Energy thresholds for the existence of breather solutions and traveling waves on lattices. *

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Abstract

We discuss the existence of breathers and of energy thresholds for their formation in DNLS lattices with linear and nonlinear impurities. In the case of linear impurities we present some new results concerning important differences between the attractive and repulsive impurity which is interplaying with a power nonlinearity. These differences concern the coexistence or the existence of staggered and unstaggered breather profile patterns.

We also distinguish between the excitation threshold (the positive minimum of the power observed when the dimension of the lattice is greater or equal to some critical value) and explicit analytical lower bounds on the power (predicting the smallest value of the power a discrete breather one-parameter family), which are valid for any dimension. Extended numerical studies in one, two and three dimensional lattices justify that the theoretical bounds can be considered as thresholds for the existence of the frequency parametrized families.

The discussion reviews and extends the issue of the excitation threshold in lattices with nonlinear impurities while lower bounds, with respect to the kinetic energy, are also discussed for traveling waves in FPU periodic lattices.

1 Introduction

The *energy threshold* for the formation of a discrete breather in a nonlinear lattice [7], is defined as the positive lower energy bound possessed by the breather. This definition was given in the remarkable paper of S. Flach, K. Kladko and R. MacKay [6]. They considered a generic class of Hamiltonian systems and showed by heuristic and numerical arguments that the energy of a discrete breather family has a positive lower bound for lattice dimension N greater than or equal to some critical dimension N_c. On the other hand, when $N < N_c$ the energy goes to zero as the amplitude goes to zero. It was further predicted that the critical dimension N_c depends on details of the system but is typically 2 and never greater than 2. Furthermore, for $N > N_c$, the minimum in energy should occur at positive amplitude and finite localization length.

Particular examples concerning the studies of [6] are the discrete nonlinear Schrödinger equation DNLS and the nonlinear Klein-Gordon lattice (DKG). For the DNLS equation [5, 12],

$$\mathrm{i}\dot{\psi}_n + \epsilon(\Delta_d\psi)_n + |\psi_n|^{2\sigma}\psi_n = 0, \ \ \sigma > 0, \ n = (n_1, n_2, \ldots, n_N) \in \mathbb{Z}^N, \tag{1.1}$$

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the results of [6] were rigorously justified by M. Weinstein in the key work [22]. 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

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

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

In [22], the existence of the energy *excitation threshold* was proved through the consideration of the constrained minimization problem

$$\mathcal{I}_{\mathcal{R}} = \inf\left\{\mathcal{H}[\phi] \;:\; \mathcal{P}[\phi] = R\right\}, \tag{1.3}$$

where $\mathcal{H}[\phi]$ and $\mathcal{P}[\phi]$ are the fundamental conserved quantities

$$\mathcal{H}[\phi] \;=\; \epsilon(-\Delta_d\phi, \phi)_2 - \frac{1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}|\phi_n|^{2\sigma+2}, \tag{1.4}$$

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

the Hamiltonian and the power, respectively. For instance, it was proved in [22, Theorem 3.1, pg. 678] that if $0 < \sigma < \frac{2}{N}$, the variational problem (1.3) has a solution for all $\mathcal{R} > 0$ and there is no excitation threshold. On the other hand, *when* $\sigma \geq \frac{2}{N}$*, there exists an excitation threshold* $\mathcal{R}_{\rm thresh}$ such that *(a) if* $\mathcal{R} > \mathcal{R}_{\rm thresh}$ *then* $\mathcal{I}_{\mathcal{R}} < 0$*, and a solution of (1.3) exists* and *(b) if* $\mathcal{R} < \mathcal{R}_{\rm thresh}$ *then* $\mathcal{I}_{\mathcal{R}} = 0$*, and there is no solution (i.e a ground state minimizer) of (1.3).*

Actually, when $-\infty < \mathcal{I}_{\mathcal{R}} < 0$ the infimum in (1.3) is attained. On the other hand, when $\mathcal{I}_{\mathcal{R}} \geq 0$ it follows that $\mathcal{I}_{\mathcal{R}} = 0$ (see [22, Proposition 3.1, pg. 679]) and there is no ground state minimizer (see [22, Proposition 4.2 (d), pg. 680].

In the light of the results of Weinstein, the critical dimension predicted by Flach, Kladko and MacKay could be defined from (1.1) as

$$N_c = \frac{2}{\sigma}. \tag{1.6}$$

However such a definition has a meaning in DNLS when it gives integer values of $N_c \geq 1$. Restricted to integer values of σ, we get that $N_c = 2$ for $\sigma = 1$ and $N_c = 1$ for $\sigma = 2$ in consistence with the predictions of [7]. When $\sigma \geq 3$, N_c from (1.6) is not an integer, however it suggests that $N_c = 1$. This implementation for integer values of σ is consistent with the predictions of [7] and in equivalence with the definition of the critical exponent (1.1). It is also verified by the numerical studies of [2, 3] and of the present paper. It is important to mention that the critical dimension N_c can be greater than 2 for a large classes of Hamiltonian systems, as it is reported in [11].

The excitation energy threshold concerns "breathers" as time-periodic solutions

$$\begin{aligned} \psi_n(t) &= e^{\mathrm{i}\omega t}\phi_n,\ \omega > 0,\ \ n \in \mathbb{Z}^N,\ \ t \in \mathbb{R}, \\ \phi_n &\in \ell^2, \end{aligned} \tag{1.7}$$

spatially localized since $\phi_n \to 0$ as $|n| \to \infty$ (as an element of ℓ^2-here $|n| = \max_{1\leq i\leq N}|n_i|$). Actually $\mathcal{R}_{\rm thresh}$ corresponds to *a minimum on the power* attained by the ground-state breather $\psi_n(t) = e^{\mathrm{i}\omega_c t}\phi_n$ for a certain ω_c (as a Lagrange multiplier associated to the ground state minimizer ϕ_n of (1.3)).

A different type of lower bounds on the power of DB for DNLS systems but with the same flavor in applications, was derived in our recent works [2, 3]. Using simple arguments based on variational methods [1] or fixed point theorems [10] to establish the existence of solutions (1.7), we were able to show the existence of *explicitly given* lower bounds on the power of breathers on either finite or infinite DNLS lattices and for different types of nonlinearities (saturable or power). Although some of them depend explicitly on the dimension, a major difference with the excitation threshold of [6, 22] existing only when $N > N_c$, is that they are valid for any dimension. Thus they do not predict the energy threhshold of [6, 22] but actually the smallest value of the power a DB can have: no periodic localized solution can have power less than the prescribed estimates. This difference becomes evident in the case of the power nonlinearity and in the case where $\sigma < 2/N$, the case where the excitation threshold of [6, 22] do not exists: The numerical studies of [2, 3] established the existence of breathers of small frequencies with power very close to the theoretical estimates, the latter becoming sharp especially for small values of σ. On the other hand, when $\sigma > 2/N$, the theoretical estimates become sharp for the power of breathers associated with large values of σ and large frequencies. Similar findings hold also for the DNLS with saturable nonlinearity. Due to these reasons it is necessary to distinguish these lower bounds from the excitation energy threshold of [6, 22].

The lower bounds are "local" in the sense that they are predicting the smallest value of power a breather can have for any given frequency ω. Thus the explicit lower bounds can be useful as a theoretical estimation from below of the minimal power (or energy) of localized excitations of prescribed frequency ω, for arbitrary values of σ, N. This fact has been justified in the examples considered in [2, 3]: Tracing out the theoretical estimates varying ω it has been justified that the lower bounds are satisfied by the DB families considered (parametrized by frequency) and in a sharp manner in many cases and members of the DB families, especially in the case where the excitation threshold do not appears.

Our aim in this work is to discuss possible extensions of our observations on the lower bounds for the energy of DB in two classes of *inhomogeneous* DNLS systems as well as to other localized structures such as traveling waves in FPU lattices. In the context of the DNLS, an important example is that of the interplay of a focusing power nonlinearity with a linear impurity, discussed in Section 2. Such mechanisms are often responsible for the excitation of impurity modes, which are spatially localized oscillatory states at the impurity sites. Our motivation was initiated from [17] and the numerous physical applications listed (arising from superconductors and the dynamics of electron-phonon interactions, to the defect modes in photonic crystals). We consider both the attractive and the repulsive impurity cases. For the existence of nontrivial breathers, we follow two alternative but equivalent approaches. For the focusing case we follow the variational approach via the mountain pass theorem and prove some first lower bounds on the power. Although the defocusing case can be reduced to the focusing one but with the opposite sign of the impurity (under a staggering transformation), the alternative approach of constrained minimization problems *revealed new and interesting conditions on the existence of breathers.* For instance, a vast difference between the attractive and the repulsive case is verified: while the repulsive case is associated only with the existence of staggered patterns, in the repulsive case we derive sufficient conditions on the the impurity parameter for the coexistence of both staggered and unstaggered patterns (Theorem 2.7-Remark 2.8). We remark that such a scenario was demonstrated in [9] for Klein-Gordon lattices. As in the mountain pass approach, the constrained minimization of the defocusing case comes together with the derivation of the lower bounds on the power of the staggered patterns in the repulsive case and the coexisting staggered and unstaggered patterns in the attractive one.

The numerical studies performed, not only verify that the lower bounds are satisfied but also justify that these exact values can be fairly used as a sharp approximation of the smallest possible value of the power in the lattice as the limiting case of small σ, ω indicate. *This limiting case is also in accordance with the observations and analysis of [6], on the behavior of DB families in the small amplitude limit.*

In the light of the numerical findings of Section 2, we continue in Section 3 the study of the DNLS lattice with nonlinear impurities [14, 15, 16, 21], initiated in [3]. We review the existence proof of the excitation threshold by generalizing the concentration compactness arguments of [22], to the most general case of sign-changing nonlinear impurities. To emphasize the differences between the excitation thresholds and the lower bounds on the power, the latter derived in [3] are also reviewed numerically in the case of nonlinearity exponents where the excitation threshold do not appears. This numerical study verifies that the value of the findings of Section 2, are justified for the DNLS with nonlinear impurities. The particular examples we consider are that of a DNLS lattice with a single and a sign changing impurity.

The thresholds of the nature discussed in the present paper can be derived alternatively by using fixed point arguments. This approach has been proved useful for the treatment of the saturable DNLS [2]. Apart from the DNLS lattices, we claim that these methods can be useful in the study of energy thresholds for other interesting localized structures in nonlinear lattices. As a first step to these extensions we derive a lower bound on the energy for traveling waves in Fermi-Pasta-Ulam (FPU) lattices. The lower bound concerns the average kinetic energy of the traveling wave for the standard polynomial anharmonic potential which includes the classical FPU study as a special case. The FPU system is considered in a periodic lattice and the lower bound concerns waves of given speed $c > c^*$. The value c^* is given explicitly, and as the lower bound, depends also on the number of lattice sites. The condition $c > c^*$ although stronger is in consistency with the restrictions imposed by the analytical results of [8, 23]. The derivation of the lower bound and its discussion is given in Section 4.

2 Existence of localized modes in finite DNLS lattices with local inhomogeneity.

This section is devoted to the DNLS model with a local inhomogeneity studied in [17], supplemented with Dirichlet boundary conditions

$$\begin{aligned} \mathrm{i}\dot{\psi}_n &+ \epsilon(\Delta_d\psi)_n + \chi_n\psi_n + \gamma|\psi_n|^{2\sigma}\psi_n = 0, \;\; ||n|| \leq K, && (2.1)\\ \psi_n &= 0, \;\; ||n|| > K, && (2.2) \end{aligned}$$

where $||n|| = \max_{1\leq i\leq N}|n_i|$ for $n = (n_1, n_2, \ldots, n_N) \in \mathbb{Z}^N$. Here $\gamma \in \mathbb{R}$ is the the anharmonicity parameter.

Problem (2.1)-(2.2) *will be treated by appropriate variatonal methods.* For the impurity χ, we consider two possible alternative cases:

(A) (*Attractive impurity*) $\chi_n > 0$, for all $n \in \mathbb{Z}^N_K$.

(R) (*Repulsive impurity*) $\chi_n < 0$, for all $n \in \mathbb{Z}^N_K$.

The case of *a single linear impurity (or single point defect)* $\chi_n = \alpha\delta_{n,n_0}$ can be treated with almost identical manner as the attractive and the repulsive impurity. This example will serve for testing numerically the theoretical results which will be presented in this section.

Preliminaries. For convenience to the reader, we recall from [2, 3] some preliminary information on various norms and quantities, that will be thoroughly used in the sequel.

The finite dimensional problem (2.11)–(2.12) is formulated in the finite dimensional subspaces of the sequence spaces ℓ^p, $1 \leq p \leq \infty$,

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

Note that in the case of the infinite lattice $\mathbb{Z}^N$

$$\begin{aligned} ||\phi||_q &\leq ||\phi||_p, \;\; 1 \leq p \leq q \leq \infty && (2.4)\\ 0 \leq \epsilon(-\Delta_d\phi, \phi)_2 &\leq 4\epsilon N \sum_{n\in\mathbb{Z}^N} |\phi_n|^2. && (2.5) \end{aligned}$$

For the finite dimensional subspaces it is needless to say that $\ell^p(\mathbb{Z}^N_K) \equiv \mathbb{C}^{(2K+1)^N}$, endowed with the norm

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

and that the well known equivalence of norms ,

$$||\phi||_q \leq ||\phi||_p \leq (2K+1)^{\frac{N(q-p)}{qp}}||\phi||_q, \;\; 1 \leq p \leq q < \infty, \tag{2.6}$$

holds. For an $1D$-lattice $n = 1, \ldots, K$, the eigenvalues of the discrete Dirichlet Laplacian $-\Delta_d\phi = \lambda\phi$, with ϕ real, are given explicitly by

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

In the case of the N-dimensional discrete Laplacian, the eigenvalues are:

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

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

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

Restricting the variational characterization of the eigenvalues of the discrete Laplacian in the finite dimensional subspaces $\ell^2(\mathbb{Z}_K^N)$, it follows that $\lambda_1 > 0$, can be characterized as

$$\lambda_1 = \inf_{\substack{\phi \in \ell^2(\mathbb{Z}_K^N) \\ \phi \neq 0}} \frac{(-\Delta_d \phi, \phi)_2}{\sum_{||n|| \leq K} |\phi_n|^2}. \tag{2.7}$$

Then (2.7) implies the inequality

$$\epsilon \lambda_1 \sum_{||n|| \leq K} |\phi_n|^2 \leq \epsilon(-\Delta_d \phi, \phi)_2 \leq 4\epsilon N \sum_{||n|| \leq K} |\phi_n|^2. \tag{2.8}$$

From (2.8), we find directly that λ_1 satisfies the bound

$$\lambda_1 \leq 4N. \tag{2.9}$$

Of course, the upper bound (2.9) follows also from the explicit formula for λ_1 given above.

2.1 Mountain pass approach in the focusing case $\gamma > 0$.

In the focusing case $\gamma > 0$, substituting the time-periodic solution

$$\psi_n(t) = e^{\mathrm{i}\Omega t} \phi_n, \quad \Omega \in \mathbb{R}, \tag{2.10}$$

to (2.1), the stationary analogue of (2.1) reads as

$$\begin{aligned} -\epsilon(\Delta_d \phi)_n &+ \Omega \phi_n - \chi_n \phi_n = \gamma |\phi_n|^{2\sigma} \phi_n, \quad ||n|| \leq K, && (2.11) \\ \phi_n &= 0, \; ||n|| > K. && (2.12) \end{aligned}$$

Attractive impurity. Motivated by [17, page 3] and considering the *case of the anticontinuum limit* $\epsilon = 0$, *it follows directly that the attractive impurity* (A) *only supports time-periodic solutions (2.10) with* $\Omega > 0$. We have the following

Theorem 2.1 *(Unstaggered patterns) We consider the DNLS equation (2.1) assuming that* (A) *is satisfied. If*

$$\max_{n \in \mathbb{Z}_K^N} \chi_n < \Omega, \tag{2.13}$$

there exists a nontrivial $\phi \in \ell^2(\mathbb{Z}_K^N)$ *such that* $\psi_n(t) = e^{\mathrm{i}\Omega t}\phi_n$, $\Omega > 0$ *is a solution of the DNLS equation (2.1). Moreover the power of the nontrivial unstaggered periodic solution satisfies the lower bound*

$$\left[\frac{\epsilon\lambda_1 + \Omega - \max_{n \in \mathbb{Z}_K^N} \chi_n}{\gamma}\right]^{\frac{1}{\sigma}} < R^2. \tag{2.14}$$

Proof: We shall follow the variational (minimax) approach of [3, 10]. For instance we seek non-trivial breathers as critical points of C^1-functional $\mathcal{E} : \ell^2 \to \mathbb{R}$ defined as

$$\mathcal{E}(\phi) = \frac{\epsilon}{2}(-\Delta_d \phi, \phi)_2 + \frac{\Omega}{2} \sum_{||n|| \leq K} |\phi_n|^2 - \frac{1}{2} \sum_{||n|| \leq K} \chi_n |\phi_n|^2 - \frac{\gamma}{2\sigma + 2} \sum_{||n|| \leq K} |\phi_n|^{2\sigma+2}, \tag{2.15}$$

showing their existence by the mountain pass Theorem (MPT). It can be verified as in [2, 3, 10] that $\mathcal{E}$ is a $C^1(\ell^2(\mathbb{Z}_K^N), \mathbb{R})$-functional. Since we are in a discrete setting it follows directly that any critical point of $\mathcal{E}$ is a solution of (2.1).

