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Abstract

Ground waves in atomic chains are traveling waves that corresponds to minimal non-trivial critical values of the underlying action functional. In this paper we study FPU-type chains with bi-monomial double-well potential and prove the existence of both periodic and solitary ground waves. To this end we minimize the action on the Nehari manifold and show that periodic ground waves converge to solitary ones. Finally, we compute ground waves numerically by a constrained gradient flow.

Keywords: *Fermi-Pasta-Ulam chain with double well potential*, *Nehari manifold*, *ground waves*

MSC (2010): 37K60, 47J30, 74J30

Contents

1 Introduction

Atomic chains with nearest neighbor interactions, which are sometimes called FPU-type chains, are ubiquitous in physics and materials science as they provide simple atomistic models for solids. They are moreover prototypical examples for nonlinear Hamiltonian lattice equations and shed light on the dynamical properties of discrete media with dispersion.

The lattice equation for infinite FPU-type chains stems from Newton's law of motion and reads

$$\ddot{x}_j = \Phi'\big(x_{j+1} - x_j\big) - \Phi'\big(x_j - x_{j-1}\big)\,, \tag{1}$$

where Φ is the interaction potential and $x_j = x_j(t) \in \mathbb{R}$ denotes the position of atom $j \in \mathbb{Z}$ at time t.

Coherent structures such as traveling waves are of particular interest in the analysis of nonlinear lattice equations since they can be regarded as the nonlinear fundamental modes and describe how energy propagates through the chain. Traveling waves are special solutions to (1) that depend on a one-dimensional phase variable $\varphi = j - \sigma t$ via the ansatz

$$x_j(t) = rj + vt + X(j - \sigma t)\,.$$

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Here σ the phase speed and r, v are some constants. The profile function X must comply with

$$\sigma^2 X''(\varphi) = \Phi'\big(r + X(\varphi+1) - X(\varphi)\big) - \Phi'\big(r + X(\varphi) - X(\varphi-1)\big)\,. \tag{2}$$

This advance-delay differential equation is equivalent to the nonlinear eigenvalue problem

$$\sigma^2 W = \mathcal{A}\Phi'(\mathcal{A}W) + \mu \tag{3}$$

for the function W defined by $W(\varphi) = r + X'(\varphi)$. Here, μ is some constant of integration and the convolution operator $\mathcal{A}$ is defined by

$$(\mathcal{A}W)(\varphi) = \int_{\varphi-1/2}^{\varphi+1/2} W(s)\,\mathrm{d}s. \tag{4}$$

Traveling waves in atomic chains have been studied intensively during the last two decades, and the existence of several types of solutions to (2) has been established for various interaction potentials by different methods. The standard references are [FW94] for constrained optimization, [SW97, PP00] for critical point techniques, [Ioo00] for bifurcation results via spatial dynamics, [FP99] for near-sonic waves, and [FM02] for the high-energy limit. For further results and a more detailed discussion, especially of the variational methods, we refer to [HR10, Her10].

In this paper we consider chains with double well potential, which play an important role in the atomistic theory of martensitic phase transitions. In order to keep the presentation as simple as possible, we restrict ourselves to bi-monomial potentials with

$$\Phi(w) = d_p\,|w|^p - d_q\,|w|^q \quad \text{with} \quad 2 < p, \quad 1 < q < p\,,$$

and by a simple scaling we can achieve that $d_p = d_q = 1$. We further restrict our considerations to the case $\mu = 0$, see the discussion below, and seek non-trivial solutions to the traveling wave equation

$$\sigma^2 W + \mathcal{A}\Psi_q(\mathcal{A}W) = \mathcal{A}\Psi_p(\mathcal{A}W), \tag{5}$$

where the function Ψ_r is defined by $\Psi_r(w) := r\,\mathrm{sgn}\,(w)\,|w|^{r-1}$. Notice that the solution set to (5) is invariant under shifts $W(\varphi) \rightsquigarrow W(\varphi+\varphi_0)$ and reflections via $W(\varphi) \rightsquigarrow W(-\varphi)$ or $W(\varphi) \rightsquigarrow -W(\varphi)$. Moreover, it always contains the trivial solutions $W \equiv -c$, $W \equiv 0$, and $W \equiv +c$, where $c \in \mathbb{R}_+$ is the unique positive solution to $\sigma^2 c + qc^{q-1} = pc^{p-1}$.

Due to the Hamiltonian nature and the shift invariance of (1), there is a variational characterization of traveling waves with prescribed σ. In fact, we readily verify that each solution $W \in \mathsf{L}^2(I_K)$ to (5) is a critical point of the action functional

$$\mathcal{L}_K(W) := \tfrac{1}{2}\sigma^2\|W\|_{2,I_K}^2 + \mathcal{Q}_K(W) - \mathcal{P}_K(W)\,.$$

The term $\frac{1}{2}\sigma^2\|W\|_{2,I_K}^2 = \frac{1}{2}\sigma^2\int_{I_K} W^2\,\mathrm{d}\varphi$ can be regarded as the kinetic energy, whereas $\mathcal{Q}_K$ and $\mathcal{P}_K$ defined by

$$\mathcal{Q}_K(W) := \int_{I_K} |\mathcal{A}W|^q\,\mathrm{d}\varphi, \qquad \mathcal{P}_K(W) := \int_{I_K} |\mathcal{A}W|^p\,\mathrm{d}\varphi\,,$$

give the two contributions to the potential energy. The parameter $K \in (0, \infty]$ can be either finite or infinite, corresponding to $2K$-periodic wave with periodicity cell $I_K := (-K, K]$ or solitary waves with $I_\infty := \mathbb{R}$, respectively. Notice that solitary waves are homoclinic via $\lim_{\varphi\to\pm\infty} W(\varphi) = 0$.

