Homoclinic standing waves in focusing DNLS equations
Variational approach via constrained optimization

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Abstract

We study focusing discrete nonlinear Schrödinger equations and present a new variational existence proof for homoclinic standing waves (bright solitons). Our approach relies on the constrained maximization of an energy functional and provides the existence of two one-parameter families of waves with unimodal and even profile function for a wide class of nonlinearities. Finally, we illustrate our results by numerical simulations.

Keywords: discrete nonlinear Schrödinger equation (DNLS), homoclinic standing waves, solitary waves, bright solitons, breathers, nonlinear lattice waves, constrained maximization

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1 Introduction

The discrete nonlinear Schrödinger equation (DNLS) is one of the most fundamental lattice equations and plays a prominent role in the theories of optical waveguides, photorefractive crystals, and Bose-Einstein condensates. For an overview on applications and results we refer the reader to [KRB01, EJ03, Kev09a, Por09] and the references therein. In this paper we aim in contributing to the mathematical theory of DNLS by giving a new variational existence proof for homoclinic standing waves.

In one space dimension the homogeneous DNLS is given by

\[ i \dot{A}_j + \alpha (A_{j+1} + A_{j-1} - 2A_j) + \beta A_j + \Psi'(|A_j|^2)A_j = 0, \]

(1)

where \( j \) is the discrete space variable, \( t \) is the time, and \( A_j = A_j(t) \) is the complex-valued amplitude or the value of the wave function. The potential function \( \Psi \) is often assumed to be monomial with \( \Psi'(x) = x \) and \( \Psi'(x) = x^2 \) for the cubic and quintic DNLS, respectively.

For our purposes it is more convenient to simplify the linear terms by means of the gauge invariance of DNLS, that is the symmetry under \( u_j \sim e^{i\varphi}u_j \) with \( \varphi \in \mathbb{R} \). More precisely, with \( A_j \sim e^{i(\beta-2\alpha)t}A_j \) we readily verify that (1) is equivalent to

\[ i \dot{A}_j + \alpha (A_{j+1} + A_{j-1}) + \Psi'(|A_j|^2)A_j = 0. \]

(2)

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It is well established that the dynamical properties of (2) strongly depend on the sign and strength of the coupling parameter $\alpha$. For convex $\Psi$, one usually refers to $\alpha > 0$ and $\alpha < 0$ as the focusing and defocusing case, respectively. In the anti-continuum limit $\alpha \to 0$ the DNLS becomes a system of uncoupled oscillators, whereas in the continuum limit $\alpha \to \pm \infty$ the DNLS can be viewed as a finite difference approximation of the nonlinear Schrödinger PDE (via the scaling $j \sim \sqrt{|1/\alpha|} j$).

During the last decades a great deal of attention has been paid to coherent structures such as travelling waves and standing waves. Standing waves can be regarded as relative equilibria which stem from the gauge invariance. They are special solutions to (2) with $A_j(t) = e^{i\sigma t} u_j(t)$, where the profile $u = (u_j)^n_j$ is assumed to take values in $\mathbb{R}$ and satisfies

$$\sigma u_j = \alpha (u_{j+1} + u_{j-1}) + \Psi'(u_j^2) u_j. \tag{3}$$

Standing waves come in different types: Periodic waves (or wave trains) satisfy $u_j = u_{j+N}$ for some periodicity length $N < \infty$. Homoclinic waves (solitons, solitary waves) are localized via $\lim_{j \to \pm \infty} u_j = 0$, and are hence also breathers. Finally, heteroclinic waves (fronts, kinks) connect different asymptotic states.

The existence of standing wave solutions to (2) has been investigated by several authors using rather different methods. Sometimes it is possible to find exact solutions, see [ELS85, KRSS05], but in general one needs more sophisticated and robust arguments. A perturbative approach to the existence problem was developed by MacKay and Aubry [MA94, Aub97] and relies on continuation method. The main idea is to start with a given solution in the anti-continuum limit $\alpha = 0$ and to show that there is a corresponding solution for small $\alpha$. Continuation arguments have been proven powerful for both analytical considerations and numerical simulations and seem to be the preferred method in the physics community.

The main limitation of any continuation methods, however, is the need of an anchor solution around which the equation is expanded. As a consequence there is a growing interest in alternative existence proofs for standing waves. Example are dynamical systems approaches [QX07, PR05], or variational methods that employ critical point techniques (linking theorems, Nehari manifolds) to establish the existence of waves with prescribed frequency $\sigma$, see [PZ01, PR08, ZP09, ZL09] and [Pan06, Pan07, SZ10] for similar results in DNLS with periodic coefficients.

### 1.1 Variational setting

In this paper we rely on a variational setting, which does not prescribe the frequency but the power of a standing wave. More precisely, we obtain homoclinic standing waves as solutions to a constrained optimization problem, in which the frequency $\sigma$ is the Lagrangian multiplier. A similar idea was used by Weinstein [Wei99] for DNLS with power nonlinearities, but we allow for a wider class of nonlinear potentials $\Psi$. Moreover, our approach provides more information about the shape of standing waves as it guarantees the existence of waves with unimodal and even profile $u$. We also emphasize that, contrary to variational methods with prescribed $\sigma$, our existence proof gives rise to an effective approximation scheme for standing waves. Finally, the restriction to the one-dimensional case is not essential but was made for the sake of simplicity.