We proceed by verifying that $\mathcal{E}$ possesses the mountain pass geometry. Since $\mathcal{E}(0) = 0$, we seek next for the existence of $z \in \ell^2(\mathbb{Z}_K^N)$ with $||z||_2^2 = \theta^2$, satisfying $\mathcal{E}(z) > 0$. Now from (2.6), (2.8) and (2.13) we have that

$$\begin{aligned} \mathcal{E}(z) &\geq \frac{\epsilon}{2}(-\Delta_d z, z)_2 + \frac{\Omega}{2} \sum_{||n|| \leq K} |z_n|^2 - \frac{\max_{n \in \mathbb{Z}_K^N} \chi_n}{2} \sum_{||n|| \leq K} |z_n|^2 - \frac{\gamma}{2\sigma + 2} \sum_{||n|| \leq K} |z_n|^{2\sigma+2} \\ &\geq \left(\epsilon\lambda_1 + \Omega - \max_{n \in \mathbb{Z}_K^N} \chi_n\right) \frac{\theta^2}{2} - \frac{\gamma \theta^{2\sigma+2}}{2\sigma + 2}. && (2.16) \end{aligned}$$

Then, it follows from (2.16) that if condition (2.13) holds, there exists $z \in \ell^2(\mathbb{Z}_K^N)$ with norm $||z||_2^2 = \theta^2$ satisfying

$$\left[\left(\frac{\sigma+1}{\gamma}\right)(\epsilon\lambda_1 + \Omega - \max_{n\in\mathbb{Z}_K^N} \chi_n)\right]^{\frac{1}{\sigma}} > \theta^2,$$

for which $\mathcal{E}(z) > 0$. We consider next the element $\zeta = t\eta \in \ell^2(\mathbb{Z}_K^N)$, for some $t > 0$ and $\eta \in \ell^2(\mathbb{Z}_K^N)$ with $||\eta||_2 = 1$ and we observe that

$$E(\zeta) = \frac{t^2}{2}\epsilon(-\Delta_d\eta,\eta)_2 + \frac{\Omega t^2}{2} - \frac{t^2}{2}\sum_{||n||\leq K}\chi_n|\eta_n|^2 - \frac{\gamma t^{2\sigma+2}}{2\sigma+2}\sum_{||n||\leq K}|\eta_n|^{2\sigma+2}. \tag{2.17}$$

Taking the limit as $t \to +\infty$ we get from condition (A), that $\mathcal{E}(t\eta) \to -\infty$. Thus, we derive the existence of $\zeta \in \ell^2(\mathbb{Z}_K^N)$ such that $\mathcal{E}[\zeta] < 0$, by setting t sufficiently large.

The final step is to verify that the functional $\mathcal{E}$ satisfies the Palais-Smale (PS) condition. That is, to show that for any sequence $\{\phi_m\}_{m\in\mathbb{N}} \in \ell^2(\mathbb{Z}_K^N)$ such that $|\mathcal{E}(\phi_m)|$ is bounded and $\mathcal{E}'(\phi_m) \to 0$ as $n \to \infty$, there exists a convergent subsequence. In fact, since $\ell^2(\mathbb{Z}_K^N)$ is finite dimensional it suffices to verify that such a sequence is bounded. Considering a sequence ϕ_m of $\ell^2(\mathbb{Z}_K^N)$ be such that $|\mathcal{E}(\phi_m)| < M'$ for some $M' > 0$ and $\mathcal{E}'(\phi_m) \to 0$ as $m \to \infty$, we get similarly to (2.16), that for m sufficiently large

$$\begin{aligned}
M' &\geq \mathcal{E}(\phi_m) - \frac{1}{2\sigma+2}\langle\mathcal{E}'(\phi_m),\phi_m\rangle \\
&= \left(\frac{1}{2} - \frac{1}{2\sigma+2}\right)\left\{\epsilon(-\Delta_d\phi_m,\phi_m)_2 + \Omega||\phi_m||_2^2\right\} - \left(\frac{1}{2} - \frac{1}{2\sigma+2}\right)\sum_{||n||\leq K}\chi_n|(\phi_m)_n|^2 \\
&\geq \frac{2\sigma}{2(2\sigma+2)}(\epsilon\lambda_1 + \Omega - \max_{n\in\mathbb{Z}_K^N}\chi_n)||\phi_m||_2^2.
\end{aligned} \tag{2.18}$$

Condition (2.13) is required once again, to get from (2.18) that the sequence $\{\phi_m\}_{m\in\mathbb{N}}$ is bounded. Therefore the functional $\mathcal{E}$ possesses the geometry required by the MPT and satisfies condition (PS), proving the existence of a nontrivial breather solution (2.10).

From (2.1) we get that

$$\epsilon(-\Delta_d\phi,\phi)_2 + \Omega\sum_{||n||\leq K}|\phi_n|^2 - \sum_{||n||\leq K}\chi_n|\phi_n|^2 - \gamma\sum_{||n||\leq K}|\phi_n|^{2\sigma+2} = 0. \tag{2.19}$$

Working similarly to (2.16), we have from (2.19) the inequality

$$\begin{aligned}
\gamma\left(\sum_{||n||\leq K}|\phi_n|^2\right)^{\sigma+1} &\geq \gamma\sum_{||n||\leq K}|\phi_n|^{2\sigma+2} \\
&\geq \epsilon(-\Delta_d\phi,\phi)_2 + \Omega\sum_{||n||\leq K}|\phi_n|^2 - \max_{n\in\mathbb{Z}_K^N}\chi_n\sum_{||n||\leq K}|\phi_n|^2,
\end{aligned}$$

implying that the power $R^2 = \sum_{||n||\leq K}|\phi_n|^2$ of the critical point satisfies

$$\gamma R^{2\sigma+2} \geq (\epsilon\lambda_1 + \Omega - \max_{n\in\mathbb{Z}_K^N}\chi_n)R^2,$$

from which the estimate (2.14), readily follows. $\square$

The results of Theorem 2.1 can be extended to the particular example of the single point defect by similar arguments.

Corollary 2.2 *(Unstaggered patterns) For the DNLS system (2.1)-(2.2) with a single point defect $\chi_n = \alpha\delta_{n,n_0}$, $\alpha > 0$ (attractive impurity), the power of the unstaggered periodic solution $\psi_n(t) = e^{i\Omega t}\phi_n$, $\Omega > 0$ with $\Omega > \alpha$, satisfies the lower bound*

$$\left[\frac{\epsilon\lambda_1 + \Omega - \alpha}{\gamma}\right]^{\frac{1}{\sigma}} < R^2, \quad \sigma > 0. \tag{2.20}$$

Remark 2.3 *Note that without considering the anticontinuum limit $\epsilon = 0$, the restriction*

$$\alpha < \Omega + \epsilon\lambda_1,$$

is derived for the existence of a nontrivial breather solution. However, since the condition holds for any arbitrary $\epsilon > 0$, *this fact clearly implies that $\alpha < \Omega$. Condition $\alpha < \Omega$ can be also derived if one considers initially the anticontinuum limit case $\epsilon = 0$.*

Repulsive impurity. It is interesting that when the impurity is repulsive (R) (cf. [17, page 3]), the *case of the anticontinuum limit $\epsilon = 0$ implies the existence of both staggered patterns and unstaggered patterns.* Staggered patterns are given in the ansatz

$$\psi_n(t) = e^{-\mathrm{i}\omega t}\phi_n, \ \ \omega > 0, \tag{2.21}$$

while the unstaggered ones are (2.10) with $\Omega > 0$ (or (2.21) with $\omega = -\Omega < 0$).

It should be pointed out that distinguishing staggered and unstaggered patterns is of physical significance [13]. *In the framework of waveguide arrays, the staggered solutions display out-of-phase fields between the neighbor noncentral waveguides (oscillators) whereas the unstaggered ones display in-phase fields in these noncentral waveguides.*

Working in a very similar manner as for the proof of Theorem 2.1, we have

Theorem 2.4 *We consider the DNLS equation (2.1) assuming that condition (R) is satisfied. (i) (Staggered patterns) For any $\omega < -\max_{n\in\mathbb{Z}_K^N}\chi_n$ there exists a nontrivial $\phi \in \ell^2(\mathbb{Z}_K^N)$ such that $\psi_n(t) = e^{-\mathrm{i}\omega t}\phi_n$, $\omega > 0$ is a solution of the DNLS equation (2.1). Moreover the power of the nontrivial staggered periodic solution satisfies the lower bound*

$$\left[\frac{\epsilon\lambda_1 - \omega - \max_{n\in\mathbb{Z}_K^N}\chi_n}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2. \tag{2.22}$$

(ii) (Unstaggered patterns). For any $\Omega > 0$ there exists a nontrivial $\phi \in \ell^2(\mathbb{Z}_K^N)$ such that $\psi_n(t) = e^{\mathrm{i}\Omega t}\phi_n$, $\Omega > 0$ is a solution of the DNLS equation (2.1). Moreover the power of the nontrivial unstaggered periodic solution satisfies the lower bound

$$\left[\frac{\epsilon\lambda_1 + \Omega - \max_{n\in\mathbb{Z}_K^N}\chi_n}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2. \tag{2.23}$$

In the case of a single point defect with a repulsive impurity we have

Corollary 2.5 *(i)(Staggered patterns) For the DNLS system (2.1)-(2.2) with a single point defect $\chi_n = \alpha\delta_{n,n_0}$, $\alpha < 0$ (repulsive impurity), the power of a staggered periodic solution $\psi_n(t) = e^{-\mathrm{i}\omega t}\phi_n$ with $0 < \omega < -\alpha$, satisfies the lower bound*

$$\left[\frac{\epsilon\lambda_1 - \omega - \alpha}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2, \ \ -\alpha > 0. \tag{2.24}$$

(ii) (Unstaggered patterns) Any unstaggered solution $\psi_n(t) = e^{\mathrm{i}\Omega t}\phi_n$ with $\Omega > 0$ satisfies the lower bound

$$\left[\frac{\epsilon\lambda_1 + \Omega - \alpha}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2, \ \ -\alpha > 0. \tag{2.25}$$

2.2 Constrained minimization problems for the defocusing case $\gamma < 0$

The defocusing case $\gamma = -\Lambda < 0$ can be reduced to the focusing one *but with the opposite sign of the impurity under the staggering transformation.* This transformation is defined as

$$\psi_n \to (-1)^{|n|}\psi_n, \quad |n| = \sum_{i=1}^{N} n_i, \tag{2.26}$$

(see [13, pg. 066606-7]). We follow this approach in this section which means that we shall consider *the defocusing DNLS*

$$\begin{aligned} \mathrm{i}\dot{\psi}_n &+ \epsilon(\Delta_d\psi)_n + \chi_n\psi_n - \Lambda|\psi_n|^{2\sigma}\psi_n, \ \ \Lambda > 0 \ \ ||n|| \leq K, \\ \psi_n &= 0, \ \ ||n|| > K. \end{aligned} \tag{2.27}$$

The reason for considering alternatively the defocusing problem is that this approach allows for a derivation *of new conditions on the impurity χ_n for the proof of a coexistence result of staggered an unstaggered solutions.* We remark that *it was not possible to observe these new conditions by the mountain pass approach of the previous section for the focusing case.* On the contrary, the derivation of these new conditions was possible by the consideration constrained minimization problems for the defocusing case, that will be used in the sequel.

We are seeking breathers again in the ansatz

$$\psi_n(t) = e^{-\mathrm{i}\Omega t}\phi_n, \ \ \Omega \in \mathbb{R}. \tag{2.28}$$

Substituting (2.28) in (2.27) we get that ϕ_n satisfies the

$$\begin{aligned} -\epsilon(\Delta_d\phi)_n &- \Omega\phi_n - \chi_n\phi_n = -\Lambda|\phi_n|^{2\sigma}\phi_n, \ \ ||n|| \leq K, \\ \phi_n &= 0, \ ||n|| > K. \end{aligned} \tag{2.29}$$

Attractive case. As it was already mentioned, considering the attractive case with the condition (A) for the impurity is equivalent with the case of the repulsive case for the focusing DNLS (2.1), due to (2.26). However *it should be emphasized that the corresponding energy functional do not possesses the mountain pass geometry.* Thus we shall consider a constrained minimization problem for the *linear energy functional.* We start by seeking for staggered patterns (2.28) with $\Omega > 0$. The existence of solutions (2.28) with $\Omega > 0$, will be given by minimizing the linear energy

$$\mathcal{E}_\Omega[\phi] = \epsilon(-\Delta_d\phi, \phi)_2 - \Omega\sum_{||n||\leq K}|\phi_n|^2 - \sum_{||n||\leq K}\chi_n|\phi_n|^2, \ \ \Omega > 0. \tag{2.30}$$

More precisely, we consider the minimization problem on $\ell^2(\mathbb{Z}^N_K)$

$$\inf\left\{\mathcal{E}_\Omega[\phi] \ : \sum_{|n|\leq K}|\phi_n|^{2\sigma+2} = M > 0\right\}. \tag{2.31}$$

The functional $\mathcal{E}_\Omega$ is bounded from below: Consider the ball

$$B = \left\{\phi \in \ell^2(\mathbb{Z}^N_K) \ : \ \sum_{|n|\leq K}|\phi_n|^{2\sigma+2} = M\right\}. \tag{2.32}$$

Then, we have that

$$\begin{aligned} \mathcal{E}_\Omega[\phi] &\geq -\Omega\sum_{|n|\leq K}|\phi_n|^2 - \sum_{||n||\leq K}\chi_n|\phi_n|^2 \\ &\geq (-\Omega - \max_{n\in\mathbb{Z}^N_K}\chi_n)C_2^2\left(\sum_{||n||\leq K}|\phi_n|^{2\sigma+2}\right)^{\frac{1}{\sigma+1}} \\ &= (-\Omega - \max_{n\in\mathbb{Z}^N_K}\chi_n)C_2^2 M^{\frac{1}{\sigma+1}}. \end{aligned}$$

As we are restricted to the finite dimensional space $\ell^2(\mathbb{Z}^N_K)$, it follows that any minimizing sequence associated with the variational problem (2.31) is precompact: any minimizing sequence has a subsequence, converging to a minimizer. Thus $\mathcal{E}_\omega$ attains its infimum at a point $\hat{\phi}$ in B.

To derive the variational equation for $\mathcal{E}_\omega$, we set

$$\mathcal{L}_R[\phi] = \sum_{|n|\leq K}|\phi_n|^{2\sigma+2},$$

recalling that

$$\langle \mathcal{L}'_R[\phi], \psi\rangle = (2\sigma+2)\mathrm{Re}\sum_{|n|\leq K} |\phi_n|^{2\sigma}\phi_n\overline{\psi},\ \text{for all}\ \ \psi\in\ell^2(\mathbb{Z}^N_K).$$

Then by the Lagrange multiplier rule,

$$\begin{aligned}\left\langle \mathcal{E}'_\Omega[\hat{\phi}] - \lambda\mathcal{L}'_R[\hat{\phi}], \psi\right\rangle &= 2(-\Delta_d\hat{\phi},\psi)_2 - 2\Omega\mathrm{Re}\sum_{||n||\leq K}\hat{\phi}_n\overline{\psi}_n - 2\mathrm{Re}\sum_{|n|\leq K}\chi_n\hat{\phi}_n\overline{\psi}_n\\ &\quad -\mu(M)\mathrm{Re}\sum_{||n||\leq K}|\hat{\phi}_n|^{2\sigma}\hat{\phi}_n\overline{\psi_n} = 0,\ \ \text{for all}\ \psi\in\ell^2(\mathbb{Z}^N_K).\end{aligned} \tag{2.33}$$

Setting $\psi=\hat{\phi}$ in (2.33), we obtain

$$\mathcal{E}_\Omega[\hat{\phi}] = (-\Delta_d\hat{\phi},\hat{\phi})_2 - \Omega\sum_{|n|\leq K}|\hat{\phi}_n|^2 - \sum_{|n|\leq K}\chi_n|\hat{\phi}_n|^2 = \frac{\mu(M)}{2}\sum_{|n|\leq K}|\hat{\phi}|^{2\sigma+2}. \tag{2.34}$$

Furthermore, since

$$\mathcal{E}_\Omega[\hat{\phi}] \leq 4\epsilon N\sum_{|n|\leq K}|\hat{\phi}_n|^2 - \Omega\sum_{|n|\leq K}|\hat{\phi}_n|^2 - \sum_{|n|\leq K}\chi_n|\hat{\phi}_n|^2, \tag{2.35}$$

we get that $\mathcal{E}_\Omega[\hat{\phi}]<0$ if

$$\Omega > 4\epsilon N - \min_{n\in\mathbb{Z}^N_K}\chi_n, \tag{2.36}$$

is satisfied. Note that condition (2.36) is fullfiled for all $\Omega>0$ if $4\epsilon N < \min_{n\in\mathbb{Z}^N_K}\chi_n$. On the other hand, it is required that $\Omega > 4\epsilon N - \min_{n\in\mathbb{Z}^N_K}\chi_n > 0$, if $4\epsilon N > \min_{n\in\mathbb{Z}^N_K}\chi_n$.