By definition, a *ground wave* is a traveling wave that corresponds to a minimal non-trivial critical value of the action functional $\mathcal{L}_K$. However, since $\mathcal{L}_K$ is unbounded from below, ground waves are not minimizers but saddle points. Our main result concerns the existence of ground waves in $\mathsf{L}^2(I_k)$ and can be summarized as follows.

Theorem 1. *Let $\sigma^2 > 0$ be given. Then, for each $K \in (0, \infty]$ there exists a ground wave $W_K \in \mathsf{L}^2(I_K) \cap \mathsf{BC}^1(\mathbb{R})$ which satisfies*

$$0 < \mathcal{L}_K(W_K) = \min \Big\{ \mathcal{L}_K(W) \;:\; W \in \mathsf{L}^2(I_K) \text{ with } \partial\mathcal{L}_K(W) = 0 \Big\} = \min_{W \in \mathsf{L}^2(I_K)} \max_{\zeta > 0} \mathcal{L}_K(\zeta W)\,,$$

and which is non-constant provided that K is sufficiently large. Moreover, solitary ground waves can be approximated (in some strong sense) by period ground waves.

In order to prove these assertions, we introduce in §2 the Nehari manifold M_K, which has co-dimension 1 and contains all non-trivial critical points of $\mathcal{L}_K$. In §3.1 we employ the direct method from the calculus of variations and show that the functional $\mathcal{L}_K$ attains its minimum on M_K for $K < \infty$. Afterwards in §3.2 we demonstrate that periodic ground waves with $K \to \infty$ provide minimizing sequences for $\mathcal{L}_\infty|_{\mathsf{M}_\infty}$ and converge to a solitary ground wave. Finally, we compute ground waves numerically in §4.

Our work is closely related to the discussion of ground waves in [Pan05, Section 3.4]. The results presented there imply the assertions of Theorem 1 for the special case $q = 2$ and are likewise based on the Nehari manifold and approximation by periodic waves. The proof, however, is different as it employs the Mountain Pass Theorem and the Palais-Smale condition for $K < \infty$; see §3 for more details.

A variant of the Mountain Pass Theorem was also used in [SZ07] to construct certain homoclinic waves for chains with double well potential. These waves satisfy $W = w_* + U$ with $U \in \mathsf{L}^2(\mathbb{R})$, where w_* is one of the local minimizer of Φ. The key idea is that the relative profile U can be regarded as solitary wave with respect to a tilted potential Φ_*. This is defined by $\Phi_*(u) = \Phi(w_* + u) - \Phi'(w_*)u - \Phi(w_*)$ and has, at least for some Φ, two increasing branches as it satisfies $u\,\Phi_*'(u) > 0$ for all u. The relation to our approach becomes apparent in the periodic case. Instead of tilting the potential we can impose the constraint $|I_K|^{-1} \int_{I_K} W \,\mathrm{d}\varphi = w_*$, and we easily check that critical points of $\mathcal{L}_K$ now satisfy the traveling wave equation (3) with Lagrangian multiplier $\mu \in \mathbb{R}$. Due to the constraint, however, the corresponding traveling waves are not ground waves for the action $\mathcal{L}_K$. Moreover, it is not clear whether these waves extend to the spinodal region of Φ, or remain confined to the convex well around w_*.

We finally mention that $\mathcal{L}_K$ has, at least for $K < \infty$, infinitely many critical points in $\mathsf{L}^2(I_K)$. In particular, each ground wave for K/n with $n \in \mathbb{N}$ is also a critical point of $\mathcal{L}_K$, but qualitatively different types of traveling waves might exist as well. Moreover, for $K = \infty$ we expect to find a plethora of waves with $W \notin \mathsf{L}^2(\mathbb{R})$. Of particular importance are phase transitions waves, which are heteroclinic connections of two period waves corresponding to either one of wells. Unfortunately, very little is known about their existence. The only available results concern bi-quadratic potentials, which allow for solving (2) by Fourier methods [TV05, SZ09]. It remains a challenging task to find alternative, maybe variational, existence proofs for phase transition waves that apply to more general double well potentials.

2 Variational setting and Nehari manifold

In this section we develop our variational framework for both finite and infinite K and introduce the Nehari manifold, on which we minimize the action in §3. To this end we denote by $\mathsf{L}^r(I_K)$ and $\mathsf{W}^{1,r}(I_K)$ the usual Sobolev spaces of I_K-periodic functions (or functions on $\mathbb{R}$ for $K = \infty$), and write

$$\|\cdot\|_{r,I_K} \quad \text{and} \quad \langle \cdot, \cdot \rangle_{I_K}$$

for the norm on $\mathsf{L}^r(I_K)$ and the scalar product in $\mathsf{L}^2(I_K)$, respectively. Notice that there is a natural embedding $\mathsf{W}^{1,r}(I_K) \hookrightarrow \mathsf{BC}(\mathbb{R})$ for all $K \in (0, \infty]$.

We first summarize some properties of the convolution operator $\mathcal{A}$. In particular, we show that $\mathcal{A}$ maps $\mathsf{L}^2(I_K)$ compactly into $\mathsf{L}^r(I_K)$ provided that $1 \le r < \infty$ and $K < \infty$.

Lemma 2. *Let $K \in (0, \infty]$ and $1 \le r < \infty$ be given. Then, the linear operator $\mathcal{A}$ maps $\mathsf{L}^r(I_K)$ continuously into $\mathsf{W}^{1,r}(I_K) \subset \mathsf{BC}(\mathbb{R})$ with*

$$\|(\mathcal{A}W)'\|_{r,I_K} \le 2\|W\|_{r,I_K}\,, \qquad \|\mathcal{A}W\|_{\infty,I_K} \le \|W\|_{r,I_K}\,, \qquad \|\mathcal{A}W\|_{r,I_K} \le \|W\|_{r,I_K}\,.$$

Moreover, $W_n \rightharpoonup W_\infty$ weakly in $\mathsf{L}^2(I_K)$ implies $\mathcal{A}W_n \to \mathcal{A}W_\infty$ pointwise for all K and also strongly in $\mathsf{L}^r(I_K)$ for $K < \infty$.