In order to sketch the main idea of our method we introduce an energy functional $\mathcal{P}$ and the power functional $\mathcal{N}$ by

$$\mathcal{P}(u) = \sum_j \Psi(u_j^2) + \alpha \sum_j (u_{j+1} + u_{j-1}) u_j, \quad \mathcal{N}(u) = \sum_j u_j^2. \tag{4}$$

Both $\mathcal{N}$ and $\mathcal{P}$ are related to conserved quantities for the Hamiltonian system (1). In fact, $\mathcal{N}$ is linked to the gauge invariance by Noether’s Theorem, and rearranging the quadratic terms we find...
\[ \mathcal{P}(u) = 2\alpha \mathcal{N}(u) - \mathcal{H}(u), \]

where

\[ \mathcal{H}(A) = \sum_j \alpha |A_{j+1} - A_j|^2 - \Psi(|A_j|^2) \]

is the Hamiltonian corresponding to (1). We readily verify that the standing wave equation (3) is equivalent to

\[ \sigma \partial \mathcal{N}(u) = \partial \mathcal{P}(u) \] (5)

where \( \partial \) denotes the variational derivative with respect to \( u \). The key observation is that (5) can be considered as the Euler–Lagrange equation of the optimization problem

\[
\begin{aligned}
\text{maximize } & \mathcal{P}(u) \text{ under the constraint } \mathcal{N}(u) = \varrho, \\
\end{aligned}
\]

where \( \sigma \) plays the role of a Lagrangian multiplier. Notice that (6) is equivalent to minimizing the energy \( \mathcal{H} \) subject to prescribed power \( \mathcal{N} \), which is a well established idea in the theory of standing waves, see \[Wei99\] for DNLS and \[Pav09, Stu09\] for dispersive Hamiltonian PDEs.

In this paper we refine the optimization problem (6) by considering only those profiles \( u \) that are non-negative, unimodal, and even. Specifically, we solve the optimization problem

\[
\begin{aligned}
\text{maximize } & \mathcal{P}(u) \text{ under the constraints } \mathcal{N}(u) = \varrho \text{ and } u \in C, \\
\end{aligned}
\]

where the convex cone \( C \) consists of all profiles \( u \) that satisfy \( u_{-j} = u_j \) and \( u_j \geq u_{j+1} \geq 0 \) for all \( j \geq 0 \). Of course, we then have to show that each solution to the so restricted optimization problem satisfies the standing wave equation (4) without further multipliers.

It is known that there exist two possible choices for the index \( j \). In the on-site (or site-centered) setting we suppose \( j \in \mathbb{Z} \), whereas in the inter-site (or bond-centered) setting we choose \( j \in \mathbb{Z} + \frac{1}{2} \). Both settings are equivalent on the level of (2), and even on the level of (6) with \( u \in \ell^2 \), but lead to different results when studying waves with even and unimodal profile \( u \in C \). In fact, on-site waves attain their maximum in an odd number of points centered around \( j = 0 \) (generically only in \( j = 0 \)), whereas the maximum of inter-site waves is realized in an even number of points (generically only in \( j = -\frac{1}{2} \) and \( j = \frac{1}{2} \)).

### 1.2 Sketch of the proof and main result

Due to the lack of strong compactness, it is not trivial to show that \( \mathcal{P} \) attains its maximum on the set of interest. A standard strategy would be to employ Lion’s concentration compactness principle \[Lio84\], see also \[Wei99, Pav09\], but we argue differently: At first we consider the analogue to (7) in the space of periodic profiles with \( u_j = u_{j+N} \). The existence of a maximiser is then granted and the invariance properties of the reversed gradient flow for \( \mathcal{P} \) ensure that the maximizer solves (5) with some multiplier \( \sigma \). In particular, there are no multipliers due to the unimodality constraint, and so we obtain periodic waves with unimodal and even profile. In the second step we then establish the existence of homoclinic waves by passing to the limit \( N \to \infty \). To this end we exploit a strict maximum condition, which replaces the concentration compactness principle and guarantees that the periodic waves are uniformly localized. We mention that approximation by periodic waves is also used in \[Pan06, Pan07\], but in a variational setting that prescribes \( \sigma \) and uses critical techniques to construct saddle points of an action integral.

Our main result on standing waves for DNLS can be summarized as follows.
**Theorem 1.** Suppose $\alpha > 0$ and that $\Psi$ satisfies the super-linear growth and regularity conditions formulated in Assumption 2. Then, in both the on-site and the inter-site setting there exists a one-parameter family of homoclinic standing waves $(u, \sigma)$ that is parametrized by $\varrho = \|u\|^2 \geq \varrho_*(\alpha) \geq 0$. For each wave, the frequency satisfies $\sigma > 2\alpha$ and the profile $u$ is non-negative, even, unimodal, and exponentially decaying.

We proceed with some remarks concerning the assumptions and assertions of Theorem 1.

1. The class of admissible $\Psi$ includes all convex functions with $\Psi'(0) = 0$. In particular, it contains power nonlinearities
   \[
   \Psi(x) = \frac{1}{\eta} x^{1+\eta}, \quad \Psi'(x) = x^\eta, \quad \eta > 0,
   \]
   but also potentials with saturable derivative such as
   \[
   \Psi(x) = x - \log (1 + x), \quad \Psi'(x) = \frac{x}{1 + x}.
   \]
   Notice that the dynamical systems approach by Qin and Xiao [QX07] also allows for arbitrary strictly convex $\Psi$ and guarantees the existence of a homoclinic wave for all $\sigma \in (2\alpha, 2\alpha + h_\infty)$ with $h_\infty = \lim_{x \to \infty} \Psi'(x)$.

2. Theorem 1 also covers some non-convex potentials as for instance
   \[
   \Psi(x) = x^3 \frac{1}{1 + x^2}, \quad \Psi'(x) = \frac{x^2 (3 + x^2)}{(1 + x^2)^2}.
   \]

3. Our results derived below imply $\varrho_*(\alpha) \to 0$ as $\alpha \to 0$. Therefore, instead of fixing $\alpha$ and choosing $\varrho$ sufficiently large we can alternatively fix $\varrho$ and choose $\alpha$ sufficiently small. We also derive explicit criteria for $\Psi$, which guarantee that $\varrho_*(\alpha) = 0$ and reflect well known results about the excitation threshold for breathers in 1D, see [FKM07, Wei99, DZC00].

