}{2}\sum_{n\in\mathcal{S}_+}|z_n|^2 + \frac{\min_{n\in\mathcal{S}_+}\{\Lambda_n\}}{2\sigma+2}\sum_{n\in\mathcal{S}_+}|z_n|^{2\sigma+2}. \end{aligned} \tag{3.6}$$

Applying (2.4) for $q = 2\sigma+2$ and $p = 2$, we get that

$$||\phi||_{2\sigma+2}^{2\sigma+2} \geq \frac{1}{(2K+1)^{N\sigma}}||\phi||_2^{2\sigma+2}. \tag{3.7}$$

Combining (3.6) with (3.7) we get that

$$\mathcal{E}[z] \geq -\frac{\Omega}{2}\sum_{n\in\mathcal{S}_+}|z_n|^2 + \frac{\min_{n\in\mathcal{S}_+}\{\Lambda_n\}}{(2\sigma+2)(2K+1)^{N\sigma}}\left(\sum_{n\in\mathcal{S}_+}|z_n|^2\right)^{\sigma+1}. \tag{3.8}$$

Then from (3.8), it follows that the requirement $\mathcal{E}[z] > 0$ holds if z satisfies (3.5) and

$$\theta^2 > \left[\frac{\Omega(2\sigma+2)(2K+1)^{N\sigma}}{2\min_{n\in\mathcal{S}_+}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}}.$$

Now consider some $\chi \in \ell^2(\mathbb{Z}_K^N)$ with $||\chi||_2 = 1$ such that

$$\{\chi_n\}_{n\in\mathbb{Z}_K^N} = \{\chi_n\}_{n\in\mathcal{S}_+} + \{\chi_n\}_{n\in\mathcal{S}_-}, \text{ where } \begin{cases} \{\chi_n\}_{n\in\mathcal{S}_+} & = 0, \\ \{\chi_n\}_{n\in\mathcal{S}_-} & > 0. \end{cases}$$

Setting $\zeta = t\chi \in \ell^2(\mathbb{Z}_K^N)$, for some $t > 0$, we observe that

$$E[\zeta] = \frac{t^2}{2}\epsilon(-\Delta_d\zeta,\zeta)_2 - \frac{\Omega t^2}{2} + \frac{t^{2\sigma+2}}{2\sigma+2}\sum_{n\in\mathcal{S}_-}\Lambda_n|z_n|^{2\sigma+2}. \tag{3.9}$$

Letting now $t \to +\infty$ we get from condition (P), that $\mathcal{E}[t\chi] \to -\infty$. Thus choosing χ as in (3.9) and t sufficiently large, we derive the existence of some $z_1 \in \ell^2(\mathbb{Z}_K^N)$ such that $\mathcal{E}[z_1] < \rho$. Furthermore, since we are restricted in the finite lattice (Z_K^N), the functional $\mathcal{E}$ satisfies Palais-Smale condition [2, Definition 4.1, pg. 130]. Hence, the conditions of MPT are satisfied, justifying the existence of nontrivial breather solution (1.4).

Since the nontrivial critical point ϕ of the functional $\mathcal{E}$ is a solution of (3.4) we may set $\psi = \phi$ in (3.4), to get that

$$\epsilon(-\Delta_d\phi,\phi)_2 - \Omega\sum_{||n||\leq K}|\phi_n|^2 + \sum_{||n||\leq K}\Lambda_n|\phi_n|^{2\sigma+2} = 0. \tag{3.10}$$

From (3.10) we get the inequality

$$\begin{aligned}\sum_{n\in\mathcal{S}_+}\Lambda_n|\phi_n|^{2\sigma+2} + \sum_{n\in\mathcal{S}_-}\Lambda_n|\phi_n|^{2\sigma+2} &= \Omega\sum_{||n||\leq K}|\phi_n|^2 - \epsilon(-\Delta_d\phi,\phi)_2 \\ &\geq (\Omega - 4\epsilon N)\sum_{||n||\leq K}|\phi_n|^2. \end{aligned} \tag{3.11}$$

Assuming that $\Omega > 4\epsilon N$ we get from (3.11) that

$$\sum_{n\in\mathcal{S}_+}\Lambda_n|\phi_n|^{2\sigma+2} > \sum_{n\in\mathcal{S}_-}\{-\Lambda_n\}|\phi_n|^{2\sigma+2}, \ \{-\Lambda_n\}_{n\in\mathcal{S}_-} \geq 0. \tag{3.12}$$