Proof. Thanks to $(\mathcal{A}W)'(\varphi) = W(\varphi + 1/2) - W(\varphi - 1/2)$ and since Hölders inequality implies

$$\big|(\mathcal{A}W)(\varphi)\big|^r \le \int_{\varphi-1/2}^{\varphi+1/2} |W(s)|^r \,\mathrm{d}s,$$

all estimates follows immediately. Moreover, the pointwise convergence $\mathcal{A}W_n \to \mathcal{A}W$ follows from the definition of $\mathcal{A}$ in (4), and implies the strong convergence for $K < \infty$ due to $\mathsf{L}^\infty(I_K) \hookrightarrow \mathsf{L}^r(I_K)$ and the Dominated Convergence Theorem. □

Lemma 2 reveals that the functionals $\mathcal{Q}_K$, $\mathcal{P}_K$, and $\mathcal{L}_K$ are well defined on $\mathsf{L}^2(I_K)$ for all $K \in (0, \infty]$. Moreover, we easily show that they are also Gâteaux-differentiable with derivatives

$$\partial\mathcal{L}_K(W) = \sigma^2 W - \partial\mathcal{Q}_K(W) + \partial\mathcal{P}_K(W), \qquad \partial\mathcal{Q}_K(W) = \mathcal{A}\Psi_q(\mathcal{A}W), \qquad \partial\mathcal{P}_K(W) = \mathcal{A}\Psi_p(\mathcal{A}W),$$

where the continuous and nonlinear functions Ψ_q and Ψ_p are defined above.

Remark 3. *For $K = \infty$ or $K \notin \pi\mathbb{Q}$, the operator $\mathcal{A} : \mathsf{L}^2(I_K) \to \mathsf{L}^2(I_K)$ has only trivial kernel.*

Proof. The operator $\mathcal{A}$ diagonalizes in Fourier space via $\mathcal{A}\mathrm{e}^{\mathrm{i}k\varphi} = \varrho(k/2)\mathrm{e}^{\mathrm{i}k\varphi}$ with $\varrho(\kappa) = \sin(\kappa)/\kappa$ for all $k \in \mathbb{R}$, and the claim follows immediately. □

2.1 Necessary condition for traveling waves

A key property of the action functional $\mathcal{L}_K$ is that its restriction to the positive ray $\zeta > 0 \mapsto \zeta W$ has a unique maximizer for every non-degenerate W. To see this, we start with an auxiliary result about the maximizers of certain tri-monomial functions.

Lemma 4. *The function $\bar{\xi}$ with*

$$\bar{\xi}(c_2, c_q, c_p) := \operatorname{argmax}_{\xi>0} c_2\xi^2 + c_q\xi^q - c_p\xi^p$$

is well-defined and continuous on $\mathbb{R}^3_+$.

Proof. For given $c = (c_2, c_q, c_p) \in \mathbb{R}^3_+$, the function $f_c(\xi) := c_2\xi^2 + c_q\xi^q - c_p\xi^p$ is continuously differentiable with

$$f_c'(\xi) > 0 \qquad \text{and} \qquad f_c'(\xi) < 0$$

for small and large ξ, respectively. The derivative f_c' has thus at least one zero $\bar{\xi}(c) > 0$, which obviously satisfies

$$0 = g_c\big(\bar{\xi}(c)\big) = 2c_2\bar{\xi}(c)^2 + qc_q\bar{\xi}(c)^q - pc_p\bar{\xi}(c)^p, \qquad g_c(\xi) := \xi f_c{}'(\xi)\,. \tag{6}$$

A further straight forward computation yields

$$\bar{\xi}(c)g_c'\big(\bar{\xi}(c)\big) = \bar{\xi}(c)^2 f_c''\big(\bar{\xi}(c)\big) = (4 - 2p)c_2\bar{\xi}(c)^2 + \big(q^2 - qp\big)c_q\bar{\xi}(c)^q < 0\,,$$

and we conclude that $\bar{\xi}(c)$ is the only zero of both g_c and f_c' in the interval $(0, \infty)$. In particular, we have $f_c'(\xi) > 0$ and $f_c'(\xi) < 0$ for $\xi < \bar{\xi}(c)$ and $\xi > \bar{\xi}(c)$, respectively, that means $\bar{\xi}(c)$ is a global maximizer of f_c. Finally, using (6) we readily verify the estimates

$$\max\left\{\left(\frac{2c_2}{pc_p}\right)^{1/(p-2)}, \left(\frac{qc_q}{pc_p}\right)^{1/(p-q)}\right\} \le \bar{\xi}(c) \le \max\left\{\left(\frac{4c_2}{pc_p}\right)^{1/(p-2)}, \left(\frac{2qc_q}{pc_p}\right)^{1/(p-q)}\right\},$$

which in turn imply the claimed continuity of $\bar{\xi}$ since we have $f_{c_n} \to f_c$ uniformly as $c_n \to c \in \mathbb{R}^3_+$ on each compact subset of $\mathbb{R}_+$. □

Corollary 5. *Let $K \in (0, \infty]$ and $W \in \mathsf{L}^2(I_K)$ be given with $\mathcal{A}W \neq 0$. Then, there exists a unique $\bar{\zeta}_K(W) \in \mathbb{R}_+$ such that*

$$0 < \mathcal{L}_K\big(\bar{\zeta}_K(W)W\big) = \max_{\zeta>0} \mathcal{L}_K(\zeta W)\,.$$

Moreover $W_n \to W$ strongly in $\mathsf{L}^2(I_K)$ with $\mathcal{A}W \neq 0$ implies $\bar{\zeta}_K(W_n) \to \bar{\zeta}(W)$.

