Proceedings of the Royal Society of Edinburgh, **140A**, 753–785, *2010*

Unimodal wavetrains and solitons in convex Fermi–Pasta–Ulam chains

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(MS received 23 January 2009; accepted 30 November 2009)

We consider atomic chains with nearest neighbour interactions and study periodic travelling waves and homoclinic travelling waves, which are called wavetrains and solitons, respectively. Our main result is a new existence proof which relies on the constrained maximization of the potential energy and exploits the invariance properties of an improvement operator. The approach is restricted to convex interaction potentials but refines the standard results, as it provides the existence of travelling waves with unimodal and even profile functions. Moreover, we discuss both the numerical approximation and the complete localization of wavetrains, and show that wavetrains converge to solitons when the periodicity length tends to infinity.

1. Introduction

We consider infinite chains of identical atoms with unit mass that are coupled by nearest neighbour interactions. The dynamics of such chains is governed by Newton's equations

$$\ddot{x}_j(t) = \Phi'(x_{j+1}(t) - x_j(t)) - \Phi'(x_j(t) - x_{j-1}(t)), \tag{1.1}$$

where $x_j(t)$ denotes the position of the jth atom at time t and Φ is the interaction potential. Restating (1.1) in terms of atomic distances $r_j(t) = x_{j+1}(t) - x_j(t)$ and atomic velocities $v_j(t) = \dot{x}_j(t)$, we find that

$$\dot{r}_j(t) = v_{j+1}(t) - v_j(t), \qquad \dot{v}_j(t) = \Phi'(r_j(t)) - \Phi'(r_{j-1}(t)). \tag{1.2}$$

We allow for arbitrary convex interaction potentials Φ and refer to (1.1) as a Fermi–Pasta–Ulam (FPU) chain, although the potential in the original paper [5] was a quartic polynomial.

FPU chains can be viewed as simple toy models for crystals and solids, and they allow some essential properties of nonlinear elastic materials to be studied. Although (1.1) is a strong simplification of a real material, it exhibits very complex behaviour and we are, at present, far from a complete understanding of its dynamical properties.

During the past few decades, a lot of research has addressed the existence and properties of travelling waves in FPU chains because they can be viewed as elementary waves and provide a lot of insight into the energy transport in nonlinear

https://doi.org/10.1017/S0308210509000146 Published online by Cambridge University Press