4. Theorem 1 provides the existence of bright solitons for $\alpha > 0$. Via the staggering transformation $u_j \leftrightarrow (-1)^j u_j$ it also implies the existence of standing waves for the defocusing case $\alpha < 0$. These resulting waves have an alternating phase structure and are called bright gap solitons, see [Kev09]. However, the most fundamental standing waves for $\alpha < 0$ are dark solitons which correspond to heteroclinic solutions to (3) and require a different variational setting. This is discussed in [Her10].

We do not claim that the constrained maximization of $P$ provides all standing wave solutions to (2). It fact, by continuation from the anti-continuum limit it is known that there exist infinitely many multipulse solitons, see [Kev09c]. However, the careful spectral analysis by Pelinovsky et al. [PKF05] indicates that most of these multipulse solitons are unstable. This is true even for unimodal inter-site waves, but at least unimodal on-site waves can be expected to be stable. We also emphasize that maximisers of the optimization problem (6) can be shown to be orbitally stable [Wei80, Wei99], for instance using the Grillakis–Shatah–Strauss theory, see [Pav09] and the references therein. Due to the additional shape constraint $u \in C$, however, this stability result does not apply directly to the waves provided by Theorem 1 because it is not clear that the optimization problems (6) and (7) have the same solution. We conjecture that this is indeed the case but a rigorous proof is still missing.

This paper is organized as follows. In §2 we formulate our assumptions on $\Psi$ and introduce some notations. We also introduce the strict maximum condition and investigate the maximum of $P$ on bounded subsets of $\ell^2$. In §3 we then prove the existence of periodic waves and pass to the limit $N \to \infty$. Finally, we present some numerical simulations in §4.
2 Setting and properties of the energy landscape

In this paper we always assume $\alpha > 0$ and rely on the following standing assumptions on $\Psi$.

**Assumption 2.** The potential $\Psi$ is continuously differentiable on $[0, \infty)$ and has the following properties.

1. $\Psi$ is normalized by $\Psi'(0) = \Psi(0) = 0$.
2. $\Psi$ is grows super-linearly, that means $x\Psi'(x) \geq \Psi(x) \geq 0$ for all $x \geq 0$.
3. $\Psi$ is non-degenerate, i.e., $\Psi(x) > 0$ for $x > 0$.

**Remark 3.**

1. Assumption 2 implies
   \[ 0 \leq x^{-1}\Psi(x) \leq \Psi'(x) \xrightarrow{x \to 0} 0, \quad \Psi(\lambda x) \geq \lambda \Psi(x) \quad \forall \ x \geq 0, \ \lambda \geq 1, \quad \Psi(x) \xrightarrow{x \to \infty} \infty. \quad (8) \]
2. Each convex and normalized potential $\Psi$ grows super-linearly since the function $\theta(x) = x\Psi'(x) - \Psi(x)$ is non-negative due to $\theta(0) = 0$ and $\theta'(x) = x\Psi''(x) \geq 0$.
3. Assumption 2 is invariant under scalings $\Psi \xrightarrow{\Pi} \hat{\Psi}$, $\hat{\Psi}(x) := a \Psi(bx^{1+c})$, where $a, b, c > 0$ are given constants. This means $\Psi$ satisfies Assumption 2 if and only if $\hat{\Psi}$ does so.

2.1 Notations

In what follows we consider real-valued sequences $u = (u_j)_{j \in J}$, called profiles, where the index set is given by $J = \mathbb{Z}$ and $J = \mathbb{Z} + \frac{1}{2}$ in the on-site and inter-site setting, respectively. Under the periodicity condition $u_j = u_{j+N}$ for all $j$ and some $N$, each profile $u$ is uniquely determined by its values on a periodicity cell $Z_N$. We choose $Z_{2M} = \{-M + 1, \ldots, -1, 0, 1, \ldots, M\}$, $Z_{2M+1} = \{-M, \ldots, -1, 0, 1, \ldots, M\}$, in the on-site setting, and $Z_{2M} = \{-M + \frac{1}{2}, \ldots, -\frac{1}{2}, \frac{1}{2}, \ldots, M - \frac{1}{2}\}$, $Z_{2M+1} = \{-M + \frac{1}{2}, \ldots, -\frac{1}{2}, \frac{1}{2}, \ldots, M + \frac{1}{2}\}$ in the inter-site setting. The symmetrized periodicity cell is abbreviated by $\hat{Z}_N = Z_N \cap (-Z_N)$ and we readily verify, see Figure 1 that

\[ (N - 1)/2 \leq \max Z_N \leq N/2, \quad \# \{ i \in Z_N : |i| \leq |j| \} = 2 |j| + 1 \quad \forall \ j \in \hat{Z}_N. \quad (9) \]

For our purposes it is convenient to identify the non-periodic case with $N = \infty$, so we write $Z_{\infty} = Z_\infty = J$. In view of (4) and (5) we introduce the discrete function spaces

\[ \ell^2_N = \left\{ u = (u_j)_{j \in J} : u_j = u_{j+N} \text{ for all } j \in J, \sum_{j \in Z_N} u_j^2 < \infty \right\} \cong \mathbb{R}^N, \]

\[ \ell^2_\infty = \left\{ u = (u_j)_{j \in J} : \sum_{j \in Z_\infty} u_j^2 < \infty \right\} \cong \ell^2(\mathbb{Z}), \]

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Figure 1: Examples for periodic profiles that are non-negative, even, and unimodal. The values in the periodicity cell are plotted in Black.

for $N < \infty$ and $N = \infty$, respectively. For both finite and infinite $N$ we denote by

$$\|u\|^2 = \sum_{j \in \mathbb{Z}_N} u_j^2, \quad \langle u, v \rangle = \sum_{j \in \mathbb{Z}_N} u_j v_j,$$

the norm and scalar product in $\ell^2_N$, so the sphere of radius $\sqrt{\varrho}$ reads

$$S_{N, \varrho} = \{u \in \ell^2_N : \|u\|^2 = \varrho\}.$$

We also define the energy functional $\mathcal{P}_N$ by

$$\mathcal{P}_N(u) = \alpha \mathcal{L}_N(u) + \mathcal{W}_N(u), \quad \mathcal{L}_N(u) = \sum_{j \in \mathbb{Z}_N} u_j(u_{j+1} + u_{j-1}), \quad \mathcal{W}_N(u) = \sum_{j \in \mathbb{Z}_N} \Psi(u_j^2),$$

and denote by

$$\mathcal{C}_N = \{u : u_j = u_{-j} \geq 0 \; \forall \; j \in \mathbb{Z}_N\} \cap \{u : u_{j-1} \geq u_j \; \forall \; 1 \leq j \in \mathbb{Z}_N\}$$

the set of all profiles $u$ that are non-negative, even and unimodal on the periodicity cell $\mathbb{Z}_N$.