Then assuming (2.36), we find that $\mu(M)<0$. The constant $\mu(M)/2$ can be scaled out from (2.34) by setting $\hat{\phi} = (-\mu(M)/2)^{-1/2\sigma}\,\tilde{\phi}$. Scaling further with $\tilde{\phi} = (1/\Lambda))^{-1/2\sigma}\,\phi$ we get that the non trivial solution of (2.29) satisfies the energy equation

$$(-\Delta_d\phi,\phi)_2 - \Omega\sum_{|n|\leq K}|\phi_n|^2 - \sum_{|n|\leq K}\chi_n|\phi_n|^2 = -\Lambda\sum_{|n|\leq K}|\phi|^{2\sigma+2}. \tag{2.37}$$

From (2.37), (2.6) and (2.8) it follows that

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

implying that the power $R^2 = \sum_{||n||\leq K}|\phi_n|^2$ of the critical point satisfies

$$\left[\frac{\Omega - 4N\epsilon + \min_{n\in\mathbb{Z}^N_K}\chi_n}{\Lambda}\right]^{\frac{1}{\sigma}} \ <\ R^2,\ \ \sigma>0. \tag{2.38}$$

The attractive impurity-defocusing case supports also unstaggered patterns. This is compatible with the approach of subsection (2.1). For convenience we set in (2.29) $\Omega=-\omega<0$. The anticontinuum limit suggests that an unstaggered pattern $\psi_n(t) = e^{\mathrm{i}\omega t}\phi_n$ exists if $0<\omega<\min_{n\in\mathbb{Z}^N_K}\chi_n$. Minimizing again the linear energy, instead of (2.36), we require that

$$0<\omega<\min_{n\in\mathbb{Z}^N_K}\chi_n - 4\epsilon N,\quad \min_{n\in\mathbb{Z}^N_K}\chi_n > 4\epsilon N. \tag{2.39}$$

This time, the power of the critical point satisfies

$$\left[\frac{\min_{n\in\mathbb{Z}_K^N}\chi_n - 4N\epsilon - \omega}{\Lambda}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \sigma > 0. \tag{2.40}$$

when (2.39) is satisfied. We summarize in

Theorem 2.7 *(i) (Staggered patterns) For the defocusing DNLS system with an attractive impurity* (A) *there exists a nontrivial staggered periodic solution* $\psi_n(t) = e^{-\mathrm{i}\Omega t}\phi_n$, $\Omega > 0$

$$\textit{for all } \Omega \quad > \quad 0, \;\; \textit{if } 4\epsilon N < \min_{n\in\mathbb{Z}_K^N}\chi_n, \tag{2.41}$$

$$\textit{for all } \Omega \quad > \quad 4\epsilon N - \min_{n\in\mathbb{Z}_K^N}\chi_n > 0, \;\; \textit{if } 4\epsilon N > \min_{n\in\mathbb{Z}_K^N}\chi_n. \tag{2.42}$$

and power satisfying the lower bound (2.38). In the case of an attractive single point defect $\chi_n = \alpha\delta_{n,n_0}$, $\alpha > 0$, *the power of a staggered periodic solution with* $\Omega > 4N\epsilon - \alpha$, *satisfies the lower bound*

$$\left[\frac{\Omega - 4N\epsilon + \alpha}{\Lambda}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \sigma > 0, \;\; \Omega > 0 \;\; \textit{if } 4\epsilon N < \alpha, \tag{2.43}$$

$$\left[\frac{\Omega - 4N\epsilon + \alpha}{\Lambda}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \sigma > 0, \;\; \Omega > 4\epsilon N - \alpha \;\; \textit{if } \alpha < 4\epsilon N. \tag{2.44}$$

(ii) (Unstaggered patterns) The defocusing DNLS system with an attractive impurity (A) *supports also unstaggered patterns*

$$\psi_n(t) = e^{\mathrm{i}\omega t}\phi_n, \;\; 0 < \omega < \min_{n\in\mathbb{Z}_K^N}\chi_n - 4\epsilon N, \;\; \textit{if } 4\epsilon N < \min_{n\in\mathbb{Z}_K^N}\chi_n,$$

with power satisfying (2.40). In the case of an attractive single point defect $\chi_n = \alpha\delta_{n,n_0}$, $\alpha > 0$, *the power of an unstaggered periodic solution with* $0 < \omega < \alpha - 4\epsilon N$, *satisfies the lower bound*

$$\left[\frac{\alpha - 4N\epsilon - \omega}{\Lambda}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \sigma > 0, \;\; 0 < \omega < \alpha - 4\epsilon N, \;\; \textit{if } 4\epsilon N < \alpha. \tag{2.45}$$

Remark 2.8 *The consideration of the defocusing DNLS with the attractive impurity revealed conditions on the impurity for coexistence of both patterns in the attractive case. Apart of verifying the coexistence result of subsection 2.1-Theorem 2.4 for the equivalent focusing DNLS with repulsive impurity, the approach on minimizing the linear energy clarified the conditions on the impurity for this coexistence. More precisely, it follows that when* $4\epsilon N < \alpha$ *we have coexistence of staggered patterns of any* $\Omega > 0$ *and unstaggered patterns at least in the range* $0 < \omega < \alpha - 4\epsilon N$. *This is a vast difference with the defocusing DNLS with repulsive impurity which supports solutions only of one sign as it was shown for its equivalent analogue, the focusing one with the attractive impurity. This it will again justified in the next paragraph.*

A similar scenario was demonstrated for Klein–Gordon lattices in Ref. [9].

Repulsive case. In the repulsive case (R), it can be easily seen by considering equation (2.29) in the anticontinuum limit $\epsilon = 0$ that DNLS (2.27) supports only staggered patterns (2.28) with $\Omega > 0$. This is in agreement with the alternative approach of subsection 2.1 which considers the focusing case. For the proof of solutions (2.28) with $\Omega > 0$ we work exactly as for the proof of Theorem 2.7. The linear energy is bounded from below since

$$\mathcal{E}_\Omega[\phi] \geq -\Omega C_2^2 M^{\frac{1}{\sigma+1}}.$$

Having the corresponding minimizer $\hat{\phi}$ at hand, we observe this time that $\mathcal{E}_\Omega[\hat{\phi}] < 0$ for frequencies

$$\Omega > 4\epsilon N - \min_{n\in\mathbb{Z}_K^N}\chi_n, \;\; -\min_{n\in\mathbb{Z}_K^N}\chi_n > 0.$$

Thus we have

Theorem 2.9 *(Staggered patterns) For the defocusing DNLS system with a repulsive impurity* (R) *there exists a nontrivial staggered periodic solution* $\psi_n(t) = e^{-\mathrm{i}\Omega t}\phi_n$, $\Omega > 0$ *for all* $\Omega > 4\epsilon N - \min_{n\in\mathbb{Z}_K^N}\chi_n > 0$. *and power satisfying the lower bound*

$$\left[\frac{\Omega - 4N\epsilon - \min_{n\in\mathbb{Z}_K^N}\chi_n}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2, \ \ \sigma > 0, \ \ -\min_{n\in\mathbb{Z}_K^N}\chi_n > 0. \tag{2.46}$$

In the case of a repulsive single point defect $\chi_n = \alpha\delta_{n,n_0}$, $\alpha < 0$, *the power of the staggered periodic solution (2.28) with* $\Omega > 4N\epsilon - \alpha$, *satisfies the lower bound*

$$\left[\frac{\Omega - 4N\epsilon - \alpha}{\Lambda}\right]^{\frac{1}{\sigma}} < R^2, \ \ \sigma > 0, \ \ \Omega > 4\epsilon N - \alpha, \ \ -\alpha > 0. \tag{2.47}$$

Note, as it is mentioned before, that the focusing DNLS with repulsive linear impurity is equivalent to this case, because of the corresponding stationary states, under a staggering transformation and a frequency change, reduces to the defocussing case with opposite sign of the impurity parameter.

2.3 Numerical studies in the linear impurity case

This section is devoted to the numerical study of the DNLS system with the local inhomogeneity (2.1)-(2.2). The presentation is focused on testing the results of the alternative approach of constrained minimization for the defocusing case $\gamma < 0$ presented in Section 2.2. Our aim is to investigate numerically the coexistence result of both staggered and unstaggered patterns in the attractive case of the single point defect $\chi_n = \alpha\delta_{n,n_0}$ of Theorem 2.7, as well as, the corresponding lower bounds (2.43)-(2.44), on the power of the staggered and (2.45) for the unstaggered breathers respectively. The numerical study concerns 1D and 2D lattices.

The first panel of pictures in Figure 1 concerns the numerical study for an 1D defocusing lattice $\gamma = -\Lambda = -1$ and attractive impurity $\alpha = 0.5$ with parameters $\epsilon = 0.1$ and $\sigma = 1$. This example corresponds to the case where the parameters are satisfying condition

$$0.4 = 4\epsilon N < \alpha = 0.5.$$

Thus, we are in the case where, according to Theorem 2.7, the sufficient conditions for coexistence of both staggered and unstaggered breathers is expected. Figures 1 (a), (b) and (c) is a full justification of these sufficient conditions. In (c) the profile of the one-site *staggered* breather centered at the impurity with frequency $\Omega = 0.6$. According to the theoretical prediction, under condition $4\epsilon N < \alpha$ we have existence of staggered solutions for any $\Omega > 0$. On the other hand we should have coexistence of unstaggered patterns of frequency at least in the range

$$0 < \omega < \alpha - 4\epsilon N = 0.1,$$

where $\omega_* = 0.1$ can be considered as the transition value of frequency for coexistence. Picture (b) shows the profile of the one-site *unstaggered* solution in the transition value $\omega_* = 0.1$ while (a) shows the profile of the *unstaggered* solution with frequency $\omega = 0.05$ within the theoretical range $0 < \omega < 0.1$. The numerical justification of the lower bounds (2.43)-(2.44) for the staggered solutions and (2.45) for the unstaggered is shown in the final picture (d), where the power of one–site breathers centered at the impurity as function of frequency ω is demonstrated. The upper picture (a) corresponds to $\epsilon = 0.01$ and the lower picture (b) to $\epsilon = 0.1$. In continuous lines we represent the numerical power, where negative frequencies correspond to the staggered solutions (note that in the text $\Omega = -\omega$) and positive frequencies to the unstaggered solutions. Dashed lines represent the theoretical lower bound given by (2.43)-(2.44) and (2.45), dash-dotted line the frequency of the linear impurity mode, dotted line the frequency given by $\omega = \alpha - 4\epsilon N$, and the dark area corresponds to the linear modes frequencies. Both cases justify that the theoretical estimates can be particularly useful as an explicit prediction of the smallest value of the power for breathers satisfying the conditions of Theorem 2.7.

In Figure 2 the same defocusing example concerning the parameters α, ϵ, N as in Figure 1 is considered, but this time for “large” nonlinearity parameter $\sigma = 10$. Figure 2 (a) shows the unstaggered solution corresponding to $\omega = 0.05$, 2 (b) the unstaggered solution corresponding to $\omega = 0.1$, the transition value predicted theoretically, and 2 (c) the staggered solution corresponding to $\Omega = 0.6$. The final figure (d) is showing the behavior of the theoretical bounds against the numerical power, and verify that the breathers corresponding to $\sigma = 10$ are the real examples of breathers with power converging in a sharp manner to the analytical lower bounds.

Figure 3 demonstrates the validity of the sufficient conditions for coexistence in the case of 2D lattices. The examples concern a 2D defocusing lattice with $\gamma = -\Lambda = -1$, an attractive impurity $\alpha = 0.5$ and $\epsilon = 0.01$. With these parameters we are again under the sufficient condition

$$0.08 = 4\epsilon N < \alpha = 0.5,$$

for coexistence of both staggered and unstaggered patterns. Figures 3 (a), (b) correspond to $\sigma = 1$. Figure 3 (a) shows the *unstaggered solution* corresponding to

$$\omega = 0.4 < \alpha - 4\epsilon N = 0.42,$$

where $\omega_* = 0.42$ is the transition value of frequency according condition (2.45) for the frequency of unstaggered solutions. Figure 3 (b) shows the profile of the the *staggered solution* corresponding to $\Omega = 0.1$. Similarly, figures 3 (c), (d) correspond to $\sigma = 10$. Figure 3 (c) shows the *unstaggered solution* corresponding to $\omega = 0.46$, and 3 (d) *the staggered solution* corresponding to $\Omega = 0.07$.

The results of the numerical study on the theoretical estimates (2.43)-(2.44)-(2.45) for 2D lattices are given in Figure 4, justifying their effectiveness. The first figure shows the power of one–site breathers centered at the impurity as function of frequency ω in the defocussing case $\gamma = -1$, attractive impurity $\alpha = 0.5$ and $\sigma = 1.0$. The upper figure (a) corresponds to $\epsilon = 0.01$ and the lower (b) to $\epsilon = 0.1$. In continuous lines we represent the power of the one–site breathers, where negative frequencies correspond to the staggered solution and positive frequencies to the unstaggered solution. Dashed lines represent the theoretical bounds given by (2.43)-(2.44)-(2.45). The second figure is for the same parameters α, ϵ, N but now $\sigma = 10$. Note that in the lower figure (b), in the case of unstaggered solutions, *the power of some numerical breathers is lower than theoretical predictions, but, in this case, the condition* $0 < \omega < \alpha - 4\epsilon N$ *is not satisfied.*

It is crucial to remark that branches of solutions on the lower-right panels of Figures, 1, 2 and 4, terminate suddenly. In fact in all the numerical simulations performed, it was observed that further continuation was not possible. While this observation do not violates the theoretical statements of Theorem 2.7, *since the conditions of the theorem are only sufficient, the termination of branches possibly indicates the existence of saddle-node bifurcations with another solution branch which can not of course be explained by the theoretical results.* The study of such a phenomenon possibly requires detailed stability analysis for the study of the bond centered breathers accompanied by careful numerical simulations, and constitutes an interesting plan for a future work.

Figure 5 is a representative presentation of the numerical power against the theoretical estimates (2.43)-(2.44)-(2.45) as functions of the frequency ω and the nonlinearity exponent σ. The examples we consider are for the defocusing case $\gamma = -\Lambda = -1$, and an attractive impurity $\alpha = 0.5$. For the nonlinearity parameter σ we consider the range $0 < \sigma < 1$. *This case is of importance in the context of the present work since for this range of* σ *we should not expect appearance of the excitation threshold in the sense of [6] and [22].* The first figure shows the power of one–site breathers centered at the impurity for $N = 1$ and $\epsilon = 0.1$. Black lines represent the numerical results, where negative frequencies correspond to the staggered solution (note that in the text $\Omega = -\omega$) and positive frequencies to the unstaggered solutions. The grey surface represents the theoretical estimate given by (2.43)-(2.44)-(2.45). In addition, the linear modes frequencies area is represented in thick lines. The second corresponds to the case $N = 2$ and $\epsilon = 0.01$. The numerical study revealed a wide range of frequencies of breathers whose power are very close to the theoretical prediction for the minimal power for existence. These members of the breather family together with the comparison of the theoretical and numerical surface indicates the usefulness of the local estimates with respect to frequency as a simple analytical prediction of the smallest power of breathers satisfying the theoretical sufficient conditions. This becomes significant in the possible absence of the excitation threshold which expected for small values of the nonlinearity exponent.