Thus in the case where $\Omega > 4\epsilon N$, the "defocusing part" of the nonlinearity "dominates" in the sense of (3.12). In this case and since $\sum_{n\in\mathcal{S}_-}\{-\Lambda_n\}|\phi_n|^{2\sigma+2} \leq 0$, we deduce that

$$\begin{aligned}(\Omega - 4\epsilon N)\sum_{||n||\leq K}|\phi_n|^2 &\leq \sum_{n\in\mathcal{S}_+}\Lambda_n|\phi_n|^{2\sigma+2} + \sum_{n\in\mathcal{S}_-}\Lambda_n|\phi_n|^{2\sigma+2} \\ &< \sum_{n\in\mathcal{S}_+}\Lambda_n|\phi_n|^{2\sigma+2} \\ &< \max_{n\in\mathcal{S}_+}\{\Lambda_n\}\sum_{n\in\mathcal{S}_+}|\phi_n|^{2\sigma+2} \\ &< \max_{n\in\mathcal{S}_+}\{\Lambda_n\}\sum_{||n||\leq K}|\phi_n|^{2\sigma+2}. \end{aligned} \tag{3.13}$$

Using (2.4) and (3.13), we find the lower bound

$$\left[\frac{\Omega - 4N\epsilon}{\max_{n\in\mathcal{S}_+}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} < R^2.$$

On the other hand, when the "focusing part" dominates in the sense of

$$\sum_{n\in\mathcal{S}_+} \Lambda_n|\phi_n|^{2\sigma+2} < \sum_{n\in\mathcal{S}_-} \{-\Lambda_n\}|\phi_n|^{2\sigma+2}, \tag{3.14}$$

we get from (3.11) that

$$\left(\frac{\Omega}{4N} - \epsilon\right)(-\Delta_d\phi, \phi)_2 \leq \Omega \sum_{||n||\leq K} |\phi_n|^2 - \epsilon(-\Delta_d\phi, \phi)_2 < 0, \tag{3.15}$$

due to (2.6). Thus (3.14) holds when the frequency of the breather solution satisfies

$$\Omega < 4\epsilon N. \tag{3.16}$$

By using (2.6), we get from (3.11) and (3.15) that

$$\begin{aligned}
(\epsilon\lambda_1 - \Omega)\sum_{||n||\leq K} |\phi_n|^2 &\leq \epsilon(-\Delta_d\phi, \phi)_2 - \Omega \sum_{||n||\leq K} |\phi_n|^2 \\
&= -\sum_{n\in\mathcal{S}_+} \Lambda_n|\phi_n|^{2\sigma+2} - \sum_{n\in\mathcal{S}_-} \Lambda_n|\phi_n|^{2\sigma+2} \\
&\leq \sum_{n\in\mathcal{S}_-} \{-\Lambda_n\}|\phi_n|^{2\sigma+2} \\
. &\leq -\min_{n\in\mathcal{S}_-}\{\Lambda_n\} \sum_{||n||\leq K} |\phi_n|^{2\sigma+2}.
\end{aligned} \tag{3.17}$$

Condition (3.16), implies that $\Omega < \epsilon\lambda_1$. In this case, we may infer from (3.17) the lower bound

$$\left[\frac{\epsilon\lambda_1 - \Omega}{-\min_{n\in\mathcal{S}_-}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} < R^2.$$

Finally, when

$$\sum_{n\in\mathcal{S}_+} \Lambda_n|\phi_n|^{2\sigma+2} = \sum_{n\in\mathcal{S}_-} \{-\Lambda_n\}|\phi_n|^{2\sigma+2}, \tag{3.18}$$

i.e. $\sum_{||n||\in\mathcal{S}_+} \Lambda_n|\phi_n|^{2\sigma+2} = 0$, then from (3.11) we get that

$$\begin{aligned}
-\Delta_d\phi_n &= \Omega\phi_n, \ \ ||n|| \leq K, \\
\phi_n &= 0, \ \ ||n|| > K.
\end{aligned}$$