From these definitions we readily draw the following conclusions.

**Lemma 4.** For both finite and infinite $N$ the following assertions are satisfied.

1. $\mathcal{P}_N$ is Gâteaux-differentiable on $\ell^2_N$ with derivative $\partial \mathcal{P}(u)_j = 2\alpha(u_{j+1} + u_{j-1}) + 2\Psi'(u_j^2)u_j$.

2. $\mathcal{C}_N$ is a positive convex cone and closed under weak convergence in $\ell^2_N$.

3. By (9) we have $u_j \leq \|u\|/\sqrt{2|j| + 1}$ for all $u \in \mathcal{C}_N$ and $j \in \mathbb{Z}_N$.

The core of our variational existence proof for standing waves is the optimization problem

$$\text{maximize } \mathcal{P}_N \text{ on the set } \mathcal{C}_N \cap S_{N, \varrho}. \quad (10)$$

For finite $N$, the existence of maximizers follows from simple compactness arguments and the invariance properties of the gradient flow of $\mathcal{P}_N$ imply that each maximizer is in fact a periodic standing wave. For infinite $N$, however, we lack compactness and construct homoclinic maximizers of $\mathcal{P}_\infty$ as limits of periodic maximizers of $\mathcal{P}_N$. 

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2.2 Energy maxima on bounded sets

In this section we investigate the function

\[ T_N(\alpha, \varrho) = \frac{1}{\alpha \varrho} \sup \{ P_N(u) : u \in \mathcal{C}_N \cap \mathcal{S}_{N, \varrho} \} , \]

and show that the strict maximum condition

\[ T_\infty(\alpha, \varrho) > 2 \]

(11)

holds if one of the following conditions is satisfied:

(A1) \( \alpha \) is sufficiently small,

(A2) \( \varrho \) is sufficiently large,

(A3) \( \Psi(x) \sim cx^{1+\eta} \) for all \( 0 \leq x < 1 \) and \( 0 < \eta < 2 \) and some \( c > 0 \).

The strict maximum condition (11) appears naturally in our existence proof for homoclinic waves, see §3.2, and guarantees that the influence of the nonlinearity \( \Psi \) is strong enough in the limit \( N \to \infty \). Specifically, if (11) is satisfied, then the optimization problem (10) has a solution for \( N = \infty \), and each minimizer is a homoclinic wave with unimodal profile. Moreover, if (11) is violated, then we have \( T_\infty(\alpha, \varrho) = 2 = \sup_{u \in \mathcal{S}_{\infty, \varrho}} \mathcal{L}_\infty(u) \), and this implies that (10) has no solution for \( N = \infty \).

We also emphasize that (11) is equivalent to

\[ \inf \left\{ \mathcal{H}(u) : u \in \ell^2(\mathbb{Z}), N(u) = \varrho \right\} < 0 , \]

which is precisely the condition used in [Wei99] to prove the existence of homoclinic standing waves for DNLS with power nonlinearity \( \Psi(x) = cx^{1+\eta} \). Moreover, condition (A3) implies that there is no excitation threshold for power nonlinearities with \( 0 < \eta < 2 \), which means there exist waves with arbitrary small \( \varrho \). This result is again in line with the findings from [Wei99].

We now summarize some elementary properties of the function \( T_N \).

**Lemma 5.** \( T_N \) is decreasing in \( \alpha \) and increasing in \( \varrho \) for both finite and infinite \( N \).

**Proof.** The monotonicity with respect to \( \alpha \) is obvious. Towards the monotonicity in \( \varrho \) let \( u \in \ell^2_N \) and \( \lambda \geq 1 \) be fixed. We have \( \mathcal{L}_N(\lambda u) = \lambda^2 \mathcal{L}_N(u) \), and

\[ \frac{d}{d \lambda} \mathcal{W}_N(\lambda u) = \sum_{j \in \mathbb{Z}_N} 2 \Psi'((\lambda^2 u^2_j) \lambda u^2_j \geq \sum_{j \in \mathbb{Z}_N} 2 \lambda \Psi((\lambda^2 u^2_j) \lambda u^2_j \geq \frac{2}{\lambda} \mathcal{W}_N(\lambda u) \]

implies \( \mathcal{W}_N(\lambda u) \geq \lambda^2 \mathcal{W}_N(u) \). Consequently, for \( \|u\| \neq 0 \) and \( \lambda > 0 \) we find

\[ T_N(\alpha, \lambda^2 \|u\|^2) \geq \frac{1}{\lambda^2 \|u\|^2} (\mathcal{L}_N(\lambda u) + \frac{1}{\alpha} \mathcal{W}_N(\lambda u)) \geq \frac{1}{\|u\|^2} (\mathcal{L}_N(u) + \frac{1}{\alpha} \mathcal{W}_N(u)) , \]

and taking the supremum over \( u \) gives \( T_N(\alpha, \lambda^2 \|u\|^2) \geq T_N(\alpha, \|u\|^2) \) .