3 Existence of localized modes in infinite DNLS lattices with nonlinear impurities

The result on the existence of excitation threshold of [22], can be extended in the case of DNLS lattices with nonlinear impurities. For instance we shall consider the (infinite) DNLS lattice

$$\mathrm{i}\dot{\psi}_n + \epsilon(\Delta_d\psi)_n + \Lambda_n|\psi_n|^{2\sigma}\psi_n \quad = 0, \;\; n \in \mathbb{Z}^N, \tag{3.1}$$

with $n \in \mathbb{Z}^N$. The excitation threshold will be proved for unstaggered breathers by adapting the methods of [22]. In the infinite lattice, we shall assume for $\Lambda_n, n \in \mathbb{Z}^N$ the condition

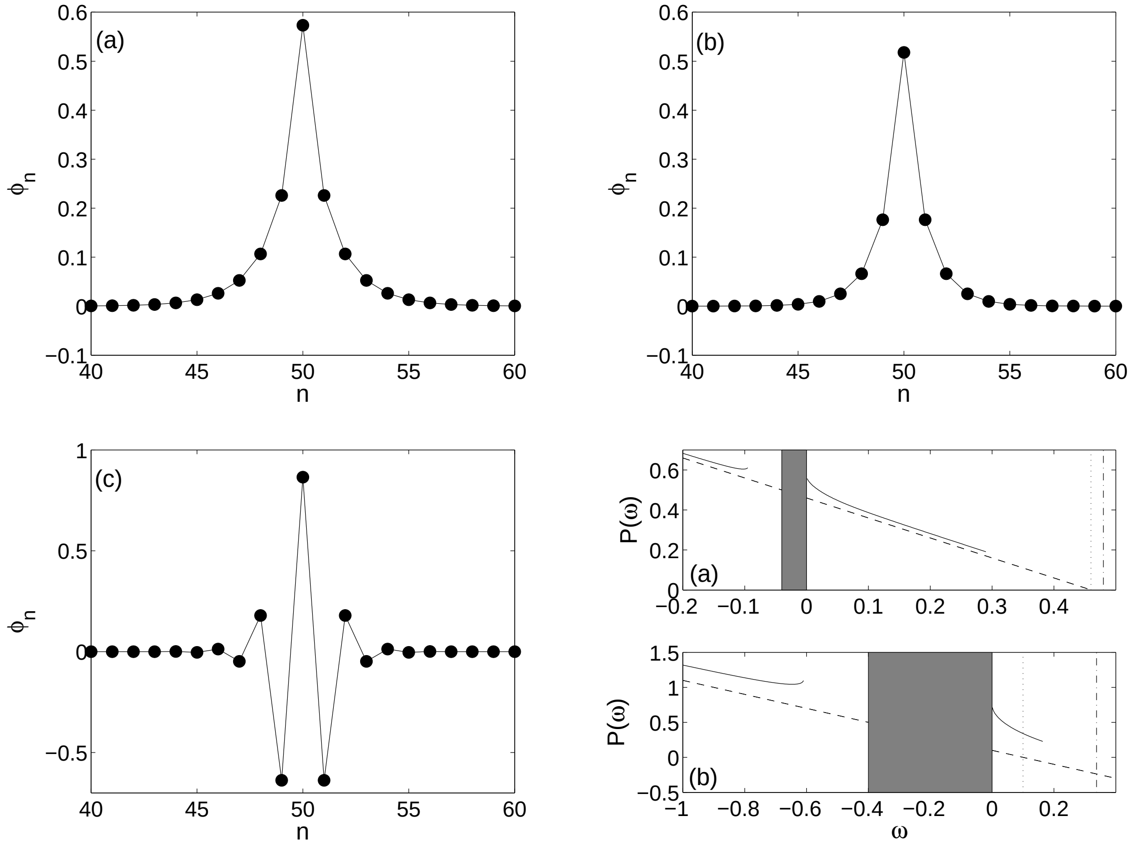

Figure 1: Transition to coexistence of both staggered and unstaggered solutions for the defocusing $\gamma = -1$ DNLS for $N = 1$, $\sigma = 1$, with attractive single point defect $\alpha = 0.5$, $\epsilon = 0.1$. (a) unstaggered solution $\omega = 0.05$, (b) unstaggered solution $\omega = 0.1$ (theoretical transition value for frequency), (c) staggered solution $\Omega = 0.6$. The final figure shows the numerical power against the theoretical estimates (2.43)-(2.44)-(2.45).

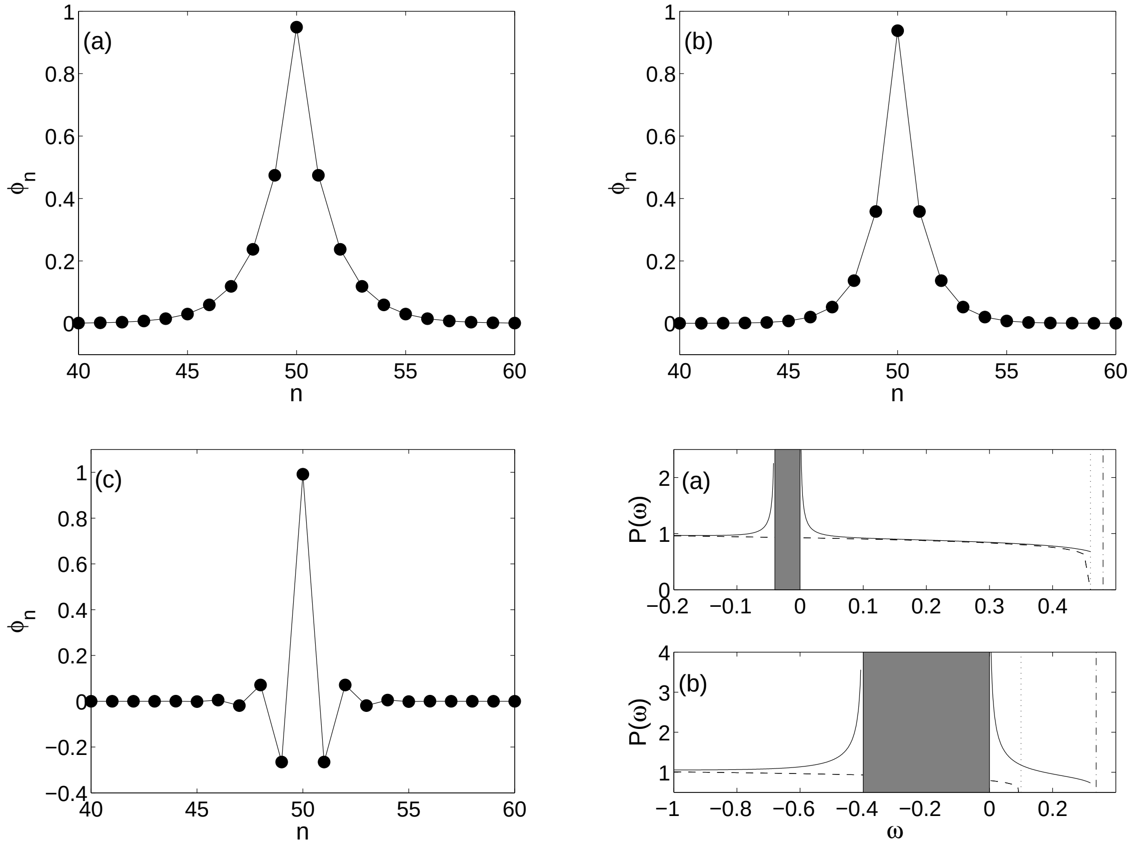

Figure 2: Transition to coexistence of both staggered and unstaggered solutions for the defocusing $\gamma = -1$ DNLS for $N = 1$, $\sigma = 10$, with attractive single point defect $\alpha = 0.5$, $\epsilon = 0.1$. (a) unstaggered solution $\omega = 0.05$, (b) unstaggered solution $\omega = 0.1$ (theoretical transition value for frequency), (c) staggered solution $\Omega = 0.6$. The final figure shows the numerical power against the theoretical estimates (2.43)-(2.44)-(2.45).

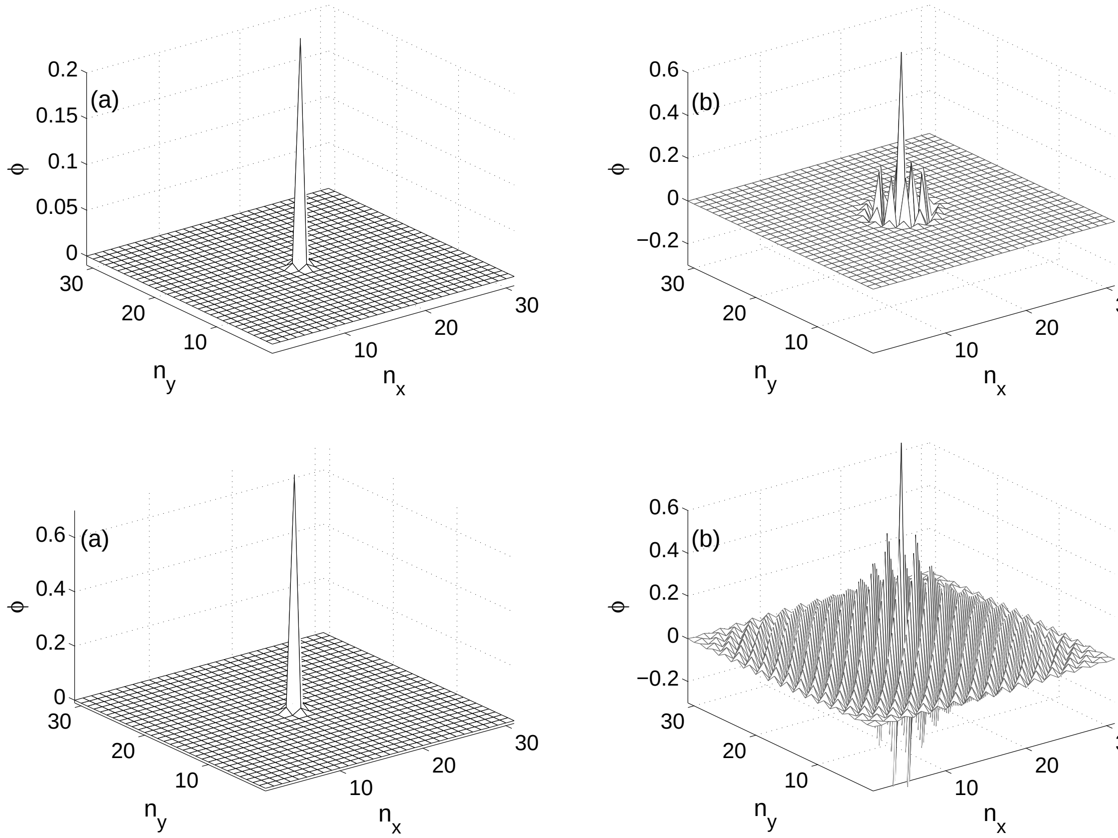

Figure 3: Coexistence of staggered and unstaggered solutions in 2D defocusing ($\gamma = -1$) lattices with attractive single point defect $\alpha = 0.5$, $\epsilon = 0.1$. (a) $\sigma = 1$, unstaggered solution $\omega = 0.4$, (b) $\sigma = 1$, staggered solution $\Omega = 0.1$, (c) $\sigma = 10$, unstaggered solution $\omega = 0.4$, (d) $\sigma = 10$, staggered solution $\omega = 0.07$.

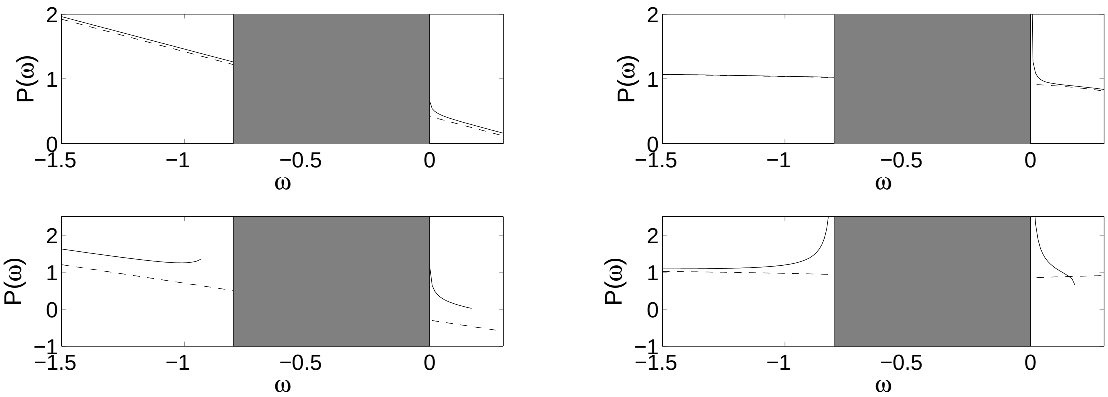

Figure 4: Numerical power against the theoretical estimates (2.43)-(2.44)-(2.45) for 2D lattices. The first set of figures is for $\sigma = 1$, attractive impurity $\alpha = 0.5$. The upper case corresponds to $\epsilon = 0.01$ and the lower case to $\epsilon = 0.1$. The second set is for $\sigma = 10$.

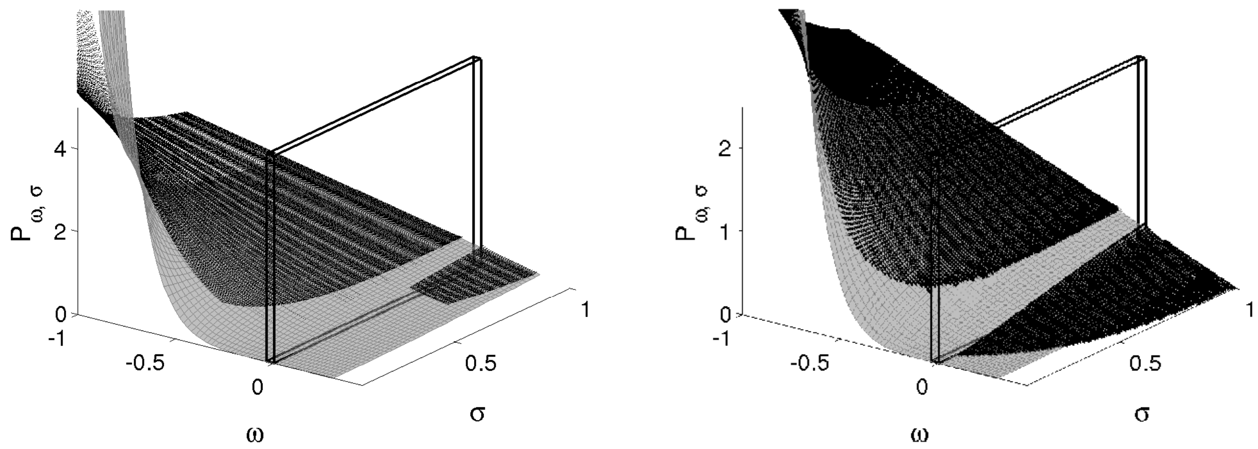

Figure 5: Numerical power against the theoretical estimates (2.43)-(2.44)-(2.45) for 1D and 2D lattices as a function of frequency ω and nonlinearity exponent $0 < \sigma < 1$. Defocusing lattice $\gamma = -1$, attractive single point defect $\alpha = 0.5$. (a) $N = 1$, $\epsilon = 0.1$ (b) $N = 2$, $\epsilon = 0.01$.

(SC_∞) (*Sign-changing case*) $\Lambda_n \in \ell^\infty$ and in some $\mathcal{S}_+ \subset \mathbb{Z}^N$, $\{\Lambda_n\}_{n\in\mathcal{S}_+} \geq 0$ and in $\mathcal{S}_- := \mathbb{Z}^N_K \setminus \mathcal{S}_+ \subseteq \mathbb{Z}^N$, $\{\Lambda_n\}_{n\in\mathcal{S}_-} \leq 0$, where $\{\Lambda_n\}_{n\in\mathcal{S}_-} \neq 0$ (not identically the zero sequence in $\mathcal{S}_-$).

For convenience we write Λ_n as

$$\Lambda_n = \begin{cases} -\alpha_n, \ \ \alpha_n \geq 0 & n \in \mathcal{S}_- \subseteq \mathbb{Z}^N, \ \ \alpha_n \neq 0, \\ \beta_n, \ \ \beta_n \geq 0 & n \in \mathcal{S}_+ = \mathbb{Z}^N \setminus \mathcal{S}_- \end{cases}$$

The existence of unstaggered breathers has been proved via the mountain pass theorem under the same condition to (SC_∞) for the sign of Λ_n but with the difference that $|\Lambda_n| \in \ell^\rho, \rho = (q-1)/(q-2)$ for some $q > 2$ [10, Theorem 2.6, pg. 125]. This restriction on the summability of Λ_n induced compactness (by considering auxiliary weighted sequence spaces). Under the relaxed condition (SC_∞), the necessary compactness will be recovered by the concentration compactness arguments of [22, Appendix,pg. 689]. Another approach concerning compactness arguments (envelope technique) has been developed in [20].

Under condition (SC_∞) we consider the functional

$$\mathcal{H}[\phi] = \epsilon(-\Delta_d\phi, \phi)_2 + \frac{1}{\sigma+1}\sum_{n\in\mathbb{Z}^N} \Lambda_n |\phi_n|^{2\sigma+2}, \tag{3.2}$$

and the variational problem on ℓ^2

$$\mathcal{I}_R = \inf\left\{\mathcal{H}[\phi] \ : \sum_{n\in\mathbb{Z}^N} |\phi_n|^2 = R > 0\right\}. \tag{3.3}$$

We have the following proposition, in analogy with [22]:

Lemma 3.1 $\mathcal{I}_R \geq 0$ *if and only if* R *satisfies the inequality*

$$-\sum_{n\in\mathbb{Z}^N} \Lambda_n |\phi_n|^{2\sigma+2} \leq (\sigma+1)\epsilon R^{-\sigma}\left(\sum_{n\in\mathbb{Z}^N} |\phi_n|^2\right)^\sigma (-\Delta_d\phi, \phi)_2, \tag{3.4}$$

for all $\phi \in \ell^2$.