Proof. All assertions follow from Lemma 4 via $\bar{\zeta}_K(W) := \bar{\xi}\big(\tfrac{1}{2}\sigma^2\|W\|^2_{2,I_K},\, \mathcal{Q}_K(W),\, \mathcal{P}_K(W)\big)$. □

In view of Corollary 5, we introduce the functional

$$\mathcal{F}_K(W) := \frac{\mathrm{d}}{\mathrm{d}\zeta}\mathcal{L}_K(\zeta W)|_{\zeta=1} = \big\langle \partial\mathcal{L}_K(W),\, W\big\rangle_{I_K} = \sigma^2\|W\|^2_{2,I_K} + q\mathcal{Q}_K(W) - p\mathcal{P}_K(W)\,,$$

which is well defined and Gâteaux differentiable on $\mathsf{L}^2(I_K)$ with

$$\partial\mathcal{F}_K(W) = 2\sigma^2 W + q\mathcal{A}\Psi_q(\mathcal{A}W) - p\mathcal{A}\Psi_p(\mathcal{A}W)\,.$$

We further define the *Nehari manifold* by

$$\mathsf{M}_K := \Big\{W \in \mathsf{L}^2(I_K) \;:\; W \neq 0, \quad \mathcal{F}_K(W) = 0\Big\}\,,$$

and notice that $\bar{\zeta}_K(W)W \in \mathsf{M}_K$ for all W with $\mathcal{A}W \neq 0$. Moreover, $W \in \mathsf{M}_K$ implies $\mathcal{A}W \neq 0$, and $\mathcal{A}W \neq 0$ implies

$$W \in \mathsf{M}_K \quad\Longleftrightarrow\quad \bar{\zeta}_K(W) = 1 \quad\Longleftrightarrow\quad \mathcal{L}_K(W) = \max_{\zeta>0}\mathcal{L}_K(\zeta W)\,.$$

Remark 6. *Each non-vanishing traveling wave $W \in \mathsf{L}^2(I_K)$ belongs to M_K and $\mathsf{BC}^1(\mathbb{R})$.*

Proof. $W \neq 0$ combined with the traveling wave equation (5) implies $\mathcal{A}W \neq 0$, and $W \in \mathsf{M}_K$ follows since testing (5) with W gives $\mathcal{F}_K(W) = 0$. Moreover, $W \in \mathsf{BC}^1(\mathbb{R})$ is a direct consequence of Lemma 2 and (5). □

Our strategy for proving the existence of ground waves is to show that $\mathcal{L}_K$ attains its minimum on M_K. We can then conclude that each minimizer satisfies the traveling wave equation (5), and Remark 6 guarantees that the minimum is in fact the smallest non-vanishing critical value of $\mathcal{L}_K$.

2.2 Properties of the Nehari manifold

We next derive some estimates for functions in the Nehari manifold.

Lemma 7. *There exist positive constants c and C, both independent of K, such that*

1. $\|W\|_{2,I_K} \geq c$ *and* $\|W\|_{2,I_K} \leq C\sqrt{\mathcal{L}_K(W)}$,
2. $\|\mathcal{A}W\|_{\infty,I_K} \geq c$ *and* $\|\mathcal{A}W\|_{\infty,I_K} \leq C\sqrt{\mathcal{L}_K(W)}$,
3. $\mathcal{L}_K(W) \geq c$,
4. $\big\langle \partial F_K(W),\, W\big\rangle_{I_K} \leq -c$,

hold for all $W \in \mathsf{M}_K$.

Proof. Employing $\mathcal{F}_K(W) = 0$ and Lemma 2 we estimate

$$q\mathcal{Q}_K(W) \leq \sigma^2\|W\|^2_{2,I_K} + q\mathcal{Q}_K(W) = p\mathcal{P}_K(W) \leq p\|\mathcal{A}W\|^{p-q}_{\infty,I_K}\mathcal{Q}_K(W)$$

and find, thanks to $\mathcal{Q}_K(W) > 0$ and Lemma 2, that

$$\|W\|_{2,I_K} \geq \|\mathcal{A}W\|_{\infty,I_K} \geq (q/p)^{1/(p-q)}. \tag{7}$$

Due to $\mathcal{F}_K(W)=0$ we also have

$$\mathcal{L}_K(W)=\sigma^2\left(\frac{1}{2}-\frac{1}{p}\right)\|W\|_{2,I_K}^2+\left(1-\frac{q}{p}\right)\mathcal{Q}_K(W)\geq\sigma^2\left(\frac{1}{2}-\frac{1}{p}\right)\|W\|_{2,I_K}^2,$$

and combining this estimate with (7) we arrive at the first three claims. Moreover, a direct computation yields

$$\begin{aligned}\big\langle\partial F_K(W),\,W\big\rangle_{I_K}&=2\sigma^2\|W\|_{2,I_K}^2+q^2\mathcal{Q}_K(W)-p^2\mathcal{P}_K(W)\\&=(2-p)\sigma^2\|W\|_{2,I_K}^2+\big(q^2-qp\big)\mathcal{Q}_K(W)\leq-\left|p-2\right|\sigma^2\|W\|_{2,I_K}^2,\end{aligned}$$

which in turn implies the final estimate. □

The fourth assertion in Lemma 7 ensures that the Nehari manifold M_K is strictly transversal to each positive ray $\zeta>0\mapsto\zeta W$ with $W\in\mathsf{M}_K$. It is therefore clear that minimizers of $\mathcal{L}_K|_{M_K}$ are critical points of $\mathcal{L}_K$. Here we give an alternative proof of this assertion that relies on the constrained gradient flow for $\mathcal{L}_K$, that is

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}W_\tau=-\partial\mathcal{L}_K(W_\tau)+\lambda_K(W_\tau)\partial F_K(W_\tau),\qquad\lambda_K(W):=\frac{\big\langle\partial\mathcal{L}_K(W),\,\partial\mathcal{F}_K(W)\big\rangle_{I_K}}{\|\partial\mathcal{F}_K(W)\|_{2,I_K}^2}\tag{8}$$

where τ is the flow time and $\tau\mapsto W_\tau$ denotes a curve in M_K. This gradient flow is also the starting point for the numerical approximation of ground waves in §4.