Thus when (3.18), it follows that Ω is an eigenvalue of the Discrete Laplacian, and ϕ behaves as a corresponding eigensolution of the discrete eigenvalue problem. $\diamond$

Remark 3.1 Working exactly as in the proof of the estimate (2.12) we may replace the estimate (3.2) of the case $\Omega > 4\epsilon N$, by

$$\mathcal{R}_{\mathrm{thresh}} \cdot \left[\frac{\Omega - 4N\epsilon}{4\epsilon M_1 N(\sigma+1)}\right]^{\frac{1}{\sigma}} \leq R^2, \ \ M_1 = \max_{||n||\leq K} |\Lambda_n| \tag{3.19}$$

which is the extension of the estimate (2.12) in the case of sign-changing anharmonic parameters.

Remark 3.2 Setting $\Omega = 0$ in (3.6), (3.8) as well as in (3.9), it can be easily checked that Theorem 3.1 can be used for the proof of existence of nontrivial steady state solutions of (1.1)-(1.2) under condition (SC) for the anharmonic parameter, i.e. solutions of the problem

$$-\epsilon(\Delta_d\phi)_n = -\Lambda_n|\phi_n|^{2\sigma}\phi_n, \ \ \Omega > 0, \ \ ||n|| \leq K, \tag{3.20}$$

$$\phi_n = 0, \ ||n|| > K. \tag{3.21}$$

The result of Theorem 3.1 if combined with [8, Theorem 2.6, pg.125] establishes the existence of periodic solutions (1.4) for any $\Omega \in \mathbb{R}$. Moreover, it is straightforward to check that inequality (3.17) is valid for $\Omega < 0$. Thus the lower bound (3.1) for the power of periodic solutions (1.4) is valid for any in $\Omega \in (-\infty, \epsilon\lambda_1)$, that is

$$\left[\frac{\epsilon\lambda_1 - \Omega}{-\min_{n\in\mathcal{S}_-}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} < R^2, \ \ \Omega \in (-\infty, \epsilon\lambda_1), \ \ \sigma > 0. \tag{3.22}$$

4 Numerical studies of the lower bounds.

We perform a numerical study to test the lower bounds derived in the previous sections. This numerical study consists in checking that the power of a numerically calculated breather is higher than the theoretical thresholds estimates. To this end, we consider single site breathers (i.e. localized solutions with only one excited site at the anti-continuous limit, $\epsilon = 0$), which are the lowest power solutions.

Figures 1-4 refers to the cases $(\sigma = 2, N = 1, \epsilon = 0.25)$, $(\sigma = 1, N = 2, \epsilon = 0.15)$, $(\sigma = 10, N = 1, \epsilon = 0.25)$ and $(\sigma = 2, N = 2, \epsilon = 0.15)$, respectively. All the cases consider the value $\sigma \geq \frac{2}{N}$ of Theorem 1.1, where the excitation threshold appears.

Figure 1 shows the power of a family of single site breathers together with the corresponding threshold estimates (2.12), (2.25), for a homogeneous lattice ($\Lambda_n = 1 \ \forall n$). The inset in each picture is a numerical verification of Theorem 1.1, demonstrating the region where the numerical power of periodic solutions (1.9) of the focusing DNLS (1.6) for the same values of σ, N, ϵ, reaches the minimum value $\mathcal{R}_{\rm thresh}$. These numerical values have been inserted in the estimate (2.12). The numerical study shows that the numerical power of periodic solutions (1.4) of the defocusing DNLS (1.1)-(1.2), fulfills the estimates. *It can also be remarked, that the numerical studies indicate that*

$$\textit{lower bound (2.12)} < \textit{lower bound (2.25)}. \tag{4.1}$$

From this numerical observation and the appearance of $\mathcal{R}_{\rm thresh}$ *in (2.12), we may guess an explicit upper bound for* $\mathcal{R}_{\rm thresh}$*,*

$$\mathcal{R}_{\rm thresh} < [4\epsilon N(\sigma+1)]^{\frac{1}{\sigma}}, \ \ \sigma \geq \frac{2}{N}. \tag{4.2}$$