Proof: Let $\psi \in \ell^2 \neq 0$ be arbitrary. Then $z = \sqrt{R}||\psi||^{-1}_{\ell^2}\psi$ is such that $\sum_{n\in\mathbb{Z}^N} |z_n|^2 = R$. Since $\mathcal{I}_R \geq 0$ if and only if

$$\epsilon(-\Delta_d\phi, \phi)_2 \geq -\frac{1}{\sigma+1}\sum_{n\in\mathbb{Z}^N} \Lambda_n |\phi_n|^{2\sigma+2}, \tag{3.5}$$

inserting z in (3.5), we derive as in [22, Proposition 3.1, pg. 679] the inequality (3.4). $\diamond$

Using (SC_∞), we remark that (3.5) is satisfied if R is such that

$$\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\le(\sigma+1)\epsilon R^{-\sigma}\left(\sum_{n\in\mathbb{Z}^N}|\phi_n|^2\right)^{\sigma}(-\Delta_d\phi,\phi)_2,\ \text{ for all }\ \phi\in\ell^2. \tag{3.6}$$

The next Proposition is a consequence of the condition (SC_∞) and [22, Theorem 4.1,pg. 682]:

Lemma 3.2 *Assuming condition (SC_∞), there exists a constant $K>0$ such that if $\sigma\ge\frac{2}{N}$, the inequality*

$$\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\le K\left(\sum_{n\in\mathbb{Z}^N}|\phi_n|^2\right)^{\sigma}(-\Delta_d\phi,\phi)_2, \tag{3.7}$$

holds for all for all $\phi\in\ell^2$.

Proof:. By condition (SC_∞) and the discrete analogue of the Sobolev-Gagliardo-Nirenberg inequality

$$\sum_{n\in\mathbb{Z}^N}|\phi_n|^{2\sigma+2}\le C\left(\sum_{n\in\mathbb{Z}^N}|\phi_n|^2\right)^{\sigma}(-\Delta_d\phi,\phi)_2, \tag{3.8}$$

of [22, Theorem 4.1,pg. 682], we have

$$\begin{aligned}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2} &\le \sup_{n\in\mathbb{Z}^N}\{\alpha_n\}\sum_{n\in\mathbb{Z}^N}|\phi_n|^{2\sigma+2}\\ &\le \sup_{n\in\mathbb{Z}^N}\{\alpha_n\}C\left(\sum_{n\in\mathbb{Z}^N}|\phi_n|^2\right)^{\sigma}(-\Delta_d\phi,\phi)_2.\end{aligned}$$

Thus $K=\sup_{n\in\mathbb{Z}^N}\{\alpha_n\}C$. $\diamond$

Let us note that under condition (SC_∞) the sign of $\sum_{n\in\mathbb{Z}^N}\Lambda_n|\phi_n|^{2\sigma+2}$ *is indefinite*. However as it is expected and shown in [3], the existence of unstaggered breathers should be supported mainly by the focusing part of the nonlinearity. Thus it is natural to claim that the existence and the global threshold for unstaggered breathers will be defined from inequality (3.7). Note that (3.7) is a stronger inequality than (3.4), since if $\phi\in\ell^2$ satisfies (3.7), then it satisfies (3.4). In analogy with [22, Eq. 4.2, pg. 680], if K_* is the infimum over all such constants, the excitation threshold denoted by R_{sc} in the case will be defined for the case $\sigma\ge\frac{2}{N}$ by the equation

$$(\sigma+1)\epsilon(R_{sc})^{-\sigma}=K_*. \tag{3.9}$$

This claim will be justified by a simple treating the defocusing part of the nonlinearity, as well as of the inequality (3.7), on the way to extend the results of [22].

Proposition 3.3 *Assume condition (SC_∞) and let $\sigma\ge\frac{2}{N}$. We define*

$$R_{sc} = \left((\sigma+1)\epsilon\mathcal{K}^{\sigma,N}\right)^{\frac{1}{\sigma}} \tag{3.10}$$

$$\textit{where }\ \mathcal{K}^{\sigma,N} = \inf\frac{\left(\sum_{n\in\mathbb{Z}^N}|\phi_n|^2\right)^{\sigma}(-\Delta_d\phi,\phi)_2}{\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}}=\frac{1}{K_*}. \tag{3.11}$$

A. *Assume that $||\phi||^2_{\ell^2}=R$. Then*

$$\mathcal{H}[\phi]\ge\epsilon(-\Delta_d\phi,\phi)_2\left[1-\left(\frac{R}{R_{sc}}\right)^{\sigma}\right]. \tag{3.12}$$

B. *If $R<R_{sc}$ then $\mathcal{I}_R=0$ and there is no ground state minimizer of (3.3).*

Proof: A. Using (SC_∞) and inequality (3.7) with its best constant K_* we derive that

$$\begin{aligned}\mathcal{H}[\phi] &= \epsilon(-\Delta_d\phi,\phi)_2+\frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_+}\beta_n|\phi_n|^{2\sigma+2}-\frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\\ &\ge \epsilon(-\Delta_d\phi,\phi)_2-\frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\\ &\ge \epsilon(-\Delta_d\phi,\phi)_2-\epsilon(R_{sc})^{-\sigma}R^{\sigma}(-\Delta_d\phi,\phi)_2,\end{aligned}$$

thus (3.12).
B. Assuming that $R < R_{thresh}$, it follows from (3.12) that $\mathcal{I}_R \geq 0$. We consider next some $\tilde{\psi} \in \ell^2$ such that

$$\begin{aligned} \{\tilde{\psi}_n\}_{n\in\mathbb{Z}^N_K} &= \{\tilde{\psi}_n\}_{n\in\mathcal{S}_+} + \{\tilde{\psi}_n\}_{n\in\mathcal{S}_-}, \text{ such that } \begin{cases} \{\tilde{\psi}_n\}_{n\in\mathcal{S}_+} & = 0, \\ \{\tilde{\psi}_n\}_{n\in\mathcal{S}_-} & \neq 0 \end{cases} \\ ||\tilde{\psi}||_{\ell^2} &= \frac{\sqrt{R}}{\lambda}, \text{ where } \lambda > 0 \text{ arbitrary.} \end{aligned}$$

Then considering $z_\lambda = \sqrt{R}||\tilde{\psi}||^{-1}_{\ell^2}\tilde{\psi}$ we observe that

$$||z_\lambda||^2_{\ell^2} = R$$

and

$$\mathcal{H}[z_\lambda] = \epsilon(-\Delta_d\tilde{\psi},\tilde{\psi})_2 - \frac{\lambda^{2\sigma+2}}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\tilde{\psi}_n|^{2\sigma+2}.$$

For λ sufficiently large, we get that $\mathcal{H}[z_\lambda] < 0$. Therefore if $R < R_{sc}$ we should have $\mathcal{I}_R = 0$. We assume that the infimum is attained at a state $\hat{\phi}$ for which

$$\begin{aligned} \epsilon(-\Delta_d\hat{\phi},\hat{\phi})_2 &= -\frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_+}\beta_n|\hat{\phi}_n|^{2\sigma+2} + \frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\hat{\phi}_n|^{2\sigma+2}, \\ \sum_{n\in\mathbb{Z}^N}|\hat{\phi}_n|^2 &= R. \end{aligned} \tag{3.13}$$

Inserting again inequality (3.7) with its best constant K_* into (3.13) we deduce that

$$\epsilon(-\Delta_d\hat{\phi},\hat{\phi})_2 \leq \frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\hat{\phi}_n|^{2\sigma+2} \leq \epsilon\left(\frac{R}{R_{sc}}\right)^\sigma < \epsilon(-\Delta_d\hat{\phi},\hat{\phi})_2. \quad \diamond$$

The last theorem concludes that R_{sc} is an excitation threshold for $\sigma \geq \frac{2}{N}$.

Theorem 3.4 *Assume condition* (SC_∞) *and let* $\sigma \geq \frac{2}{N}$. *If* $R > R_{sc}$ *then* $\mathcal{I}_R < 0$ *and there exists a minimizer of the variational problem (3.3).*

Proof: We shall justify first that if $R > R_{sc}$ then $\mathcal{I}_R < 0$: By the definitions (3.10-(3.11) of R_{sc} and $\mathcal{K}^{\sigma,N}$ it follows that a $\phi^* \in \ell^2$ must exist which do not satisfy inequality (3.7), hence

$$\sum_{n\in\mathcal{S}_-}\alpha_n|\phi^*_n|^{2\sigma+2} \geq (\sigma+1)\epsilon R^{-\sigma}\left(\sum_{n\in\mathbb{Z}^N}|\phi^*_n|^2\right)^\sigma(-\Delta_d\phi^*,\phi^*)_2, \quad R > R_{sc}. \tag{3.14}$$

Then (3.14) clearly implies that

$$\sum_{n\in\mathcal{S}_-}\alpha_n|\phi^*_n|^{2\sigma+2} \geq (\sigma+1)\epsilon R^{-\sigma}\left(\sum_{n\in\mathcal{S}_-}|\phi^*_n|^2\right)^\sigma(-\Delta_d\phi^*,\phi^*)_{\mathcal{S}_-}, \quad R > R_{sc}, \tag{3.15}$$

where $(\cdot,\cdot)_{\mathcal{S}_-}$, denotes the piece of $(\cdot,\cdot)_2$ in the part $\mathcal{S}_-$ of the lattice. Now we consider the element $\zeta \in \ell^2$, defined as

$$\zeta = \sqrt{R}||\theta||^{-1}_{\ell^2}\theta, \text{ where } \theta_n = \begin{cases} \phi^*_n, & n \in \mathcal{S}_- \\ 0, & n \in \mathcal{S}_+. \end{cases}$$

Then we observe that

$$\begin{aligned} \mathcal{H}[\zeta] &= \epsilon R||\theta||^{-2}_{\ell^2}(-\Delta_d\phi^*,\phi^*)_{\mathcal{S}_-} - \frac{R^{\sigma+1}}{\sigma+1}||\theta||^{-2\sigma-2}_{\ell^2}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi^*_n|^{2\sigma+2} \\ &< \epsilon R||\theta||^{-2}_{\ell^2}(-\Delta_d\phi^*,\phi^*)_{\mathcal{S}_-} - R^{\sigma+1}||\theta||^{-2\sigma-2}_{\ell^2}\epsilon R^{-\sigma}\left(\sum_{n\in\mathcal{S}_-}|\phi^*_n|^2\right)^\sigma(-\Delta_d\phi^*,\phi^*)_{\mathcal{S}_-} = 0 \end{aligned}$$

since $||\theta||_{\ell^2}^2 = \sum_{n\in\mathcal{S}_-} |\phi_n^*|^2$. Hence $\mathcal{I}_R < 0$.

We proceed by showing the existence of a minimizer. Clearly, $\mathcal{I}_R$ is bounded form below since

$$\begin{aligned}
\mathcal{H}[\phi] &\geq -\frac{1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\\
&\geq -\frac{1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\alpha_n|\phi_n|^{2\sigma+2}\\
&\geq -\frac{1}{\sigma+1}\sup_{n\in\mathbb{Z}^N}\{\alpha_n\}\sup_{n\in\mathbb{Z}^N}|\phi_n|^{2\sigma}\sum_{n\in\mathbb{Z}^N}\alpha_n|\phi_n|^2\\
&\geq -\frac{1}{\sigma+1}R^{\sigma+1}.
\end{aligned}$$

The final step is to prove that every minimizing sequence associated with the variational problem (3.3) is precompact modulo phase translations (cf. [22, Theorem 2.1, pg. 677]. Let $\{\psi^m\}_{m\in\mathbb{N}}$ a minimizing sequence. Then by the fact that $\mathcal{I}_R < 0$, we have that

$$\mathcal{H}[\psi^m] \leq \frac{\mathcal{I}_R}{2}, \text{ for } m \text{ large enough.} \tag{3.16}$$

Then it follows from (3.16) that

$$||\phi^m||_{\ell^2}^{2\sigma+2}\sup_{n\in\mathbb{Z}^N}|\Lambda_n| \geq -\sum_{n\in\mathbb{Z}^N}\Lambda_n|\phi_n^m|^{2\sigma+2} \geq -\frac{\sigma+1}{2}\mathcal{I}_R > 0. \tag{3.17}$$

The lower bound (3.17) shows that the vanishing scenario [22, Theorem 7.1 (2), pg. 689] is excluded for a minimizing sequence. Now we consider a sequence $\{\phi^m\}_{m\in\mathbb{N}}$ in ℓ^2 such that

$$||\phi^m||_{\ell^2}^2 \to \rho, \text{ and } \mathcal{H}[\phi^m] \to \mathcal{I}_R. \tag{3.18}$$

The sequence

$$\psi^m = \sqrt{R}||\phi^m||_{\ell^2}^{-1}\phi^m,$$

is a minimizing sequence and satisfies (3.17), thus $\rho > 0$. We prove that

$$\rho = R. \tag{3.19}$$

By contradiction, we suppose that

$$0 < \rho < R. \tag{3.20}$$

We consider the sequences $\{\zeta^m\}_{m\in\mathbb{N}}, \{\eta^m\}_{m\in\mathbb{N}}$ satisfying the dichotomy scenario [22, Theorem 7.1 (3), pg. 689]: This means that for all $\epsilon > 0$, there exists $m_0 \geq 1$ such that for all $m > m_0$

$$\begin{aligned}
||\psi^{m_k} - (\zeta^k + \eta^k)||_{\ell^2} &\leq \epsilon,\\
\left|||\zeta^k||_{\ell^2}^2 - \rho\right| &\leq \epsilon,\\
\left|||\eta^k||_{\ell^2}^2 - (R-\rho)\right| &\leq \epsilon,
\end{aligned} \tag{3.21}$$

with disjoint supports satisfying distance(supp$\{\zeta^k\}$, supp$\{\eta^k\}$) $\to \infty$. Note that there exists $c > 0$ such that

$$\begin{aligned}
&\left|\sum_{n\in\mathbb{Z}^N}\Lambda_n|\psi_n^{m_k}|^{2\sigma+2} - \sum_{n\in\mathbb{Z}^N}\Lambda_n|\zeta_n^k|^{2\sigma+2} - \sum_{n\in\mathbb{Z}^N}\Lambda_n|\zeta_n^k|^{2\sigma+2}\right|\\
&\leq c\sup_{n\in\mathbb{Z}}|\psi_n^{m_k} - \zeta_n^k - \eta_n^k|\sum_{n\in\mathbb{Z}^N}|\psi_n^{m_k}|^{2\sigma+1} \to 0, \text{ as } k \to \infty,
\end{aligned} \tag{3.22}$$

due to (3.21) and (2.4). Similarly, by (3.21) and (2.5) we can verify that

$$\left|(-\Delta_d\psi^{m_k}, \psi^{m_k})_2 - (-\Delta_d\zeta^k, \zeta^k)_2 - (-\Delta_d\eta^k, \eta^k)_2\right| \to 0, \text{ as } k \to \infty. \tag{3.23}$$

Using both (3.22) and (3.23), one yields

$$\lim_{k\to\infty}\mathcal{H}[\psi^{m_k}] = \lim_{k\to\infty}\mathcal{H}[\zeta^k] + \lim_{k\to\infty}\mathcal{H}[\eta^k], \tag{3.24}$$

$$\lim_{k\to\infty}\mathcal{H}[\zeta^k] + \lim_{k\to\infty}\mathcal{H}[\eta^k] = \mathcal{I}_R. \tag{3.25}$$

We can easily see that for any $\phi \in \ell^2$ and $\lambda > 0$,

$$\begin{aligned}\mathcal{H}[\phi] &= \frac{1}{\lambda^2}\mathcal{H}[\lambda\phi] - \frac{\lambda^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathcal{S}_+}\beta_n|\phi_n|^{2\sigma+2} + \frac{\lambda^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathcal{S}_-}\alpha_n|\phi_n|^{2\sigma+2}\\ &= \frac{1}{\lambda^2}\mathcal{H}[\lambda\phi] - \frac{\lambda^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\phi_n|^{2\sigma+2}.\end{aligned}$$

Setting $\lambda_k = \frac{\sqrt{R}}{||\zeta^k||_{\ell^2}}$, $\mu_k = \frac{\sqrt{R}}{||\eta^k||_{\ell^2}}$ we have $||\lambda_k\zeta^k||^2_{\ell^2} = R$ and $||\mu_k\eta^k||^2_{\ell^2} = R$ and

$$\begin{aligned}\mathcal{H}[\zeta^k] &= \frac{1}{\lambda_k^2}\mathcal{H}[\lambda_k\zeta^k] - \frac{\lambda_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\zeta_n^k|^{2\sigma+2} \geq \frac{\mathcal{I}_R}{\lambda_k^2} - \frac{\lambda_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\zeta_n^k|^{2\sigma+2},\\ \mathcal{H}[\eta^k] &= \frac{1}{\mu_k^2}\mathcal{H}[\mu_k\zeta^k] - \frac{\mu_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\eta_n^k|^{2\sigma+2} \geq \frac{\mathcal{I}_R}{\mu_k^2} - \frac{\mu_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\eta_n^k|^{2\sigma+2}.\end{aligned}$$

From these inequalities and the definition of $\mathcal{I}_R$ it follows that

$$\mathcal{H}[\zeta^k] + \mathcal{H}[\eta^k] \geq \mathcal{I}_R\left(\frac{1}{\lambda_k^2} + \frac{1}{\mu_k^2}\right) - \frac{\lambda_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\zeta_n^k|^{2\sigma+2} - \frac{\mu_k^{2\sigma}-1}{\sigma+1}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\eta_n^k|^{2\sigma+2}. \tag{3.26}$$