Lemma 8. *For each $K\in(0,\,\infty]$, the initial value problem to the M_K-valued ODE* (8) *is well-posed. Moreover, $\mathcal{L}_K$ is strictly decreasing along each non-stationary trajectory and each stationary point solves the traveling wave equation* (5).

Proof. Let some initial datum $W_0\in\mathsf{M}_K$ be given. Lemma 7 implies $\partial\mathcal{F}_K(W_0)\neq0$, and by continuity there exists a small ball $B\subset\mathsf{L}^2(I_K)$ around W_0 such that the multiplier λ_K is a well defined and Lipschitz continuous function on B. Consequently, there exists a local solution $\tau\in[0,\,\tau_1)\mapsto W_\tau\in\mathsf{L}^2(I_K)$. The definition of λ_K implies

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{F}_K(W_\tau)=\big\langle\partial\mathcal{F}_K(W_\tau),\,\tfrac{\mathrm{d}}{\mathrm{d}\tau}W_\tau\big\rangle_K=0,$$

so M_K is indeed invariant under the flow of (8). Moreover, a direct computation gives

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{L}_K(W_\tau)&=\big\langle\partial\mathcal{L}_K(W_\tau),\,\tfrac{\mathrm{d}}{\mathrm{d}\tau}W_\tau\big\rangle_{I_K}\\&=\frac{\|\partial\mathcal{L}_K(W_\tau)\|_{2,I_K}^2\|\partial\mathcal{F}_K(W_\tau)\|_{2,I_K}^2-\big\langle\partial\mathcal{L}(W_\tau),\,\partial\mathcal{F}(W_\tau)\big\rangle_{I_K}^2}{\|\partial\mathcal{F}_K(W_\tau)\|_{2,I_K}^2}\geq0,\end{aligned}$$

where the inequality is strict provided that $\partial\mathcal{L}_K(W_\tau)$ and $\partial\mathcal{F}_K(W_\tau)$ are not co-linear, that means as long as the right hand side in (8) does not vanish. Finally, suppose that $W_\tau\equiv W\in\mathsf{M}_K$ is stationary under the flow of (8). Then we have

$$\partial\mathcal{L}_K(W)=\lambda_K(W)\partial\mathcal{F}_K(W),$$

and testing this identity with W we find

$$0=\big\langle\partial\mathcal{L}_K(W),\,W\big\rangle_{I_K}=\lambda_K(W)\big\langle\partial\mathcal{F}_K(W),\,W\big\rangle_{I_K}.$$

Lemma 7 now implies $\lambda_K(W)=0$, and hence $\partial\mathcal{L}_K(W)=0$. □

A particular consequence of Lemma 8 is that each minimizer of $\mathcal{L}_K|_{M_K}$ is a stationary point of (8), and thus in fact a traveling wave.

3 Ground waves as Nehari minimizers of the action

In this section we finish the proof of Theorem 1 by showing that $\mathcal{L}_K$ attains its minimum on the Nehari manifold M_K. To this end we employ the direct method for $K < \infty$, and pass afterwards to the limit $K \to \infty$. For the proofs we define

$$\ell_K := \inf \mathcal{L}_K|_{\mathsf{M}_K}$$

and recall that Lemma 7 provides a constant $c > 0$ such that $\ell_K \geq c$ for all $K \in (0, \infty]$.

3.1 Existence of periodic ground waves

We now fix $0 < K < \infty$ and employ the compactness of $\mathcal{A}$ to show that each minimizing sequence for $\mathcal{L}_K|_{\mathsf{M}_K}$ contains a subsequence that converges to a minimizer. Alternatively, we could employ critical point techniques as follows. Using similar estimates as in the proof of Lemma 7, one easily shows that the action landscape has a *mountain pass geometry* via

$$\mathcal{L}_K(0) = 0, \qquad \|W\|_{2,I_K} = 1 \implies \mathcal{L}_K(W) \geq \tfrac{1}{2}\sigma^2, \qquad \mathcal{A}W \neq 0 \implies \lim_{\zeta \to \infty} \mathcal{L}_K(\zeta W) = -\infty\,,$$

and the compactness of $\mathcal{A}$ ensures that $\mathcal{L}_K$ satisfies the Palais-Smale condition. The existence of non-vanishing critical values is hence implied by the Mountain Pass Theorem, and the Palais-Smale condition guarantees that there is a minimal critical value. The details for this line of argument can, for the special case $q = 2$, be found in [Pan05, Section 3.4.1].

Theorem 9. *For each $0 < K < \infty$ there exists a minimizer of $\mathcal{L}_K|_{\mathsf{M}_K}$.*

Proof. Let $(W_n)_{n\in\mathbb{N}} \subset \mathsf{M}_K$ be any minimizing sequence for $\mathcal{L}_K|_{\mathsf{M}_K}$. By construction and Lemma 7, we then have

$$c \leq \|W_n\|_{2,I_K} \leq C, \qquad c \leq \mathcal{L}_K(W_n) \leq C$$

for some constants $0 < c < C < \infty$ independent of n. By passing to a (not relabeled) subsequence we can assume that $W_n \rightharpoonup W$ weakly in $\mathsf{L}^2(I_K)$, and that $\lim_{n\to\infty} \|W_n\|_{2,I_K}^2$ exists. Our strategy is now to show that W minimizes $\mathcal{L}_K$ on M_K.