Testing the estimate with the values for the parameters in figure 1, we get for (a) $\mathcal{R}_{\rm thresh} < 1.732$*, for (b)* $\mathcal{R}_{\rm thresh} < 2.4$*, for (c)* $\mathcal{R}_{\rm thresh} < 1.270$ *and for (c)* $\mathcal{R}_{\rm thresh} < 1.897$*. In all cases the numerical calculated* $\mathcal{R}_{\rm thresh}$ *satisfies the above estimates. We remark that in the vicinity of* $\Omega = 1$*, the numerical power tends to infinity when* $N = 1$ *and* $\sigma > 2$ *and to a finite value for the cases* $N = 1$*,* $\sigma = 2$ *and* $N = 2$*,* $\sigma \geq 1$*. Explanations for this behavior are not straightforward, we refer to [12] for a detailed discussion.*

Figure 2, demonstrates the results of the numerical study for the DNLS (1.1)-(1.2) for the case of a single nonlinear impurity $\Lambda_n = \delta_{n,0}$. For the estimate (2.12) the values of $R_{\rm thresh}$ of figure 1 have been used. As it is shown, both theoretical estimates can serve as satisfactory predictions of a lower bound for the numerical power of the breathers. In comparison with the case of constant anharmonic parameter, the accuracy of both estimates is increased. In this case also (4.1) is also satisfied.

Figure 3 present the results of a numerical study for a DNLS lattice with sign-changing anharmonic parameter. We choose as an example, a random DNLS lattice (1.1)-(1.2). The random site dependent anharmonic parameter Λ_n is given by a random uniform distribution of $+1$ and -1. The figure shows the numerical power of breathers against the estimates (3.2) and (3.19) (here $M_1 = \max_{||n||\leq K}|\Lambda_n| = 1$), for the random DNLS lattice. Both figures justify that both theoretical estimates, are fulfilled as a lower bounds for the power of breathers with frequency $\Omega > 4\epsilon N$, also in the case of the random DNLS lattice.

The results of the numerical study checking the estimate (3.1) and especially (3.22) for the random DNLS lattice, are presented in figure 4. For $\Omega < 0$ as well as for the case $0 \leq \Omega < \epsilon\lambda_1$, it follows that the lower bound (3.22) gives satisfactory quantitative predictions for lower bounds on the real power of the breathers of