**Remark 6.** For power nonlinearities \( \Psi(x) = cx^{1+\eta} \) with \( c, \eta > 0 \) we have \( T_N(\alpha, \lambda^2 \varrho) = N(\lambda^{-2\eta} \alpha, \varrho) \) and hence

\[ T_N(\alpha, \varrho) = T_N(\alpha \varrho^{-\eta}, 1) = T_N(1, \alpha^{-1/\eta} \varrho) \]

for all \( \alpha, \varrho, \lambda > 0 \) and both \( N < \infty \) and \( N = \infty \).
For finite $N$, the constant profile with $u_j = \sqrt{\varrho/N}$ for all $j$ belongs to $\mathcal{C}_N \cap \mathcal{S}_{N, \varrho}$, and using (8) we readily verify that
\[
P_N(\sqrt{\varrho/N}) = 2\alpha \varrho + \varrho N \Psi(\varrho/N) \xrightarrow{N \to \infty} 2\alpha \varrho.
\] (12)

In particular, due to $\Psi(\varrho/N) > 0$ we have
\[
T_N(\alpha, \varrho) \geq P_N(\sqrt{\varrho/N}) > 2
\] (13)
for all $N < \infty, \alpha > 0, \varrho > 0$. The case $N = \infty$ is a bit more delicate.

**Lemma 7.** We have $T_\infty(\alpha, \varrho) \geq 2$ with strict inequality provided that (A1) or (A2) is satisfied.

**Proof.** We start with the proof in the on-site setting and define $u_m \in \mathcal{C}_\infty \cap \mathcal{S}_\infty, \varrho$ by
\[
u_{m,j} = \frac{\sqrt{\varrho}}{\sqrt{2m+1}} \begin{cases} 1 & \text{for } |j| \leq m, \\ 0 & \text{for } |j| > m. \end{cases}
\]
A direct calculation shows
\[
L_\infty(u_m) = \frac{2m}{2m+1} \varrho, \quad P_\infty(u_m) = (2m+1) \Psi\left(\frac{\varrho}{2m+1}\right),
\]
and hence
\[
T_\infty(\alpha, \varrho) \geq \frac{\alpha L_\infty(u_m) + P_\infty(u_m)}{\alpha \varrho}
= 2 - \frac{1}{\varrho} + \frac{1}{2m+1} \varrho N \Psi\left(\frac{\varrho}{2m+1}\right) \geq 2 - \frac{1}{\varrho} + \frac{1}{2m+1} \varrho.
\] (14)

This gives $T_\infty(\alpha, \varrho) \geq 2$ by passing to the limit $m \to \infty$ and using (8).

We have now two possibilities to show $T_\infty(\alpha, \varrho) > 2$. First, for given $\varrho$ and $m$ we can choose $\alpha$ small. Second, for fixed $\alpha$ and any $\varrho > 1$ we choose $m = m(\varrho)$ such that $2m-1 < \varrho < 2m+1$, so (14) gives
\[
T_\infty(\alpha, \varrho) \geq 2 - \frac{1}{\varrho} + \frac{c}{\alpha}
\]
for some $c > 0$, and the claim follows with $\varrho \to \infty$.

Finally, in the inter-site setting we define $u_m$ by
\[
u_{m,j} = \frac{\sqrt{\varrho}}{\sqrt{2m}} \begin{cases} 1 & \text{for } |j| \leq m - \frac{1}{2}, \\ 0 & \text{for } |j| > m - \frac{1}{2}, \end{cases}
\]
and argue analogously.

We now show that the strict maximum conditions is always satisfied if $\Psi$ is sufficiently nonlinear for $x \approx 0$. The key idea in our proof is also used in [Wei99] to disprove the existence of an excitation thresholds for power nonlinearities with $0 < \eta < 2$.

**Lemma 8.** (A3) implies $T_\infty(\alpha, \varrho) > 2$. 

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Proof. We present the arguments for the on-site setting; the proof for the inter-site setting is similar. For fixed $\alpha > 0$, $\varrho > 0$ but arbitrary $0 < \zeta \ll 1$ we consider $u_\zeta \in C_\infty \cap S_\infty, \varrho$ defined by

$$u_{\zeta, j} = \sqrt{\varrho \tanh \zeta} \exp (-\zeta \abs{j}),$$

which has small amplitudes due to $\tanh \zeta = \zeta + O(\zeta^3)$. By direct computations we find

$$L_\infty(u_\zeta) = \frac{2\varrho}{\cosh \zeta} = \varrho \left( 2 - \zeta^2 + O(\zeta^4) \right),$$

as well as

$$W_\infty(u_\zeta) = (1 + o(1)) \sum_{j \in J_\infty} c u_j^{2+2\eta} = (1 + o(1)) c (\varrho \tanh \zeta)^{1+\eta} \frac{1 + \exp (-2\zeta(1 + \eta))}{1 - \exp (-2\zeta(1 + \eta))},$$

where $o(1)$ means arbitrary small for small $\zeta$. We now conclude that

$$T_\infty(\alpha, \rho) \geq P_\infty(u_\zeta) = 2 + (1 + o(1)) \left( \frac{c\varrho^{\eta}}{\alpha(1 + \eta)} \zeta^\eta - \zeta^2 \right),$$

and the claim follows from choosing $\zeta$ sufficiently small. \qed

We finally establish the convergence $T_N(\alpha, \varrho) \to T_\infty(\alpha, \varrho)$ as $N \to \infty$. To this end we denote elements of $\ell_2^N$ by $u_N = (u_{N, j})_j$ and introduce two operators $R_N$ and $E_N$ which act on profiles $u$ as follows. $R_N u$ is the restriction of $u$ to the symmetrized periodicity cell $\tilde{Z}_N$, i.e.,

$$(R_N u)_j = \begin{cases} u_j & \text{for } j \in \tilde{Z}_N, \\ 0 & \text{otherwise,} \end{cases}$$

and $E_N u$ is defined as the periodic continuation of $R_N u$. Notice that we allow for small embedding errors. In fact, for non-symmetric periodicity cells with $\tilde{Z}_N \neq Z_N$ we have $E_N u_N \neq u_N$ for $u_N \in \ell_2^N$, but the embedding error is small due to the decay estimate from Lemma 4.