The properties of $\mathcal{A}$, see Lemma 2, guarantee that $\mathcal{A}W_n \to \mathcal{A}W$ pointwise and strongly in $\mathsf{L}^r(I_K)$ for all $1 < r < \infty$, so by Lemma 7 we have $\mathcal{A}W \neq 0$ and hence $W \neq 0$. By definition of M_K, we also have $\max_{\zeta>0} \mathcal{L}_K(\zeta W_n) = \mathcal{L}_K(W_n) = \ell_K$, and the above convergencies imply

$$\mathcal{L}_K(\zeta W) \leq \frac{1}{2}\sigma^2\Big(\|W\|_{2,I_K}^2 - \lim_{n\to\infty} \|W_n\|_{2,I_K}^2\Big) + \ell_K \quad \text{for all} \quad \zeta > 0\,.$$

Taking the maximum over $\zeta > 0$ gives

$$\ell_K \leq \max_{\zeta>0} \mathcal{L}_K(\zeta W) \leq \frac{1}{2}\sigma^2\Big(\|W\|_{2,I_K}^2 - \lim_{n\to\infty} \|W_n\|_{2,I_K}^2\Big) + \ell_K\,,$$

and we conclude that

$$\ell_K = \max_{\zeta>0} \mathcal{L}_K(\zeta W), \qquad \|W\|_{2,I_K} = \lim_{n\to\infty} \|W_n\|_{2,I_K}\,.$$

These identities imply the strong convergence $W_n \to W$ as well as $W \in \mathsf{M}_K$ with $\mathcal{L}_K(W) = \ell_K = \lim_{n\to\infty} \mathcal{L}_K(W_N)$. ☐

To complete our existence proof for periodic ground waves we finally derive an upper bound for ℓ_K which in turn implies that minimizer of $\mathcal{L}_K$ are non-trivial for large K.

Lemma 10. *We have $\limsup_{K\to\infty} \ell_K < \ell_\infty$.*

Proof. Let $W_\infty \in \mathsf{M}_\infty$ be given. For each $1 < K < \infty$ we define $V_K \in \mathsf{L}^2(\mathbb{R})$

$$V_K(\varphi) := \begin{cases} W_\infty(\varphi) & \text{for } |\varphi| < K-1, \\ 0 & \text{else,} \end{cases}$$

and $W_K \in \mathsf{L}^2(I_K)$ as periodic continuation of $V_K|_{I_K}$. This implies $\|V_K - W_\infty\|_{2,\mathbb{R}} \to 0$, and by continuity of $\mathcal{L}_\infty$ and $\bar{\zeta}_\infty$ we get

$$\mathcal{L}_\infty(W_\infty) = \lim_{K\to\infty} \mathcal{L}_\infty\big(V_K\big), \qquad 1 = \bar{\zeta}_\infty(W_\infty) = \lim_{K\to\infty} \bar{\zeta}_\infty\big(V_K\big).$$

Moreover, the properties of $\mathcal{A}$ ensure that $(\mathcal{A}V_K)(\varphi) = (\mathcal{A}W_K)(\varphi)$ for all $\varphi \in I_K$, and thus we find

$$\mathcal{L}_K(W_K) = \mathcal{L}_\infty\big(V_K\big), \qquad \bar{\zeta}_K\big(W_K\big) = \bar{\zeta}_\infty(V_K).$$

Consequently, we have $\mathcal{L}_\infty(W_\infty) = \lim_{K\to\infty} \mathcal{L}_K\big(\bar{\zeta}_K(W_K)W_K\big)$, and $\ell_K \le \mathcal{L}_K\big(\bar{\zeta}(W_K)W_K\big)$ yields $\limsup_{K\to\infty} \ell_K \le \mathcal{L}_\infty(W_\infty)$. The thesis now follows since $W_\infty \in \mathsf{M}_\infty$ was arbitrary. □

Corollary 11. *Let $K < \infty$ be sufficiently large. Then, each minimizer of $\mathcal{L}_K|_{\mathsf{M}_K}$ is non-constant.*

Proof. The only constant function in M_K is given by the unique maximizer $\bar{\zeta} := \bar{\xi}\big(\sigma^2/2,\, 1,\, 1\big) > 0$ of the function

$$\zeta \mapsto \tfrac{1}{2}\sigma^2\zeta^2 + \zeta^q - \zeta^p = \frac{\mathcal{L}_K\big(\zeta\big)}{2K},$$

see Lemma 4. In particular, for all sufficiently large K we have $\mathcal{L}_K\big(\bar{\zeta}\big) = K\mathcal{L}_1\big(\bar{\zeta}\big) > \ell_\infty$, and hence $\mathcal{L}_K\big(\bar{\zeta}\big) > \ell_K$ due to Lemma 10. □

Combing Theorem 9 and Lemma 8 with Remark 6 and Corollary 11 we now obtain our existence result on periodic ground waves as formulated in Theorem 1.

3.2 Convergence to solitary ground waves

Our final goal is to prove that $\mathcal{L}_\infty$ attains its minimum on M_∞. Since the operator $\mathcal{A}$ is no longer compact, we cannot argue as in the proof of Theorem 9. Instead, we construct minimizers as limit of period ground waves. The same strategy was used in [Pan05, Section 3.4.2] and some of our key arguments are inspired by those presented there.

Theorem 12. *$\mathcal{L}_\infty$ attains its minimum on M_∞ and we have $\ell_\infty = \lim_{K\to\infty} \ell_K$. In particular, each unbounded sequence $(K_m)_{m\in\mathbb{N}}$ has at least one subsequence $(K_n)_{n\in\mathbb{N}}$ with the following property: There exists a corresponding sequence $(W_n)_{n\in\mathbb{N}}$ of period ground waves $W_n \in \mathsf{M}_{K_n} \cap \mathsf{BC}^1(\mathbb{R})$ that converges to a solitary ground wave $W_\infty \in \mathsf{M}_\infty \cap \mathsf{BC}^1(\mathbb{R})$ in the sense of*

$$\|W_\infty - V_n\|_{2,\mathbb{R}} \xrightarrow{n\to\infty} 0,$$

where $V_n \in \mathsf{L}^2(\mathbb{R})$ is defined by $V_n(\varphi) = W_n(\varphi)$ for $\varphi \in I_{K_n}$ and $V_n(\varphi) = 0$ for $\varphi \notin I_{K_n}$.