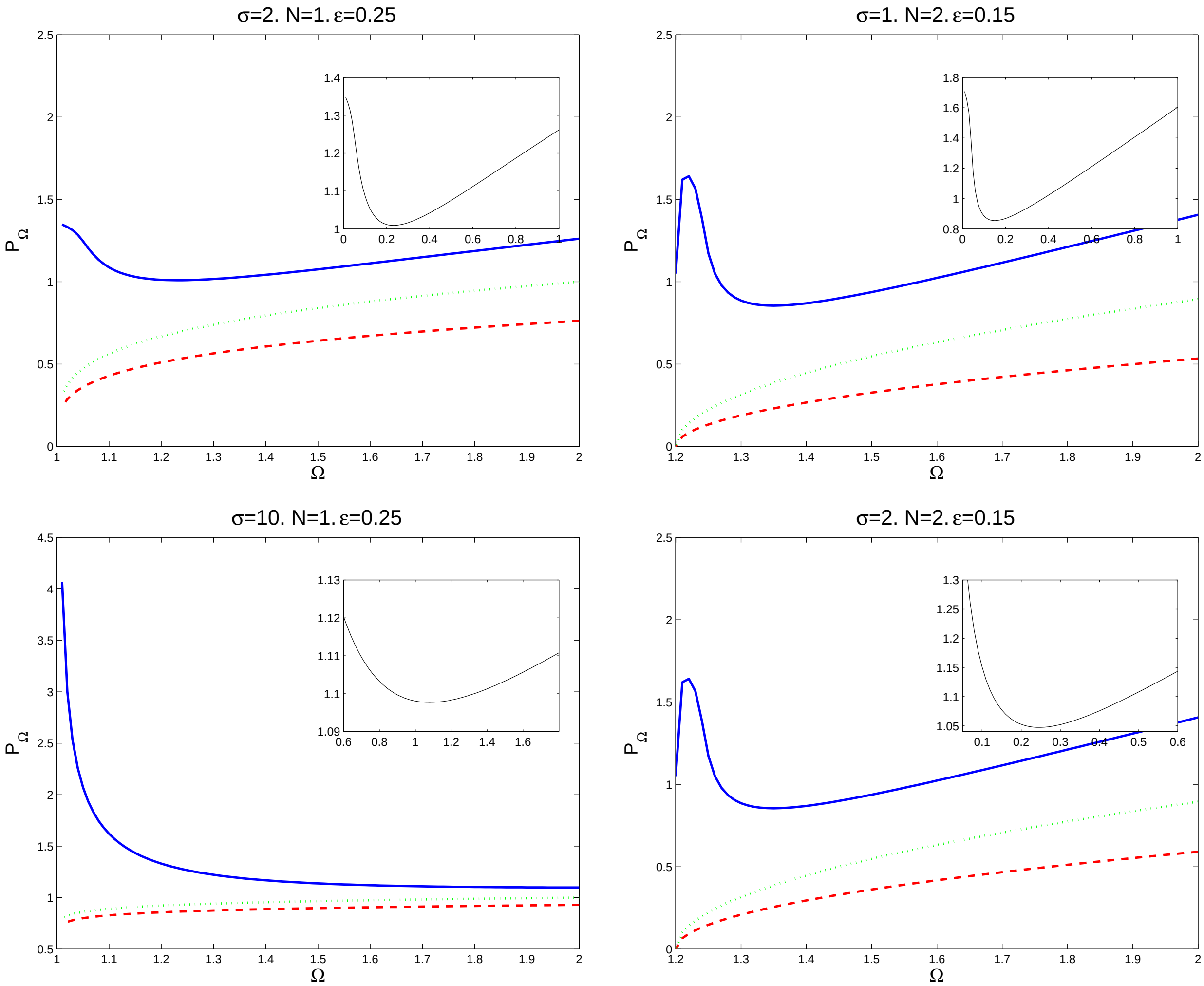

Figure 1: Numerical power for solutions (1.4), of the *defocusing* DNLS (1.1)-(1.2), with constant anharmonic parameter $\Lambda_n = 1$. (a) $\sigma = 2$, $N = 1$ ($\sigma = \frac{2}{N}$), (b) $\sigma = 1$, $N = 2$ ($\sigma = \frac{2}{N}$), (c) $\sigma = 10$, $N = 1$ ($\sigma > \frac{2}{N}$), (d) $\sigma = 2$, $N = 2$ ($\sigma > \frac{2}{N}$). The inset in each case, shows a magnification of the region where the power of periodic solutions (1.9) of the *focusing* DNLS (1.6), reaches its minimum value. In case (a), $\mathcal{R}_{\rm thresh} = 1.009$, in case (b), $\mathcal{R}_{\rm thresh} = 0.855$, in case (c), $\mathcal{R}_{\rm thresh} = 1.098$ and in case (d), $\mathcal{R}_{\rm thresh} = 1.047$. Full line corresponds to the numerical calculated single site breathers, dashed line to the estimate (2.12) and dotted line to the estimate (2.25).