We readily verify that $E_N$ and $R_N$ are linear operators with

$$R_N : C_N \to C_\infty, \quad E_N : C_\infty \to C_N,$$

and $\|R_N u_N\| \leq \|u_N\|$ and $\|E_N u_\infty\| \leq \|u_\infty\|$.

Lemma 9. We have

$$|P_N(u_N) - P_\infty(R_N u_N)| \leq O(\|u_N\|/\sqrt{N}), \quad P_N(E_N u_\infty) \xrightarrow{N \to \infty} P_\infty(u_\infty)$$

for all $u_N \in C_N$ and $u_\infty \in C_\infty$.

Proof. The first claim is a consequence of [9] and Lemma [4]. The second one follows from $R_N u_\infty \to u_\infty$ as $N \to \infty$. \qed

We are now able to prove the convergence of maxima.

Lemma 10. We have $T_N(\alpha, \varrho) \to T_\infty(\alpha, \varrho)$ as $N \to \infty$. 

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Proof. For fixed \( u_\infty \in C_\infty \cap S_{\infty, \varrho} \), Lemma 5 and Lemma 9 provide
\[
\mathcal{P}_\infty(u_\infty) \leq \mathcal{P}_N(E_Nu_\infty) + o(1) \leq \alpha \varrho T_N(\alpha, \|E_Nu_\infty\|^2) + o(1),
\]
with \( o(1) \) being arbitrary small for large \( N \). Passing to the limit \( N \to \infty \) and taking the supremum over \( u_\infty \) gives \( T_\infty(\alpha, \varrho) \leq \liminf_{N \to \infty} T_N(\alpha, \varrho) \). Towards the reverse estimate, we denote the maximizer of \( \mathcal{P}_N \) in \( C_N \cap \hat{S}_{N, \varrho} \) by \( \hat{u}_N \), and thanks to Lemma 9 we find
\[
\alpha \varrho T_N(\alpha, \varrho) = \mathcal{P}_N(\hat{u}_N) \leq \mathcal{P}_\infty(E_N\hat{u}_N) + o(1) \leq \alpha \varrho T_\infty(\alpha, \varrho) + o(1),
\]
which implies \( \limsup_{N \to \infty} T_N(\alpha, \varrho) \leq T_\infty(\alpha, \varrho) \). \( \square \)

3 Existence of standing waves

3.1 Periodic waves

We now prove the existence of periodic waves with \( N < \infty \). To this end we consider the reversed gradient flow for \( \mathcal{P}_N \) under the constraint \( \|u\|^2 = \varrho \), that is
\[
\frac{d}{d\tau} u = F_N(u), \quad F_N(u) = \partial \mathcal{P}_N(u) - \sigma_N(u)u, \quad \sigma_N(u) = \frac{\langle \partial \mathcal{P}_N(u), u \rangle}{\|u\|^2},
\]
where \( \tau \geq 0 \) denotes the flow time, and \( \sigma_N \) is a (dynamical) Lagrangian multiplier. Constrained gradient flows are well known in the context of ground states for Schrödinger equations and sometimes referred to as imaginary time methods, see [BD04, YL07] and references therein.

Lemma 11. The gradient flow (16) has the following properties:

1. \( S_{N, \varrho} \) is an invariant set.
2. \( \mathcal{P}_N(u) \) is strictly increasing on each non-stationary trajectory.
3. Each stationary point \( u \in \ell_N^2 \) of (16) is a standing wave with frequency \( \sigma = \sigma_N(u) \).

Proof. The definition of \( \sigma \) implies \( \frac{d}{d\tau} \|u\|^2 = \langle F_N(u), u \rangle = 0 \), so \( \|u\| \) is conserved under the flow. By a direct computation we find
\[
\frac{d}{d\tau} \mathcal{P}_N(u) = \langle \partial \mathcal{P}_N(u), F_N(u) \rangle = \frac{1}{\|u\|^2} \left( \|\partial \mathcal{P}_N(u)\|^2 \|u\|^2 - |\langle \partial \mathcal{P}_N(u), u \rangle|^2 \right) \geq 0
\]
with \( \frac{d}{d\tau} \mathcal{P}_N(u) = 0 \) if and only if \( u \) and \( \partial \mathcal{P}_N(u) \) are collinear, i.e., \( \partial \mathcal{P}_N(u) = \sigma_N(u)u \). \( \square \)

The next result provides a key ingredient for our existence result.

Lemma 12. \( C_N \) is invariant under the gradient flow (16).

Proof. Within this proof let \( u(0) \in C_N \) be some fixed initial data and denote by \( u(\tau) \in \ell_N^2 \) with \( \tau \geq 0 \) the corresponding forward in time solution to (16). We first note that
\[
\mathcal{E}_N = \{ u : u_j = u_{-j} \quad \forall \quad j \in Z_N \},
\]
the set of all even profiles, is a closed linear subspace of \( \ell_N^2 \) and moreover invariant under \( \mathcal{F}_N \). We thus conclude that \( u(0) \in \mathcal{E}_N \) implies \( u(\tau) \in \mathcal{E}_N \) for all \( \tau \). In order to show the remaining assertions we proceed as usual and consider the perturbed initial value problem
\[
\frac{d}{d\tau} v = F_N(v) + \varepsilon, \quad v(0) = u(0) + \varepsilon
\]
where the perturbation $\varepsilon = (\varepsilon_j)_j$ is supposed to be an inner point of $\mathcal{C}_N$ with respect to the induced topology of $\mathcal{E}_N$. First suppose for contradiction that there exist $\tau_0 > 0$ and $j_0 \in \mathbb{Z}_N$ such that

$$v_{j_0}(\tau_0) = 0 \quad \text{and} \quad v_j(\tau) \geq 0 \quad \text{for all} \quad j \in \mathbb{Z}_N \quad \text{and} \quad 0 \leq \tau < \tau_0.$$ 