We shall pass to the limit in (3.26) as $k \to \infty$: We observe that

$$\lim_{k\to\infty}\left(\frac{1}{\lambda_k^2} + \frac{1}{\mu_k^2}\right) = \frac{\rho}{R} + \frac{R-\rho}{R} = 1,$$

as well as, that due to the assumption (3.20)

$$\begin{aligned}\lim_{k\to\infty}\lambda_k^{2\sigma} &= \frac{R^\sigma}{\rho^\sigma} > 1,\\ \lim_{k\to\infty}\mu_k^{2\sigma} &= \frac{R^\sigma}{(R-\rho)^\sigma} > 1.\end{aligned}$$

Then by using (3.22) we infer that

$$\lim_{k\to\infty}\mathcal{H}[\zeta^k] + \mathcal{H}[\eta^k] \geq \mathcal{I}_R - \frac{\xi-1}{\sigma+1}\lim_{k\to\infty}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\psi_n^{m_k}|^{2\sigma+2},\ \ \xi = \min\left\{\frac{R^\sigma}{\rho^\sigma}, \frac{R^\sigma}{(R-\rho)^\sigma}\right\}.$$

Application of the lower bound (3.17) to ψ^{m_k} implies the inequality

$$\mathcal{I}_R - \frac{\xi-1}{\sigma+1}\lim_{k\to\infty}\sum_{n\in\mathbb{Z}^N}\Lambda_n|\psi_n^{m_k}|^{2\sigma+2} \geq \mathcal{I}_R - \frac{\xi-1}{2}\mathcal{I}_R > \mathcal{I}_R,$$

since $\mathcal{I}_R < 0$. In conclusion,

$$\lim_{k\to\infty}\mathcal{H}[\zeta^k] + \mathcal{H}[\eta^k] > \mathcal{I}_R,$$

which contradicts (3.25). Henceforth the dichotomy scenario must be excluded. $\diamond$

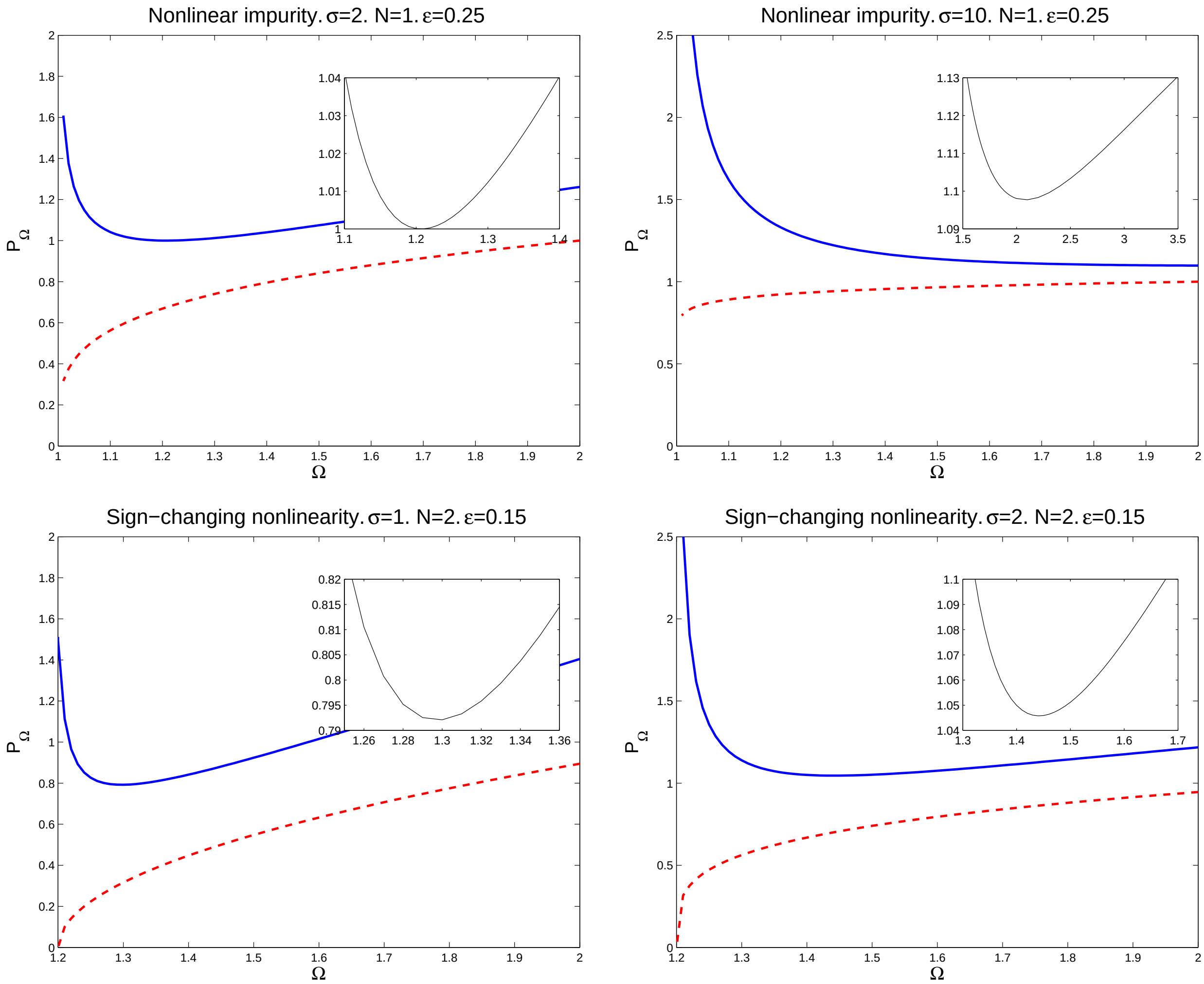

Figure 6: Numerical power for single site breathers centered at the nonlinear impurity site for $N = 1, 2$. (a) Single nonlinear impurity $\sigma = 2$, $N = 1$ ($\sigma = \sigma_{\text{crit}}$), (b) Single nonlinear impurity $\sigma = 10$, $N = 1$ ($\sigma > \sigma_{\text{crit}}$), (c) Sign-changing impurity $\sigma = 1$, $N = 2$ ($\sigma = \sigma_{\text{crit}}$), (d) Sign-changing impurity $\sigma = 2$, $N = 2$ ($\sigma > \sigma_{\text{crit}}$). The insets show magnifications of the region where the power of periodic solutions attains the excitation threshold $\mathcal{R}_{sc}$ of Theorem 3.4.

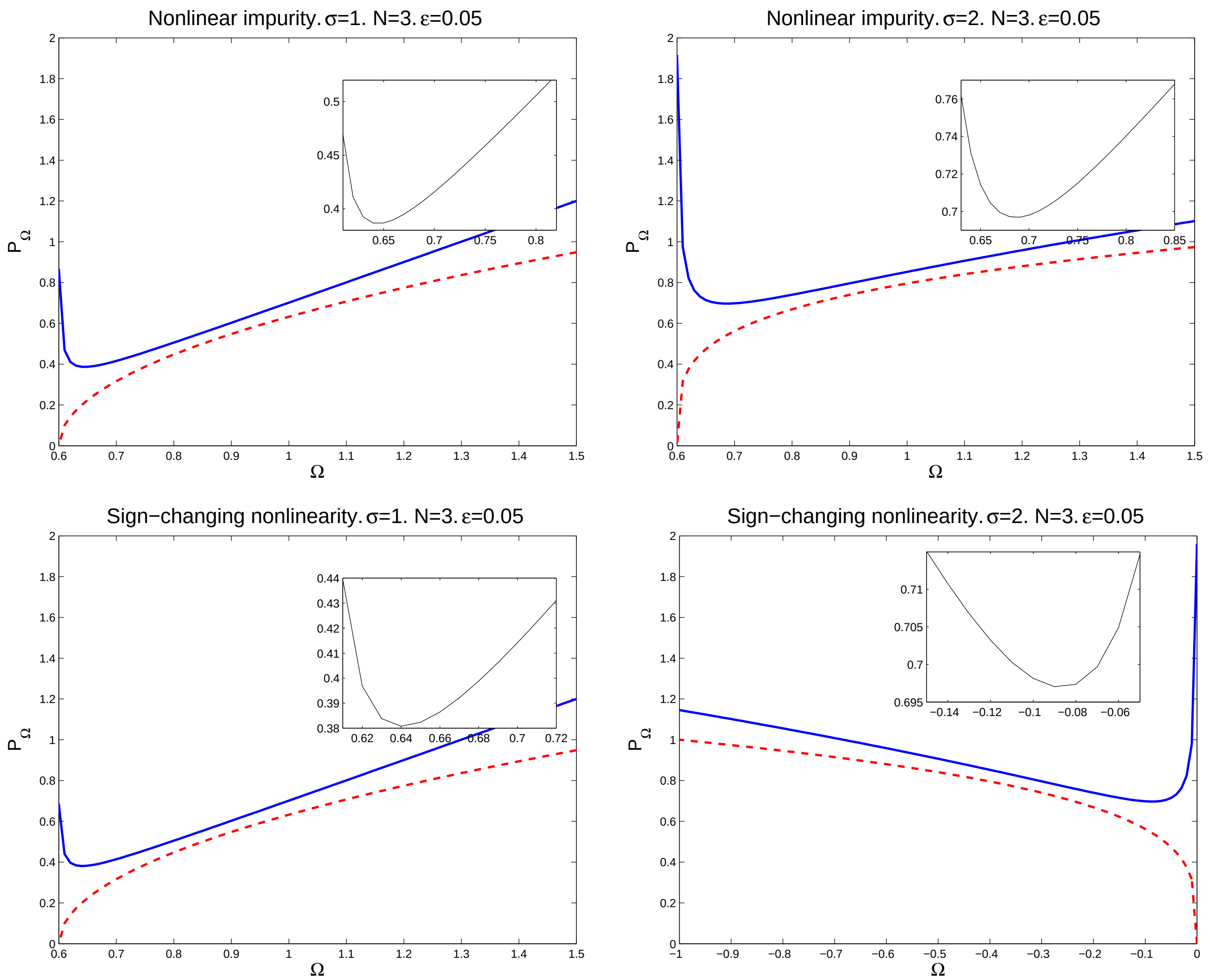

Figure 7: 3D DNLS lattices with nonlinear impurities. (a) Numerical power for single site breathers centered at the nonlinear impurity site for the single nonlinear impurity $\sigma = 1$, $N = 3$ ($\sigma > \sigma_{\mathrm{crit}}$), (b) for the single nonlinear impurity $\sigma = 2$, $N = 3$ ($\sigma > \sigma_{\mathrm{crit}}$), (c) for the sign-changing impurity $\sigma = 1$, $N = 3$. (d) Numerical power for single site unstaggered breathers far from the sign-changing impurity $\sigma = 2$, $N = 3$. The insets show magnifications of the region where the power of each breather family attains the excitation threshold $\mathcal{R}_{sc}$ of Theorem 3.4 in the 3D case.

3.1 Numerical studies in the case of nonlinear impurities

In this section we present numerical studies for the DNLS lattices with nonlinear impurities with a twofold purpose. The first aim is to present the numerical verification on the existence of the excitation threshold. The second is to review the lower bounds derived in [3], emphasizing the differences between the lower bounds and the excitation thresholds. The present study is also extended to 3D-lattices, thus covering all the cases of physical significance with respect to the dimension. The models we consider are those of a single nonlinear impurity, $\Lambda_n = \delta_{n,0}$ [14, 15, 16, 21], and of a sign-changing anharmonic parameter. In the latter, we have considered the simplest case where all sites have $\Lambda_n = 1$ except for one of them which is -1.

The panel of pictures in figure 6, demonstrates the results of the numerical study for 1D and 2D lattices. For these cases, the critical exponent $\sigma_{\mathrm{crit}} = 2/N$ for the nonlinearity exponent σ is

$$\sigma_{\mathrm{crit}} = 2, \quad \text{for} \quad N = 1$$
$$\sigma_{\mathrm{crit}} = 1, \quad \text{for} \quad N = 2,$$

and the study concerns cases $\sigma \geq \sigma_{\mathrm{crit}}$ where the excitation threshold appears. This numerical study gives the numerical verification of Theorem 3.4 on the generalization of the existence of the excitation threshold in the

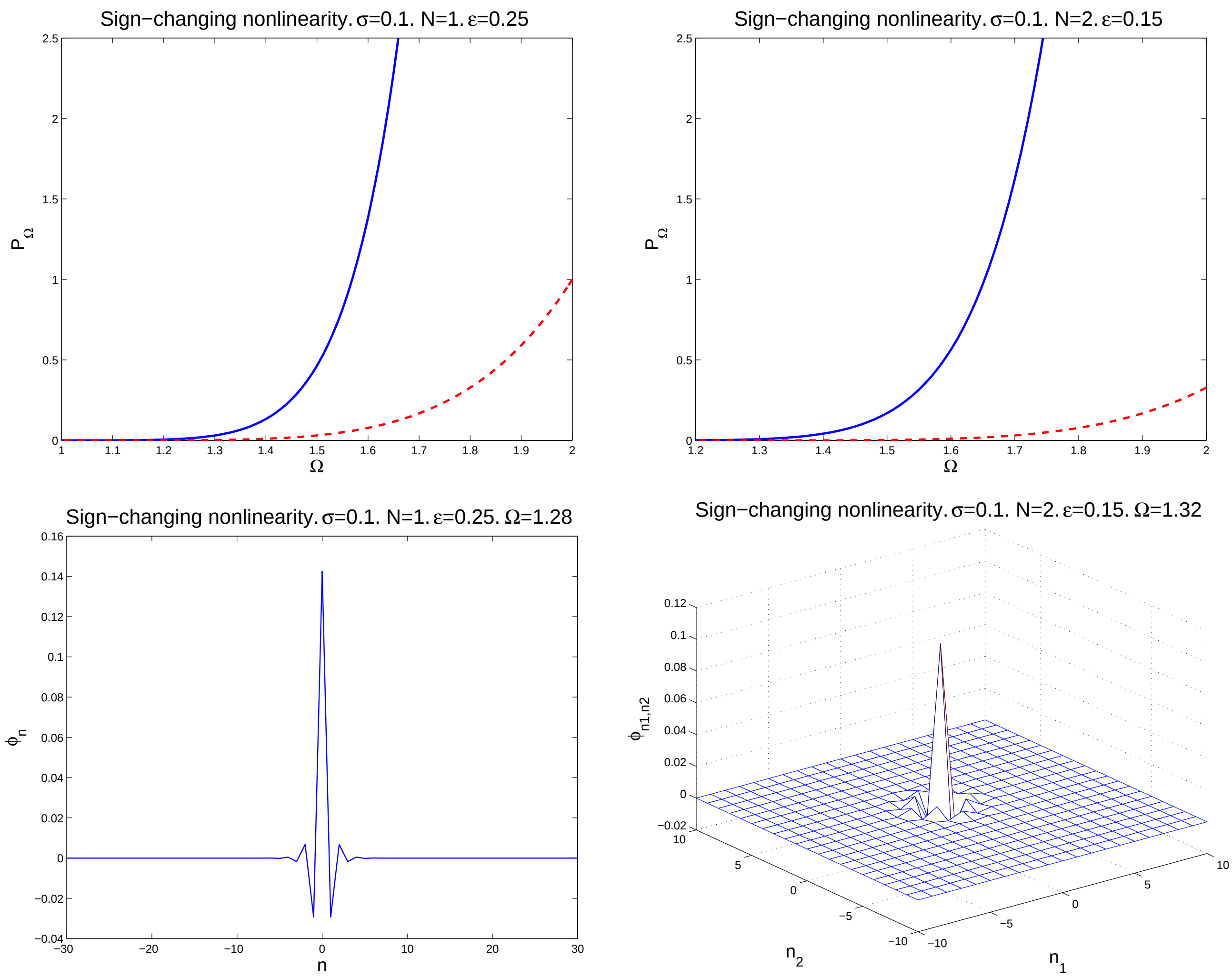

Figure 8: Numerical power for single site staggered breathers centered at the nonlinear impurity site, for the DNLS with sign-changing impurity for $\sigma = 0.1 < \sigma_{\mathrm{crit}}$. (a) $N = 1$, (b) $N = 2$. The lower bound $\mathcal{R}_{\mathrm{lb}}(\Omega)$ is fulfilled. (c), (d) Breather profiles with power close to the lower bound.

case of nonlinear impurities. The inset in each picture demonstrates the positive lower energy bound $\mathcal{R}_{sc}$ of Theorem 3.4. The numerical power as well as the excitation threshold $\mathcal{R}_{sc}$ has been calculated for *staggered breathers* of the defocusing DNLS. The numerical power has been drawn against the theoretical lower bound

$$\mathcal{R}_{\mathrm{lb}} := \left[\frac{\Omega - 4N\epsilon}{\max_{n\in\mathcal{S}_+}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \Omega > 4\epsilon N, \;\; \sigma > 0, \tag{3.27}$$

derived in [3, Theorem 3.1, pg. 77], and justifies that $\mathcal{R}_{\mathrm{lb}}$ is fulfilled for breathers with frequency $\Omega > 4\epsilon N$. Picture (b) indicates that $\mathcal{R}_{\mathrm{lb}}(\Omega)$ is becoming a satisfactory estimate for large σ and for large values of frequencies Ω, as an Ω-dependent lower bound for existence.