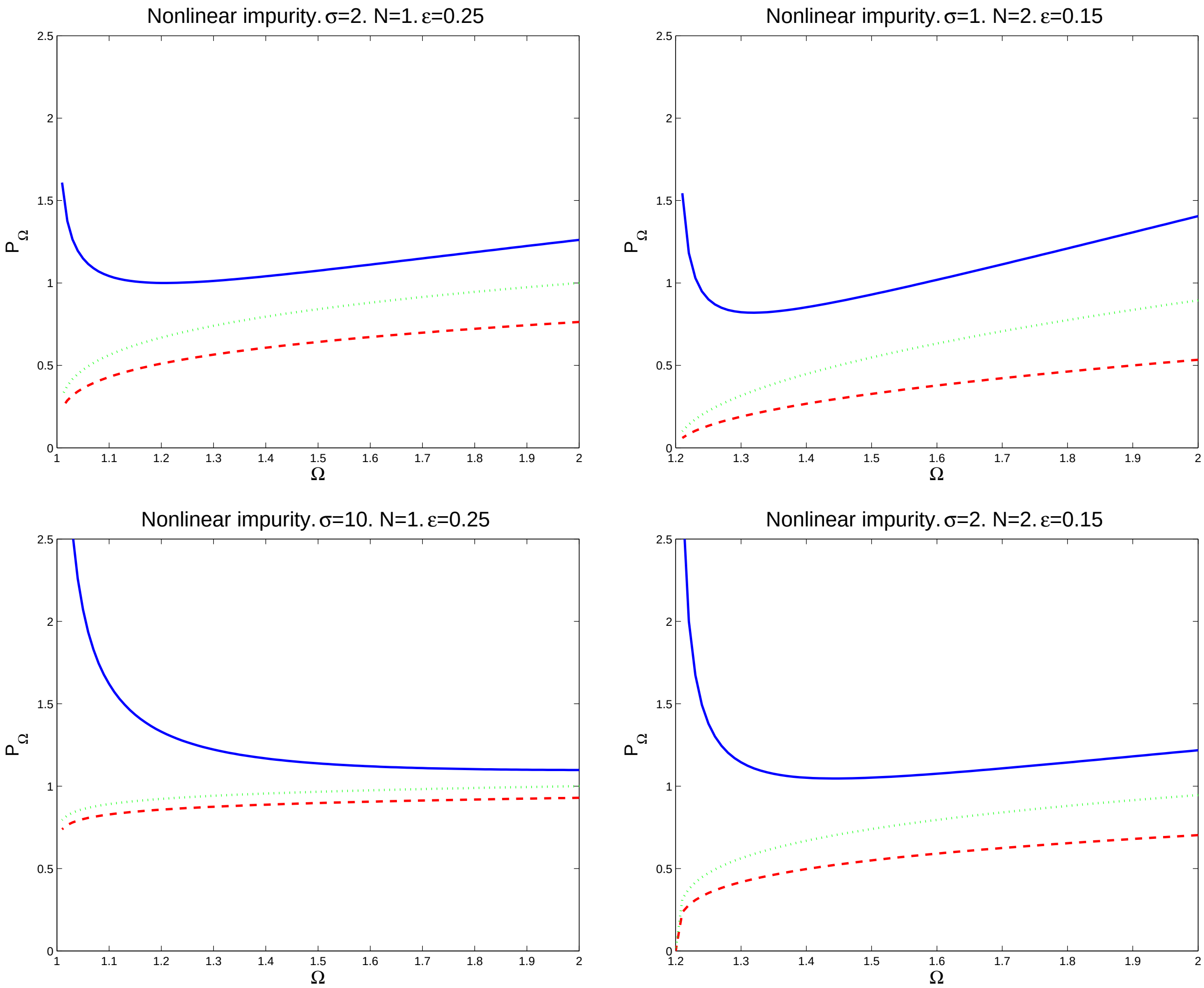

Figure 2: Numerical power for single site breathers centered at the nonlinear impurity site (1.4), of the *defocusing* DNLS (1.1)-(1.2) with a nonlinear impurity $\Lambda_n = \delta_{n,0}$.