This implies $\frac{d}{d\tau}v_{j_0}(\tau_0) \leq 0$, so (17) provides

$$\frac{d}{d\tau}v_{j_0}(\tau_0) = F_{N,j_0}(v(\tau_0)) + \varepsilon_{j_0} = \alpha(v_{j_0+1}(\tau_0) + v_{j_0-1}(\tau_0)) + \varepsilon_{j_0} \geq \varepsilon_{j_0} > 0,$$

which is the desired contradiction. Secondly, assuming

$$v_{j_0-1}(\tau_0) = v_{j_0}(\tau_0) \quad \text{and} \quad v_{j-1}(\tau) \geq v_j \quad \text{for all} \quad 1 \leq j \leq \max \mathbb{Z}_N \quad \text{and} \quad 0 \leq \tau < \tau_0,$$

we find a contradiction by

$$0 \geq \frac{d}{d\tau}v_{j_0-1}(\tau_0) - \frac{d}{d\tau}v_{j_0}(\tau_0) = \alpha(v_{j_0-2} + v_{j_0} - v_{j_0+1} - v_{j_0-1}) + \varepsilon_{j_0-1} - \varepsilon_{j_0} \geq \varepsilon_{j_0-1} - \varepsilon_{j_0} > 0.$$

In conclusion, we have shown $v(\tau) \in \mathcal{C}_N$ for all $\tau \geq 0$ and all perturbations $\varepsilon$, and $u(\tau) \in \mathcal{C}_N$ follows by $\|\varepsilon\| \to 0$.

**Theorem 13.** For each $\varrho > 0$ there exists a standing wave $(u, \sigma)$ with $u \in \mathcal{C}_N \cap \mathcal{S}_{N,\varrho}$ and $\sigma \varrho \geq P_N(u) = \alpha \varrho T_N(\alpha, \varrho) > 2\alpha \varrho$.

**Proof.** Due to $N < \infty$ the set $\mathcal{S}_{N,\varrho} \cap \mathcal{C}_N$ is compact in $\ell^2_N$, and hence there exist a maximizer $u$ for $P_N$ on this set. Lemma 11 combined with Lemma 12 then implies that $u$ is stationary point of (16) and solves the standing wave equations (3) with frequency $\sigma = \sigma_N(u)$. Finally, testing (3) with $u$ gives

$$\sigma_N(\varrho) = \alpha \mathcal{L}_N(u) + \sum_{j \in \mathbb{Z}_N} \Psi(u_j^2)u_j^2 \geq \alpha \mathcal{L}_N(u) + \sum_{j \in \mathbb{Z}_N} \Psi(u_j^2) = P_N(u)$$

due to Assumption 2 and (13) completes the proof.

We conclude this section with two remarks.

1. **Theorem** 13 provides the existence of two families of periodic waves as it holds in both the on-site and the inter-site setting.

2. **Theorem** 13 does not exclude that the maximizer is equal to the constant profile $\sqrt{\varrho/N}$. However, Lemma 7 combined with Lemma 10 and (12), ensures that the profile is non-constant for large $N$, provided that (A1), (A2), or (A3) is satisfied.

### 3.2 Homoclinic waves

In this section we prove that the period waves from Theorem 13 converge to homoclinic waves provided that the strict maximum condition (11) is satisfied. To this end we fix $\varrho > 0$ and consider a sequence of profiles $(u_N)_N \subset \mathcal{C}_\infty$ such that

1. $u_N$ is the image of a maximizer of $P_N$ on $\mathcal{C}_N \cap \mathcal{S}_{N,\varrho}$ under the restriction map $R_N$ from (15),

2. $\sigma_N$ is the corresponding frequency.
According to these definitions and Lemma 4 we have
\[ 0 \leq u_{N,j} = \sqrt{\varrho/(2|j| + 1)} \quad \forall j, \quad u_{N,j} = 0 \quad \forall |j| \geq (N + 1)/2. \] (18)

Moreover, Lemma 10 and Theorem 13 provide
\[ \sigma_N u_{N,j} = \alpha(u_{N,j+1} + u_{N,j-1}) + \Psi'(u_{N,j}^2)u_{N,j} \quad \text{for all } j, N \text{ with } |j| \leq (N - 1)/2, \] (19)
as well as
\[ \sigma_N \varrho \geq P_\infty(u_N) + o(1) = \alpha \varrho T_\infty(\alpha, \varrho) + o(1). \] (20)

We next show by using the strict maximum condition that the profiles \( u_N \) are localized.

**Lemma 14.** Suppose that (11) is satisfied. Then,
\[ \sigma = \liminf_{N \to \infty} \sigma_N > 2\alpha \]
and there exist two positive constants \( C \) and \( d \) such that
\[ u_{N,j} \leq C \exp(-d |j|) \] (21)
holds for all \( j, N \).

**Proof.** The first claim follows from (20). Now choose \( \bar{\sigma} > 2\alpha > \sigma_\star \in (2\alpha, \sigma) \) such that
\[ \sup_{0 \leq x \leq \varrho/(2j_\star + 1)} \Psi'(x) \leq \bar{\sigma} - \sigma_\star. \]
Combining this with (18), (19), and \( u_{N,j} \geq u_{N,j+1} \) gives
\[ (\sigma_\star - \alpha)u_{N,j} \leq (\sigma_N - \Psi'(u_{N,j}^2) - \alpha)u_{N,j} \leq \sigma_N u_{N,j} - \Psi'(u_{N,j}^2)u_{N,j} - \alpha u_{N,j+1} \leq \alpha u_{N,j+1} \]
and hence \( u_{N,j} \leq \kappa^{-j} \sqrt{\varrho} \) with \( \kappa = \frac{\alpha}{\sigma_\star - \alpha} < 1 \) for all \( j \) with \( j_\star < j < N/2 - 2 \). Finally, (21) follows with \( d = -\ln \kappa \) and \( C \) sufficiently large.