Proof. Step 1: According to Theorem 9 and Remark 6, for each m there exists a periodic traveling wave $W_m \in \mathsf{M}_{K_m} \cap \mathsf{BC}(\mathbb{R})$ which minimizes $\mathcal{L}_{K_m}|_{\mathsf{M}_{K_m}}$. Since (5) is invariant under shifts $W \rightsquigarrow W(\cdot + \varphi_0)$ and reflections $W \rightsquigarrow -W$, we can assume that

$$(\mathcal{A}W_m)(0) = \|\mathcal{A}W_m\|_{\infty,I_{K_m}}. \tag{9}$$

By Lemma 7 and Lemma 10 we also have

$$c \le \mathcal{L}_{K_m}(W_m) \le C, \qquad c \le \|W_m\|_{2,I_{K_m}} \le C \qquad c \le \|\mathcal{A}W_m\|_{\infty,I_{K_m}} \le C \tag{10}$$

for some constants $0 < c < C < \infty$ independent of m. Moreover, from the traveling wave equation (5) we infer, using Lemma 2 and (10), that

$$\|(\mathcal{A}W_m)'\|_{\infty,I_{K_m}} \le 2\|W_m\|_{\infty,I_{K_m}} \le C\|\mathcal{A}W_m\|_{\infty,I_{K_m}}\,.$$

In view of (9) we thus obtain

$$W_m(\varphi) = W_m(0) + \int_0^{\varphi} (\mathcal{A}W_m)'(s)\,\mathrm{d}s \ge d \quad \text{for all} \quad |\varphi| \le d, \tag{11}$$

for some constant d independent of m.

Step 2: By definition, we have $\|V_m\|_{2,\mathbb{R}} = \|W_m\|_{2,I_{K_m}} \le C$ and

$$(\mathcal{A}V_n)(\varphi) = (\mathcal{A}W_n)(\varphi) \quad \text{for} \quad |\varphi| < K_n - \tfrac{1}{2}. \tag{12}$$

We now choose a subsequence $(K_n)_{n\in\mathbb{N}}$ such that $V_n \rightharpoonup W_\infty \in \mathsf{L}^2(\mathbb{R})$, and Lemma 2 provides the pointwise convergence

$$(\mathcal{A}W_\infty)(\varphi) = \lim_{n\to\infty} (\mathcal{A}V_n)(\varphi) = \lim_{n\to\infty} (\mathcal{A}W_n)(\varphi).$$

Moreover, thanks to (5) and (12) we conclude that the sequence $(V_n)_{n\in\mathbb{N}}$ converges pointwise, and combining this with $V_n \rightharpoonup W_\infty$ we arrive at the pointwise convergence

$$W_\infty(\varphi) = \lim_{n\to\infty} V_n(\varphi) = \lim_{n\to\infty} W_n(\varphi)\,.$$

In particular, $W_\infty \in \mathsf{L}^2(\mathbb{R})$ is a traveling wave. Thanks to (11) and Remark 3 we also have $W_\infty \ne 0$ with $\mathcal{A}W_\infty \ne 0$, so Remark 6 yields $W_\infty \in \mathsf{M}_\infty \cap \mathsf{BC}^1(\mathbb{R})$.

Step 3: For each $0 < D < \infty$ and $1 \le r < \infty$ we have

$$\int_{-D}^{D} |\mathcal{A}W_\infty|^r\,\mathrm{d}\varphi = \lim_{n\to\infty}\int_{-D}^{D} |\mathcal{A}W_n|^r\,\mathrm{d}\varphi \le \liminf_{n\to\infty}\int_{I_{K_n}} |\mathcal{A}W_n|^r\,\mathrm{d}\varphi$$

due to (10) and the Dominated Convergence Theorem, and the limit $D \to \infty$ gives

$$\mathcal{Q}_\infty(W_\infty) \le \liminf_{n\to\infty} \mathcal{Q}_{K_n}(W_n), \qquad \mathcal{P}_\infty(W_\infty) \le \liminf_{n\to\infty} \mathcal{P}_{K_n}(W_n). \tag{13}$$

Similarly, using Fatou's Lemma and passing afterwards to $D \to \infty$ we prove that

$$\|W_\infty\|_{2,\mathbb{R}}^2 = \lim_{D\to\infty}\int_{-D}^{D} W_\infty(\varphi)^2\,\mathrm{d}\varphi \le \lim_{D\to\infty}\liminf_{n\to\infty}\int_{-D}^{D} W_n(\varphi)^2\,\mathrm{d}\varphi \le \liminf_{n\to\infty}\|W_n\|_{2,I_{K_n}}^2. \tag{14}$$

Combining (13) and (14) with $W_n \in \mathsf{M}_{K_n}$ for all $n \in \mathbb{N}\cup\{\infty\}$ we now estimate

$$\begin{aligned}\ell_\infty \le \mathcal{L}_\infty(W_\infty) &= \sigma^2\Big(\frac{1}{2}-\frac{1}{p}\Big)\|W_\infty\|_{2,\mathbb{R}}^2 + \Big(1-\frac{q}{p}\Big)\mathcal{Q}_\infty(W_\infty)\\ &\le \sigma^2\Big(\frac{1}{2}-\frac{1}{p}\Big)\liminf_{n\to\infty}\|W_n\|_{2,I_{K_n}}^2 + \Big(1-\frac{q}{p}\Big)\liminf_{n\to\infty}\mathcal{Q}_n(W_n)\\ &= \liminf_{n\to\infty}\mathcal{L}_{K_n}(W_n) = \liminf_{n\to\infty}\ell_{K_n}.\end{aligned} \tag{15}$$