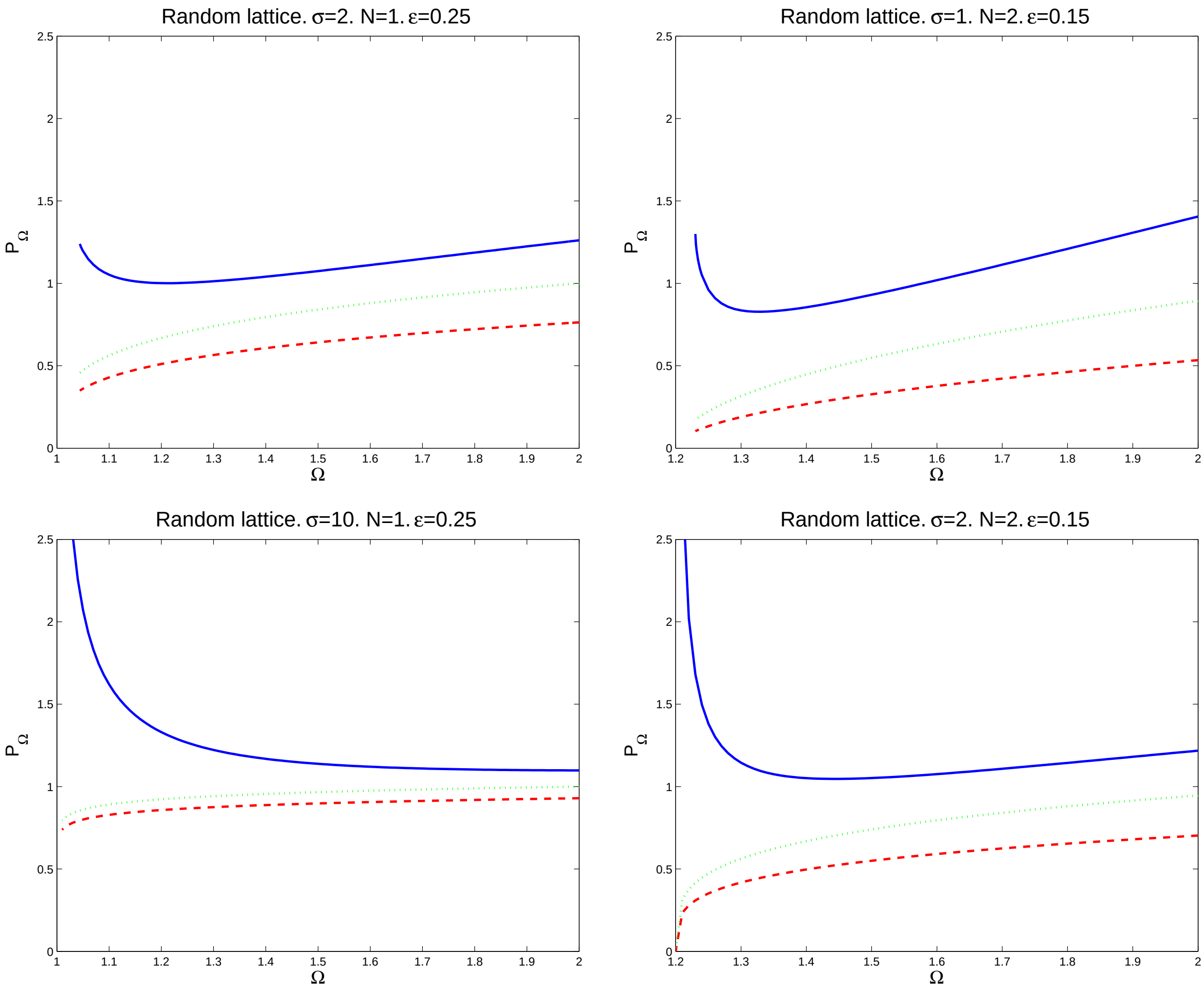

Figure 3: Numerical power for solutions (1.4) for the random DNLS lattice (1.1)-(1.2) against the theoretical estimates (3.2) and (3.19). The numerical solutions are single site breathers centered at $n = 0$, for which $\Lambda_n = +1$.