**Corollary 15.** Suppose that \( \alpha \) and \( \varrho \) are chosen such that (11) is satisfied. Then, the sequence \( (u_N) \) is strongly compact and each accumulation point \( u_\infty \) satisfies \( u_\infty \in C, \|u_\infty\|^2 = \varrho \), and \( P_\infty(u_\infty) = \alpha \varrho T_\infty(\alpha, \varrho) \). Moreover, \( u_\infty \) decays exponentially and is a standing wave with frequency \( \sigma_\infty > 2\alpha \).

**Proof.** By compactness we can extract a (not relabelled) subsequence such that \( u_N \rightharpoonup u_\infty \in C \) in \( \ell^2_\infty \), and this yields the pointwise convergence \( u_{N,j} \to u_\infty,j \) for all \( j \). The uniform tail estimate (21) then implies \( \|u_\infty\|^2 = \varrho \) and that \( u_\infty \) decays exponentially for \( j \to \pm \infty \). We conclude that \( u_N \to u_\infty \) strongly in \( \ell^2_\infty \) as well as \( P_\infty(u_\infty) = \lim_{N \to \infty} P_\infty(u_N) = \alpha \varrho T_\infty(\alpha, \varrho) > 2\alpha \varrho \), where we used (20). Moreover, (19) with fixed \( j \) and (20) imply \( \sigma_N \to \sigma_\infty \) for some \( \sigma_\infty > 2\alpha \), and exploiting (19) for all \( j \) we infer that \( u_\infty \) is a standing wave with frequency \( \sigma_\infty \).

We have now finished the existence proof for standing waves. In particular, Theorem 1 follows from Lemma 7, Lemma 8, Theorem 13 and Corollary 15. We finally recall that for given \( \alpha > 0 \) the condition (A3) on \( \Psi \) implies (11) for all \( \varrho > 0 \), and hence the existence of homoclinic waves with arbitrary small energy.
4 Numerical examples

In this section we illustrate our analytical results by numerical simulations of standing waves with $N < \infty$. To this end we define a map $I : S_{N, \varrho} \rightarrow S_{N, \varrho}$ by

$$I(u) = \sqrt{\varrho} \frac{u + \tau F_N(u)}{\|u + \tau F_N(u)\|},$$

where $\tau > 0$ is sufficiently small, and construct standing waves as limits of the iteration

$$u_0 = u_{\text{ini}}, \quad u_{k+1} = I(u_k). \quad (22)$$

This scheme preserves the constraint $\|u\|^2 = \varrho$ exactly, and is a discrete analogue to the gradient flow due to $I(u) = u + \tau F_N(u) + o(\tau^2)$. In order to compute a good guess for the initial profile $u_{\text{ini}}$ we start with the ansatz

$$u_{\text{ini},j} = \kappa_1 + \kappa_2 \chi_j + \kappa_3 (1 + \cos(\pi j/N)) + \kappa_4 \exp(-20(j/N)^2), \quad \chi_j = \begin{cases} 1 & \text{for } |j| < 1, \\ 0 & \text{otherwise}, \end{cases}$$

where the parameters $\kappa_i$ are positive and coupled by the constraint $\|u_{\text{ini}}\|^2 = \varrho$. Then we sample the set of all admissible parameters by about 100 points, and solve the discrete maximization $P_n(u_{\text{ini}}(\kappa_i)) \rightarrow \max$ to find the optimal values for the parameters $\kappa_i$.

![Initial profile](image1.png)

![Profile after 30 steps](image2.png)

![Residual after 30 steps](image3.png)

Figure 2: Periodic on-site (top row, $N = 25$) and inter-site (bottom row, $N = 24$) waves for the data from (23) with $\tau = 1$.

![Profile for $\varrho = 2.38$](image4.png)

![Profile for $\varrho = 2.4$](image5.png)

![$P_{N-2a\varrho}$ versus $\varrho$](image6.png)

Figure 3: Periodic on-site waves for the data from (24) with $\tau = 1$ and $N = 41$.

Figure 2 shows numerical results for

$$\Psi(x) = x - \arctan x, \quad \alpha = 1, \quad \varrho = 10, \quad (23)$$

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and provides evidence that the algorithm (22) produces a standing wave in both the on-site and inter-site setting. Notice that \( \Psi \) satisfies Assumption 2 and is saturable due to \( \lim_{x \to \infty} \Psi'(x) = 1 \).

A second example concerns

\[
\Psi(x) = \exp(x) - \frac{1}{2}x^2 - x - 1, \quad \alpha = 1, \quad \varrho \in [2, 3].
\]  

(24)

and is shown in Figure 3. The simulations indicate that the periodic on-site waves for (24) exhibit quite different properties for small and large values of \( \varrho \): For \( \varrho \leq 2.38 \) we observe that almost all lattice sites are excited and that the profile has small amplitude and is almost constant. Moreover, the energy \( P_N = P_N(u_N) \) is only slightly larger than \( 2\alpha\varrho \). For \( \varrho \geq 2.4 \), however, the profile is strongly localized and \( P_N \) is considerably larger than \( 2\alpha\varrho \). We therefore expect that for \( N \to \infty \) the periodic waves converge pointwise to zero and a non-trivial homoclinic wave for small and large \( \varrho \), respectively. Notice that this is in accordance with our theoretical results: Since we have \( \Psi(x) \sim \frac{1}{6}x^3 \) for small \( x \), the existence of homoclinic waves is guaranteed only for sufficiently large \( \varrho \).

A similar phenomenon can be observed in Figure 4, which illustrates the limit \( N \to \infty \) for \( \Psi(x) = x^4, \quad \alpha \in \{1/2, 2\}, \quad \varrho = 2 \).

(25)

For sufficiently large \( \alpha \) we have \( P_N \to 2\alpha\varrho \) as \( N \to \infty \) and the periodic waves converge (weakly in \( \ell^2 \)) to zero. If \( \alpha \) is sufficiently small, however, we have \( \lim_{N \to \infty} \sigma_N > 2\alpha\varrho \) and the periodic waves converge (strongly in \( \ell^2 \)) to a non-trivial homoclinic wave.

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