On the other hand, by Lemma 10 we have $\limsup_{n\to\infty}\ell_{K_n} \le \ell_\infty$, and thus we find

$$\ell_\infty = \mathcal{L}_\infty(W_\infty) = \liminf_{n\to\infty}\ell_{K_n} = \limsup_{n\to\infty}\ell_{K_n}\,.$$

Consequently, W_∞ is in fact a solitary ground wave and we have an equality sign in (15). This implies

$$\|W_\infty\|_{2,\mathbb{R}} = \lim_{n\to\infty}\|W_n\|_{2,I_n} = \lim_{n\to\infty}\|V_n\|_{2,\mathbb{R}},$$

which in turn provides the strong convergence $V_n \to W_\infty$. Finally, $\ell_\infty = \lim_{K\to\infty}\ell_K$ holds since we have already shown that any unbounded sequence $(K_m)_{m\in\mathbb{N}}$ has a subsequence $(K_n)_{n\in\mathbb{N}}$ with $\ell_\infty = \lim_{n\to\infty}\ell_{K_n}$. □

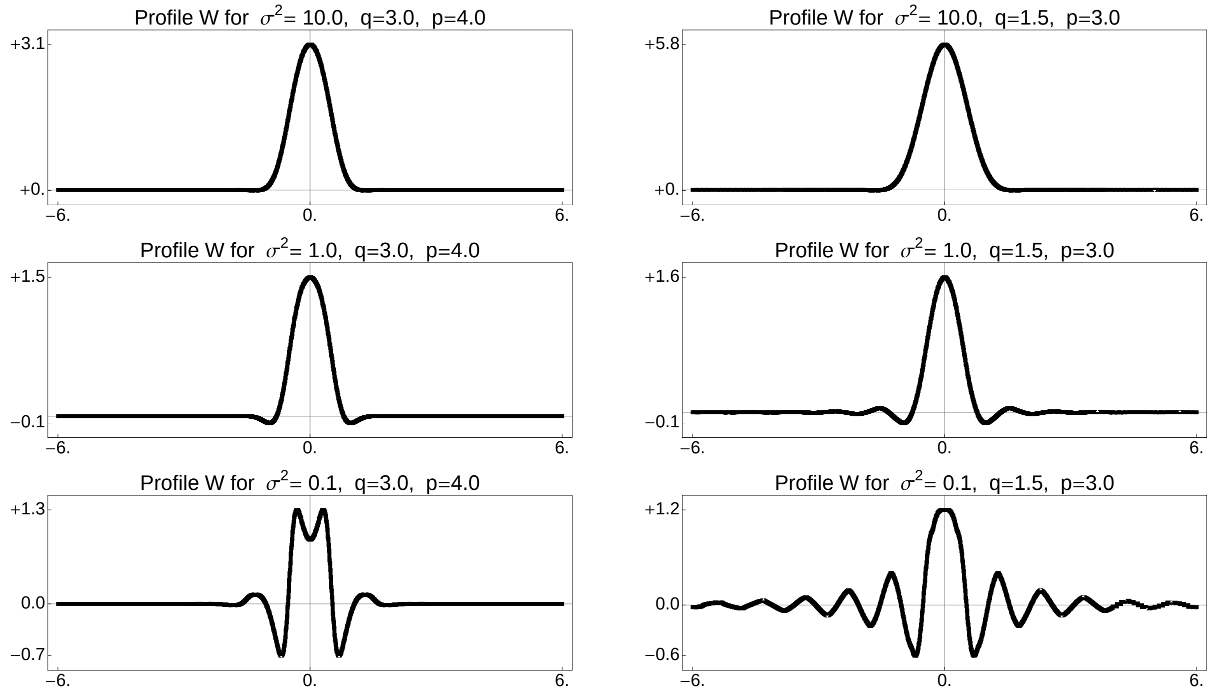

Figure 1: Numerical approximations of ground wave for different values of σ^2 and $q = 3, p = 4$ (left column) or $q = 3/2, p = 3$ (right column). The numerical parameters are $K = 6$, $N = 2400$, and $\triangle\tau \geq 0.0005$.

4 Numerical solutions

In order to illustrate our theoretical findings we implemented the following discretization of the constrained gradient flow for $\mathcal{L}_K|_{\mathsf{M}_K}$:

1. Given $0 < K < \infty$, we divide the periodicity cell $[-K, K)$ into N equidistant grid points and approximate all integrals by Riemann sums.
2. We choose a small flow time $\triangle\tau$ and minimize the action on M_K by iterating the following two steps:
   (a) We compute an explicit Euler step for (8), that means we update W tangential to M_K via
   $$W \mapsto W - \triangle\tau\Big(\partial\mathcal{L}_K(W) - \lambda_K(W)\partial\mathcal{F}_K(W)\Big).$$
   (b) We update in radial direction via
   $$W \mapsto \big(1 + \triangle\tau\mathcal{F}_K(W)\big)W$$
   to enforce the constraint $\mathcal{F}_K(W) = 0$.
3. We initialize the iteration by discretizing reasonable initial data, as for instance $W(\varphi) = \exp\big(-\varphi^2\big)$ for $|\varphi| < K$.

Although this scheme is rather simple, it exhibits good convergence properties provided that the flow time $\triangle\tau$ is sufficiently small. Moreover, numerical simulations indicate that each time-discrete trajectory converges to a limit that is independent of the particular choice of the initial data, and thus we expect that this limit approximates a global minimizer of $\mathcal{L}_K|_{\mathsf{M}_K}$.

Typical numerical solutions for $K = 6$ are displayed in Figure 1. We clearly observe that periodic ground waves are localized but have rather different shapes for large and small speeds, respectively. If σ^2 is sufficiently large, the double well structure of Φ is less important and the wave looks like a unimodal wave for the convex potential $\Phi(w) = w^p$, see [Her10] for details. For small σ^2, however, the contributions from the different monomials balance and W has several local extrema.

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