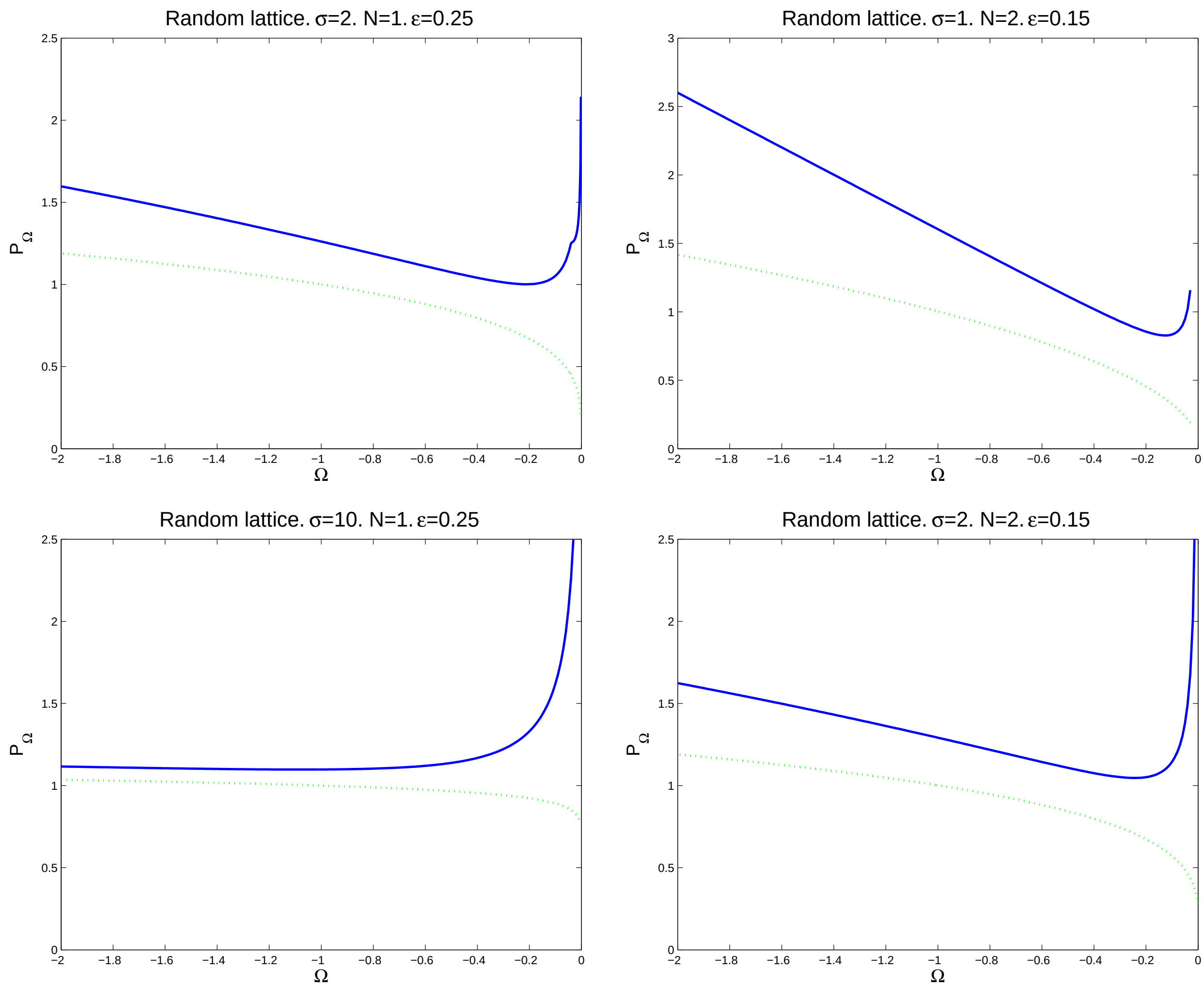

Figure 4: Numerical power for solutions (1.4) for the random DNLS lattice (1.1)-(1.2) against the theoretical estimate (3.22). The numerical solutions are single site breathers centered at $n = 1$, for which $\Lambda_n = -1$.

the random DNLS lattice. Notice that the Ω is always below 0 because single site breathers in random lattices always bifurcate with another breather solution for $\Omega < 0$ (see Refs. [20] and [21]). We also refer to [19], on the application of numerical methods, for calculating power thresholds of localized excitations in DNLS lattices.

Remark 4.1 *The results of [17] prove the existence of an excitation threshold, which appears for the case $\sigma \geq 2/N$, as well the existence of a frequency $\omega^* > 0$ on which this threshold value on the power is achieved. The corresponding solution $\psi_n(t) = e^{i\omega^* t}\phi_n$ is a ground state having power $\mathcal{P}_{\mathrm{thresh}}$-the excitation threshold value. However, the thresholds we have calculated in the paper are "local" ones, i.e. they are value above which the power of each breather with given Λ_n, ϵ, σ, and Ω must be. On the other hand, noting that the numerical power approaches in a quite sharp manner the theoretical estimates, for "limiting" large values of of the nonlinearity exponent $\sigma > 2/N$ (as it is observed in the case $\sigma = 10$) and large frequencies, can be considered also as "global" in the sense that they predict the smallest value a breather can have for any Ω, σ, N satisfying the assumptions for the derivation of the estimates. We remark that similar "global" bounds have been shown in [3] for the case $\sigma < 2/N$ which is the case of nonexistence of the excitation threshold of [17], as well as for the saturable nonlinearity.*

Finally, we note that the phonon band of the defocusing DNLS equation extends to the interval $[0, 4N\epsilon]$. Then breathers frequencies must lie in the intervals $\Omega > 4N\epsilon$, or $\Omega < 0$. It is the former case which we consider in this paper (except in Figure 4, where the latter is considered).

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