The effectiveness and strength of the theoretical explicit lower bounds become even more apparent in the 3D-lattices. In Figure 7, the numerical study of (3.27) for the cases $N = 1, 2$ in [3] is extended to the case $N = 3$. For the 3D-lattice, the critical exponent is

$$\sigma_{\mathrm{crit}} = \frac{2}{3}, \;\; \text{for} \;\; N = 3.$$

The examples considered $\sigma = 1, 2$ correspond to the supercritical case $\sigma > \sigma_{\mathrm{crit}}$ and the insets in each picture justify numerically the appearance of the excitation threshold $\mathcal{R}_{sc}$ in the three dimensional lattice. The range of frequencies $0.8 < \Omega < 1$ in pictures (a), (b), (c), corresponds to the members of the *staggered breather family* with power approaching the lower bound $\mathcal{R}_{\mathrm{lb}}(\Omega)$ with increased accuracy and in a quite sharp manner for $\sigma > \sigma_{\mathrm{crit}}$. The insets in each picture justify numerically the appearance of the excitation threshold $\mathcal{R}_{sc}$ in the three dimensional lattice. To elucidate further the difference between the excitation threshold $\mathcal{R}_{sc}$ and the lower bound $\mathcal{R}_{\mathrm{lb}}(\Omega)$, let us remark that the example of frequencies $0.8 < \Omega < 1$ corresponds to frequencies $\Omega > \Omega_{\mathrm{thresh}}$ =the frequency of the minimizer on which the excitation threshold $\mathcal{R}_{sc}$ is attained. In the example (c), it is found that $\mathcal{R}_{sc} = 0.6968$ at $\Omega_{\mathrm{thresh}} = 0.69$. Picture (d) in particular, shows the numerical power of the family of *unstaggered breathers which are infinitely far from the sign-changing impurity* against the theoretical estimate

$$\hat{\mathcal{R}}_{\mathrm{lb}}(\Omega) = \left[\frac{\epsilon\lambda_1 - \Omega}{-\min_{n\in\mathcal{S}_-}\{\Lambda_n\}}\right]^{\frac{1}{\sigma}} \quad < \quad R^2, \;\; \Omega \in (-\infty, \epsilon\lambda_1), \;\; \sigma > 0,$$

of [3, Remark 3.2, pg. 80]. Estimate (3.28) is valid for any unstaggered breather $\psi_n(t) = e^{-\mathrm{i}\Omega t}\phi_n$, for any $\Omega < 0$. The range of frequencies $-0.5 < \Omega < -0.2$ in (d), corresponds to the members of the unstaggered breather family far from the impurity with power very close to the lower bound $\hat{\mathcal{R}}_{\mathrm{lb}}(\Omega)$. For this breather family it is found that $\mathcal{R}_{sc} = 0.6970$ at $\Omega_{\mathrm{thresh}} = -0.09$. We remark here that a complete study of $\hat{\mathcal{R}}_{\mathrm{lb}}(\Omega)$ requires also the study of the unstaggered breathers which are centered at the site adjacent to the impurity, since our numerical studies revealed that there is a range of frequency for which the smallest power breather is attained for this kind of breather family.

Figure 8 considers the example of DNLS lattices with sign-changing impurity in the case $\sigma = 0.1$, a "limiting case" of $\sigma < \sigma_{\mathrm{crit}}$ *where the excitation threshold do not exist.* This study shows that although there is no excitation threshold $\mathcal{R}_{sc}$, breathers with $\Omega > 4\epsilon N$ have power fulfilling $\mathcal{R}_{\mathrm{lb}}(\Omega)$. Breathers with frequency $1 < \Omega < 1.3$ and $1.2 < \Omega < 1.4$ in the 1D and 2D case respectively, are the real examples with power approaching sharply to the theoretical lower bound $\mathcal{R}_{\mathrm{lb}}(\Omega)$, justifying that this bound can be considered as a theoretical prediction of the smallest power for any breather family. Pictures (c) and (d) show two members of these families. In Figure 9, where the 3D case is considered, we observe that the range of frequencies for breathers close to the lower bound is increased. The results of the numerical study can be summarized in Figure 10, where the power of staggered breathers has been plotted as a function of Ω and σ. The upper (blue) surface corresponds to the numerical power while the lower (red) surface to the lower bound (3.27). The comparison between both surfaces makes evident the effectiveness of the theoretical estimates as a local prediction with respect to the frequency, of the smallest power for breathers in DNLS lattices with nonlinear impurities.

4 Lower bounds on the kinetic energy of traveling waves of periodic FPU lattices

In this section, we prove the existence of a lower bound on the kinetic energy for the existence of traveling waves of prescribed speed, on a finite lattice, supplemented with periodic boundary conditions. For instance, we shall

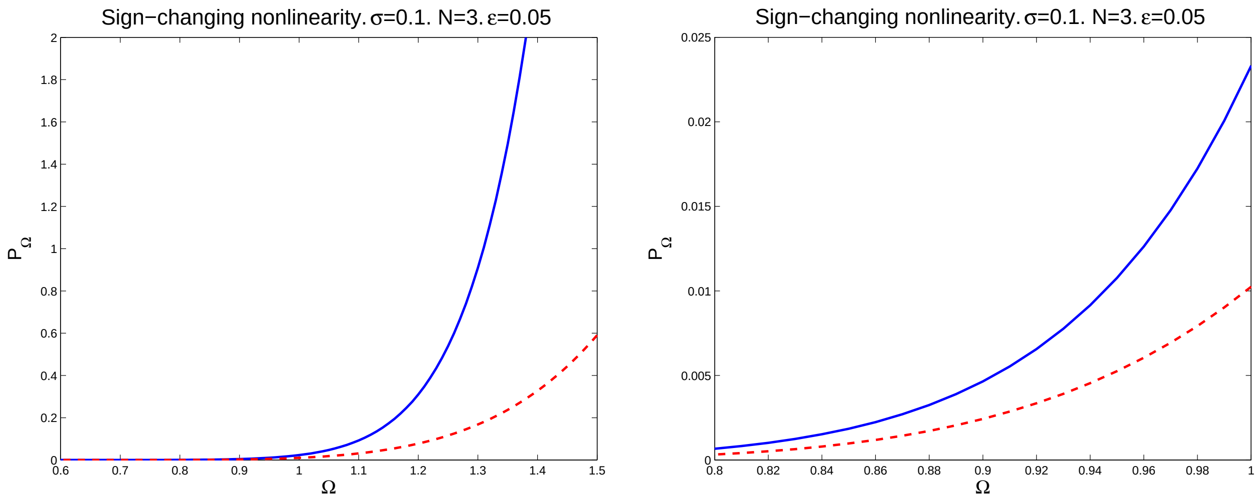

Figure 9: (a) Numerical power for single site staggered breathers centered at the nonlinear impurity site, for the DNLS with sign-changing impurity for $\sigma = 0.1 < \sigma_{\text{crit}}$ for $N = 3$. (b) Magnification for the range of frequencies $0.8 < \Omega < 1$.

consider the equation of motion

$$\ddot{q_n} = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}), \tag{4.1}$$

where q_n denotes the displacement of the nth particle from its equilibrium position, and $V(q_{n+1} - q_n)$ is the anharmonic interaction potential. The Hamiltonian of system (4.1) is

$$H = \sum_n \left(\frac{1}{2}\dot{q}_n^2 + V(q_{n+1} - q_n) \right). \tag{4.2}$$

A solitary wave of (4.1) is a solution of the form

$$q_n(t) = u(n - ct) = u(z), \text{ with } u(z) \to 0 \text{ as } |z| \to \infty. \tag{4.3}$$

Substitution of (4.3) in (4.1) results in the forward-backward differential-difference equation

$$c^2 u''(z) = V'[u(z+1) - u(z)] - V'[u(z) - u(z-1)]. \tag{4.4}$$

We refer to the monograph [18] for rigorous results on the analysis of periodic oscillations and traveling waves of FPU lattices.

In this first investigation will shall consider the case of a *periodic* lattice of $2L$ particles, $-L \leq n \leq L$. This case is of the same importance for numerical simulations with periodic boundary conditions, since the infinite lattice cannot be modeled numerically. We shall consider the case of the potential

$$V(u) = \gamma^2 \frac{u^2}{2} + \alpha^2 \frac{u^p}{p}, \quad \gamma \geq 0, \quad p > 2, \tag{4.5}$$

which covers the case of the classical Fermi, Pasta and Ulam study (FPU). In the FPU study $p = 3$ or 4, [4]. It is important at this point, to remark some important results on the existence of traveling waves for the system (4.1). In the case of the potential (4.5) the existence of non-trivial traveling waves in infinite lattices, has been resolved through the study of (4.4) by variational methods in [8, 23].The approach of [8] is based on minimizing the *average kinetic energy*

$$T(u) := \frac{1}{2} \int_{\mathbb{R}} u'(z)^2 dz, \tag{4.6}$$

subject to the constraint $\int_{\mathbb{R}} V[u(z-1) - u(z)]dz = K$ (prescribed average potential energy). The speed c of the wave is given by an unknown Lagrange multiplier. The approach of [23] is based on the application of the

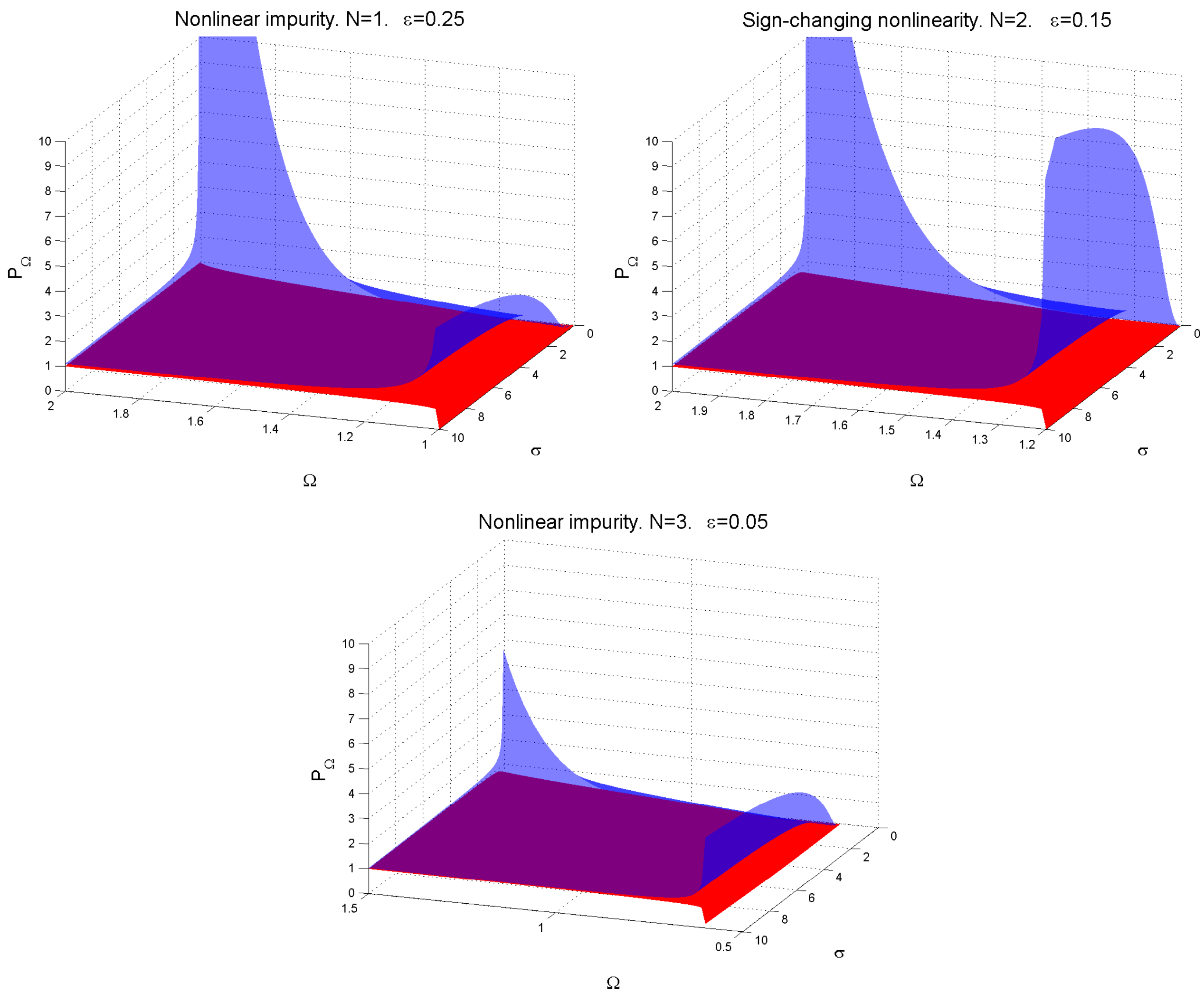

Figure 10: Numerical power against the theoretical lower bound, as a function of Ω, σ. (a) Single nonlinear impurity $N = 1$ (b) Sign-changing impurity $N = 2$ (c) Single-nonlinear impurity $N = 3$.

mountain pass theorem, providing the existence of nontrivial traveling waves of *prescribed speed c*. For instance:
(a) in the case of the potential (4.5) with $p = 2m + 1$, $m \in \mathbb{N}$, equation (4.4) has a nontrivial *nondecreasing* solution for every $c > \gamma$.
(b) In the case of the potential (4.5) with $p = 2m$, $m \in \mathbb{N}$, equation (4.4) has a pair of opposite nontrivial solutions, one *nondecreasing and the other nonincreasing*, for every $c > \gamma$.

We remark that monotonicity properties are considered in the sense that the corresponding wave profile is a monotone function or, equivalently, the relative displacement profile is either positive or negative (see [18], [19, pg. 1225], [23, Section 3 & pg. 274]). This notion of monotonicity has a physical implementation. Increasing waves are expansion waves while decreasing waves are compression waves [18, pg. 78].

The case of the periodic lattice was considered in [19]. The existence of periodic traveling waves with prescribed speed and arbitrary period is proved with mountain pass arguments, while the existence of waves with minimal possible averaged action (ground waves) is proved by the Nehari variational principle.

Motivated by these existence results, we shall apply the fixed-point argument of [2], this time to the problem (4.4)-(4.5), to derive an explicit lower bound T_{thresh} on the average kinetic energy (4.6) satisfied by traveling waves *of sufficiently large speed* $c > c^*$. The lower bound T_{thresh} is a threshold for the existence of traveling waves of speed $c > c^*$ in the sense that we should not expect traveling waves $q_n(t) = u(z)$ of speed $c > c^*$ with average kinetic energy $T(u) \leq T_{\text{thresh}}$. This result is given in Theorem 4.5.

4.1 Derivation of the lower bound on the average kinetic energy

Problem (4.4) in the periodic lattice is naturally formulated in Sobolev spaces of periodic functions used in [19]: For instance, (4.4) will be considered in the Hilbert space of periodic functions

$$\mathcal{X}_1 := \left\{ u \in \dot{H}^1(\mathbb{R}) \ : \ u'(z + 2L) = u'(z), \ \ u(0) = 0 \right\},$$

endowed with the scalar product and induced norm

$$(u, v)_1 = \int_{-L}^{L} u'(z)v'(z)dt, \ \ ||u||_1^2 = \int_{-L}^{L} u'(z)^2 dt.$$

It can be easily checked that with the normalizing condition $u(0) = 0$, the Poincaré inequality

$$\int_{-L}^{L} u(z)^2 dt \leq \tilde{C}(L) \int_{-L}^{L} u'(z)^2 dt, \tag{4.7}$$

holds with $\tilde{C}(L) = L^2$, while the optimal constant $\tilde{C}(L) = \frac{L^2}{\pi^2}$ can be used when one considers the Hilbert space of $2L$-periodic functions. We rewrite equation (4.4) as

$$-u''(z) = \frac{1}{c^2} \left\{ V'[u(z) - u(z-1)] - V'[u(z+1) - u(z)] \right\}. \tag{4.8}$$

To apply the fixed point argument, we shall need the existence of solutions to *an auxiliary problem related to (4.4)-(4.5).* For convenience to the reader we recall Friedrich's extension Theorem.

Theorem 4.2 *Let $\mathcal{L}_0 : D(\mathcal{L}_0) \subseteq \mathcal{X}_0 \to \mathcal{X}_0$ be a linear symmetric operator on the Hilbert space $\mathcal{X}_0$ with its domain $D(\mathcal{L}_0)$ being dense in $\mathcal{X}_0$. Assume that there exists a constant $c > 0$ such that*

$$(\mathcal{L}_0 u, u)_{\mathcal{X}_0} \geq c||u||^2_{\mathcal{X}_0} \ \ \textit{for all} \ \ u \in D(\mathcal{L}_0).$$

Then $\mathcal{L}_0$ has a self-adjoint extension $\mathcal{L} : D(\mathcal{L}) \subseteq \mathcal{X}_1 \subseteq \mathcal{X}_0 \to \mathcal{X}_0$ where $\mathcal{X}_1$ denotes the energy Hilbert space endowed with the energy scalar product $(u, v)_{\mathcal{X}_1} = (\mathcal{L}u, v)_{\mathcal{X}_0}$ for all $u, v \in \mathcal{X}_1$ and the energy norm $||u||^2_{\mathcal{X}_1} = (\mathcal{L}u, v)_{\mathcal{X}_0}$. Furthermore, the operator equation

$$\mathcal{L}u = f, f \in \mathcal{X}_0,$$

has a unique solution $u \in D(\mathcal{L})$. In addition, if $\hat{\mathcal{L}} : \mathcal{X}_1 \to \mathcal{X}_1^*$ denotes the energy extension of $\mathcal{L}$, then $\hat{\mathcal{L}}$ is the canonical isomorphism from $\mathcal{X}_1$ to its dual $\mathcal{X}_1^*$ and the operator equation

$$\hat{\mathcal{L}}u = f, f \in \mathcal{X}_1^*,$$

has also a unique solution $u \in \mathcal{X}_1$.

It is well known that Theorem 4.2 is applicable to the operator $\mathcal{L}_0 : D(\mathcal{L}_0) \subseteq L^2(-L,L) \to L^2(-L,L)$, $\mathcal{L}_0 u = -u''(z)$, with domain of definition the space $D(\mathcal{L}_0)$ the space of C^∞-functions on $[-L,L]$. Since $D(\mathcal{L}_0)$ is dense in $\mathcal{X}_0$, and inequality (4.7) holds, the Friedrich's extension of $\mathcal{L}_0$ is the operator $\mathcal{L} : D(\mathcal{L}) \to \mathcal{X}_0$ where

$$D(\mathcal{L}) = \left\{u \in \mathcal{X}_1 \;:\; \mathcal{L}u \in L^2(-L,L)\right\}.$$

The operator equation

$$-u''(z) = f, \;\text{ for every }\; f \in L^2(-L,L) \tag{4.9}$$

has a unique solution in $D(\mathcal{L})$. Thus as an auxiliary problem we shall consider the equation

$$-u''(z) = \frac{1}{c^2}\left\{V'[\psi(z)-\psi(z-1)] - V'[\psi(z+1)-\psi(z)]\right\}, \tag{4.10}$$

for some fixed $\psi \in \mathcal{X}_1$. We also recall the following key lemma [19, Lemma 1,pg. 1225].

Lemma 4.3 *The linear operators*

$$A_1 u = u(z+1) - u(z) = \int_z^{z+1} u'(s)ds, \;\; A_2 u(z) = u(z) - u(z-1) = \int_{z-1}^{z} u(s)ds,$$

are continuous from $\mathcal{X}_1$ *to* $L^2(-L,L) \cap L^\infty(-L,L)$ *and* $||A_i u||_\infty \leq ||u||_1$, $||Au||_0 \leq ||u||_1$, $i = 1,2$.

With Lemma 4.3 in hand we may proceed to the proof of

Proposition 4.4 *For any* $\psi \in \mathcal{X}_1$*, the equation (4.10) has a unique solution* $u \in D(\mathcal{L})$.

Proof: Equation (4.10) can be rewritten as

$$-u''(z) = \frac{1}{c^2}\left\{V'[A_2\psi(z)] - V'[A_1\psi(z)]\right\}, \tag{4.11}$$

where $V'(s) = \gamma^2 s + s^{p-1}$. Note that

$$\begin{aligned}\int_{-L}^{L} |V'[A_2\psi(z)] - V'[A_1\psi(z)]|^2 dz \;\; &\leq \;\; \gamma^4 \int_{-L}^{L} |A_2\psi(z) - A_1\psi(z)|^2 dz \\ &+ \;\; \alpha^4 \int_{-L}^{L} \left|[A_2\psi(z)]^{p-1} - [A_1\psi(z)]^{p-1}\right|^2 dz. \end{aligned}\tag{4.12}$$

To estimate the second term of the right-hand side of (4.12) we shall use the inequality

$$\int_{-L}^{L} |s_1^{p-1} - s_2^{p-1}|^2 \;\; \leq \;\; (p-1)^2 \int_{-L}^{L} \left\{\int_0^1 |\xi|^{p-2}|s_1 - s_2| d\theta\right\}^2, \tag{4.13}$$

where $s_1,\; s_2 \in \mathbb{R}$, and $\xi = \theta s_1 + (1-\theta)s_2$, $\theta \in (0,1)$. Then, we have that

$$\int_{-L}^{L} \left|[A_2\psi(z)]^{p-1} - [A_1\psi(z)]^{p-1}\right|^2 dz \leq (p-1)^2 ||\xi||_\infty^{2(p-2)} \int_{-L}^{L} |A_2\psi(z) - A_1\psi(z)|^2 dz, \tag{4.14}$$

where $\xi = \theta A_2\psi(z) + (1-\theta)A_1\psi(z)$. By using Lemma 4.3, we deduce that $||\xi||_\infty^{2(p-2)} \leq ||\psi||_1^{2(p-2)}$ and from (4.12) and (4.14) the inequality

$$\begin{aligned} ||V'[A_2\psi] - V'[A_1\psi]||_0^2 \;\; &\leq \;\; (\gamma^4 + \alpha^4 ||\psi||_1^{2(p-2)})||A_2\psi - A_1\psi||_0^2 \\ &\leq \;\; 4(\gamma^4 + \alpha^4 ||\psi||_1^{2(p-2)})||\psi||_1^2. \end{aligned}$$

Thus $\mathcal{V}[\psi(z)] = V'[A_2\psi(z)] - V'[A_1\psi(z)]$ defines a map $\mathcal{V} : \mathcal{X}_1 \to L^2(-L,L)$. Thus, from Friedrich's extension Theorem 4.2, equation (4.10)

$$-u''(z) = \frac{1}{c^2}\mathcal{V}[\psi(z)], \tag{4.15}$$

for any $\psi \in \mathcal{X}_1$ has a unique solution $u \in H^2(-L, L) \cap \mathcal{X}_1$. □

Let us now consider for some $R > 0$ the closed ball of $\mathcal{X}_1$, $\mathcal{B}_R := \{\psi \in \mathcal{X}_1 : ||\psi||_1 \leq R\}$. Proposition 4.4 shows that the map $\mathcal{S} : \mathcal{X}_1 \to \mathcal{X}_1$ defined as

$$\mathcal{S}[\psi] = u,$$

where u is the unique solution of the auxiliary problem (4.15), is well defined. Hence we may consider $\psi_1, \psi_2 \in \mathcal{B}_R$ such that

$$u = \mathcal{S}[\psi_1] \quad \text{and} \quad v = \mathcal{S}[\psi_2].$$

Then the difference $U = u - v$ satisfies the equation

$$\begin{aligned} -U''(z) &= \frac{1}{c^2} \{\mathcal{V}[\psi_1(z)] - \mathcal{V}[\psi_2(z)]\} \\ &= \frac{1}{c^2} \{V'[A_1\psi_2(z)] - V'[A_1\psi_1(z)] + V'[A_2\psi_1(z)] - V'[A_2\psi_2(z)]\}. \end{aligned} \tag{4.16}$$

From Lemma 4.3 the linear operators $A_i : \mathcal{X}_1 \to L^2(-L, L) \cap L^\infty(-L, L)$ are globally Lipschitz,

$$\begin{aligned} ||A_i\psi_1 - A_i\psi_2||_0 &\leq ||\psi_1 - \psi_2||_1, \\ ||A_i\psi_1 - A_i\psi_2||_\infty &\leq ||\psi_1 - \psi_2||_1. \end{aligned} \tag{4.17}$$

Using once again the inequality (4.13) we get that

$$\int_{-L}^{L} \left|[A_1\psi_2(z)]^{p-1} - [A_1\psi_1(z)]^{p-1}\right|^2 dz \leq (p-1)^2 ||\Psi||_\infty^{2(p-2)} \int_{-L}^{L} |A_1\psi_2(z) - A_1\psi_1(z)|^2 dz, \tag{4.18}$$

where this time $\Psi = \theta A_1\psi_2(z) + (1-\theta)A_1\psi_1(z)$. From Lemma 4.3, we have

$$\begin{aligned} ||\Psi||_\infty &\leq \theta ||A_1\psi_2||_\infty + (1-\theta)||A_1\psi_1||_\infty \\ &\leq \theta ||\psi_2||_1 + (1-\theta)||\psi_1||_1. \end{aligned}$$

Therefore, since $\psi_1, \psi_2 \in \mathcal{B}_R$, we have that $||\Psi||_\infty \leq R$. Thus by using (4.17) and (4.18) we deduce the inequality

$$||V'[A_1\psi_1] - V'[A_1\psi_2]||_0 \leq \gamma^2 ||\psi_1 - \psi_2||_1 + \alpha^2(p-1)R^{p-2}||\psi_1 - \psi_2||_1.$$

By the same token,

$$||V'[A_2\psi_1] - V'[A_2\psi_2]||_0 \leq \gamma^2 ||\psi_1 - \psi_2||_1 + \alpha^2(p-1)R^{p-2}||\psi_1 - \psi_2||_1.$$

Hence, for the right-hand side of (4.16) we get

$$||\mathcal{V}[\psi_1(z)] - \mathcal{V}[\psi_2(z)]||_0 \leq 2(\gamma^2 + \alpha^2(p-1)R^{p-2})||\psi_1 - \psi_2||_1. \tag{4.19}$$

Next, by multiplying (4.16) in the $L^2(-L, L)$-scalar product and the usual trick, the estimate

$$\begin{aligned} ||U||_1^2 &\leq \frac{1}{c^2} ||\mathcal{V}[\psi_1(z)] - \mathcal{V}[\psi_2(z)]||_0 \, ||U||_0 \\ &\leq \frac{2\tilde{C}^{\frac{1}{2}}}{c^2}(\gamma^2 + \alpha^2(p-1)R^{p-2})||\psi_1 - \psi_2||_1 \, ||U||_1 \\ &\leq \frac{1}{2}||U||_1^2 + \frac{2\tilde{C}}{c^4}(\gamma^2 + \alpha^2(p-1)R^{p-2})^2 ||\psi_1 - \psi_2||_1^2, \end{aligned} \tag{4.20}$$

follows. Note that the Poincaré inequality (4.7) has been used. From (4.20), we conclude with

$$||U||_1^2 = ||\mathcal{S}[\psi_1] - \mathcal{S}[\psi_2]||_1^2 \leq \frac{4\tilde{C}}{c^4}(\gamma^2 + \alpha^2(p-1)R^{p-2})^2 ||\psi_1 - \psi_2||_1^2. \tag{4.21}$$

From (4.21), we observe that if the Lipschitz constant

$$\frac{2\sqrt{\tilde{C}}}{c^2}(\gamma^2 + \alpha^2(p-1)R^{p-2}) < 1, \tag{4.22}$$

the map $\mathcal{S} : \mathcal{B}_R \rightarrow \mathcal{B}_R$ is a contraction. Hence the map $\mathcal{S}$ satisfies the assumptions of the Banach-fixed point theorem and has a unique fixed point. By (4.5), we have that $\mathcal{V}(0) = 0$. Therefore we deduce that if (4.22) holds, the unique fixed point is the trivial one. *Thus nontrivial solutions exist only if (4.22) is violated, that is when*

$$\frac{2\sqrt{\tilde{C}}}{c^2}(\gamma^2 + \alpha^2(p-1)R^{p-2}) > 1. \tag{4.23}$$

On the account of (4.23), we may summarize in

Theorem 4.5 *Consider the system (4.1)-(4.5) in the periodic lattice of $2L$ particles, $-L \leq n \leq L$. Every nontrivial traveling wave solution $q_n(t) = u(n - ct) = u(z)$ with speed*

$$c > \sqrt{2}\tilde{C}^{\frac{1}{4}}\gamma = c^* \tag{4.24}$$

must have average kinetic energy $T(u) = \frac{1}{2}\int_{-L}^{L} u'(z)^2 dz$ satisfying the lower bound

$$T_{\rm thresh} := \frac{1}{2}\left(\frac{c^2 - 2\sqrt{\tilde{C}}\gamma^2}{2\alpha^2(p-1)L}\right)^{\frac{2}{p-2}} < T(u). \tag{4.25}$$

Clearly (4.24) do not contradicts the the condition $c > \gamma$ for the existence of traveling waves in the case of the potential (4.5). We may implement (4.25) as a threshold value on the average kinetic energy for the existence of traveling waves of relatively high-speed $c > c^*$.

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References

[1] S. N. Chow and J. K. Hale. *Methods of Bifurcation Theory*, Grundlehren der mathematischen Wissenschaften – A series of Comprehensive Studies in Mathematics 251, Springer-Verlag, New-York, 1982.

[2] J. Cuevas, J. C. Eilbeck and N. I. Karachalios. *Thresholds for time periodic solutions on the Discrete Nonlinear Schrödinger Equation with saturable and power nonlinearity.* Discrete Cont. Dyn. Syst. **21** (2) (2008), 445-475.

[3] J. Cuevas, J. C. Eilbeck and N. I. Karachalios. *A lower bound for the power of periodic solutions of the defocusing discrete nonlinear Schrödinger equation.* Dyn. Partial Differ. Equ. **5** (2008), no. 1, 69–85.

[4] D. B. Duncan, J. C. Eilbeck, H. Feddersen and J. A. D. Wattis. *Solitons on lattices.* Phys. D **68** (1993), 1-11.

[5] J. C. Eilbeck and M. Johansson. *The Discrete Nonlinear Schrödinger Equation-20 Years on.* "Localization and Energy transfer in Nonlinear Systems, eds L. Vázquez, R.S. MacKay, M.P. Zorzano. World Scientific, Singapore, (2003), 44-67.

[6] S. Flach, K. Kladko and R. MacKay. *Energy thresholds for discrete breathers in one-, two-, and three dimensional lattices.* Phys. Rev. Lett. **78** (1997), 1207-1210.

[7] S. Flach and A. V. Gorbach. *Discrete breathers – Advances in theory and applications.* Physics Reports **467** (2008), No. 1-3, 1-116.

[8] G. Friesecke and J. D. Wattis. *Existence Theorem for Solitary waves on lattices.* Commun. Math. Phys. **161** (1994), 391-418.

[9] G. James, B. Sánchez–Rey and J. Cuevas. *Breathers in inhomogeneous nonlinear lattices : an analysis via centre manifold reduction* . Rev. Math. Phys. **21** (2009), 1-58.

[10] N. I. Karachalios. *A remark on the existence of breather solutions for the Discrete Nonlinear Schrödinger Equation: The case of site dependent anharmonic parameter*, Proc. Edinburgh Math. Society **49** no.1, (2006), 115-129.

[11] M. Kastner. *Energy Thresholds for Discrete Breathers*, Phys. Rev. Lett **92**, no. 10, (2004) 104301.

[12] P. G. Kevrekidis, K. Ø. Rasmussen and A. R. Bishop. *The discrete nonlinear Schrödinger equation: A survey of recent results*, Int. Journal of Modern Physics B **15** (2001), 2833-2900.

[13] P. G. Kevrekidis, H. Susanto and Z. Chen. *High-order-mode soliton structures in two-dimensional lattices with defocusing nonlinearity*, Phys. Rev. E **74** (2006), 066606.

[14] M. I. Molina. *Nonlinear Impurity in a square lattice*, Phys. Rev. B **60** (1999), 2276-2280.

[15] M. I. Molina and H. Bahlouli. *Conductance through a single nonlinear impurity*, Phys. Lett. A **294** (2002), 87-94.

[16] M. I. Molina. *Nonlinear Impurity in a lattice: Dispersion effects*, Phys. Rev. B **67** (2003), 054202.

[17] F. Palmero, R. Carretero-González, J. Cuevas, P. Kevrekidis and W. Królikowski. *Solitons in one dimensional nonlinear Schrödinger lattices with a local inhomogeneity.* Physical Review E **77** (2008), 036614.

[18] A. A. Pankov. Travelling waves and periodic oscillations in Fermi-Pasta-Ulam lattices. Imperial College Press 2005.

[19] A. A. Pankov and K. Pflüger. *Travelling waves in Lattice Dynamical systems.* Math. Meth. Appl. Sc. **23** (2000), 1223-1235.

[20] A. A. Pankov and N. Zakharchenko. *On some discrete variational problems, Special issue dedicated to Antonio Avantaggiati on the occasion of his 70th birthday.* Acta Appl. Math. **65** (2001), 295303.

[21] G. P. Tsironis, M. I. Molina and D. Hennig. *Generalized nonlinear impurity in a linear chain*, Phys. Rev. E **50**, (1994), 2365-2368.

[22] M. Weinstein. *Excitation thresholds for nonlinear localized modes on lattices*, Nonlinearity **12** (1999), 673-691.

[23] M. Willem and D. Smets. *Solitary Waves with prescribed speed on lattices.* J. Funct. Anal, **149** (1997), 266-275.

[24] E. Zeidler. *Nonlinear functional analysis and its applications, Vol. II/A. Linear Monotone Operators.* Springer-Verlag, New York, 1990.