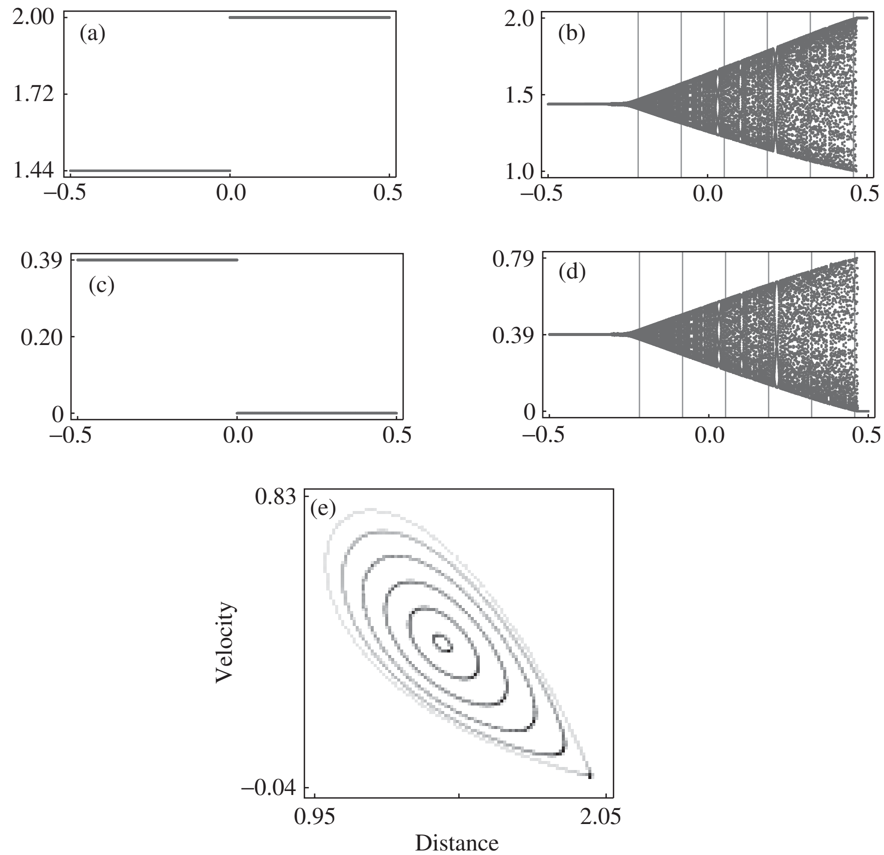

Figure 1. The atoms in a dispersive shock self-organize into modulated travelling waves. Parts (a)–(d) depict snapshots of atomic distances and velocities against the scaled particle index for different macroscopic times. (a) distances, time = 0, (b) distances, time = 0.5, (c) velocities, time = 0, (d) velocities, time = 0.5. Part (e) depicts the corresponding family of wavetrains with supersonic soliton as the 'homoclinic limit'. The picture shows the density plots of six local distribution functions in the (r, v)-plane. Modulation theory predicts that each of these local distribution functions corresponds to a travelling wave whose parameters depend on macroscopic time and particle index.

media. Such travelling waves solve nonlinear advance–delay differential equations, and characterizing the solution set to those equations is a fundamental problem in mathematics.

A further motivation for the study of travelling waves is related to atomistic Riemann problems and self-thermalization of FPU chains: starting with piecewise constant initial data for atomic distances and velocities, solutions to (1.2) are self-similar on a macroscopic scale and involve *dispersive shocks*, which are fan-like structures with strong microscopic oscillations (see figure 1). It is known from the theory of integrable systems and numerical simulations that the oscillations within a dispersive shock can be described by *modulated travelling waves* (see [1, 6] and the references therein).

1.1. Travelling waves and main results

Travelling waves are exact solutions to (1.2) and satisfy the ansatz[1]

$$r_j(t) = R(\varphi), \quad v_j(t) = V(\varphi), \quad \varphi = kj + \omega t, \tag{1.3}$$

with phase φ, wavenumber k, (negative) frequency ω and profile functions R and V. Inserting (1.3) into (1.2), we obtain the nonlinear advance–delay differential equations

$$\omega \frac{\mathrm{d}}{\mathrm{d}\varphi} R = \nabla_k^+ V, \tag{1.4\,a}$$

$$\omega \frac{\mathrm{d}}{\mathrm{d}\varphi} V = \nabla_k^- \Phi'(R), \tag{1.4\,b}$$

where ∇_k^+ and ∇_k^- respectively denote the forward- and backward-difference operators with shift k. Depending on the properties of the profile functions, we distinguish the following cases.

(i) *Wavetrains* or *periodic waves*: R and V are periodic.

(ii) *Solitons* or *homoclinic waves*: R and V are localized over a constant background state.

(iii) *Fronts* or *heteroclinic waves*: R and V connect different constant background states.

(iv) *Oscillatory fronts*: R and V connect different asymptotic wavetrains.

Note that our usage of 'soliton' is quite sloppy: localized travelling waves are sometimes called 'solitary waves', and 'soliton' then refers to a solitary wave that survives collisions with other such waves unchanged.

We show the existence of wavetrains and solitons with unimodal and even profile functions R and V, where *even* means invariance under $\varphi \rightsquigarrow -\varphi$ as usual, and *unimodal* functions are monotone for both $\varphi \leqslant 0$ and $\varphi \geqslant 0$. Our main result can be stated as follows.

THEOREM 1.1. *Under natural regularity assumptions on the convex potential Φ there exists a four-parameter family of wavetrains, and if Φ additionally satisfies some superquadratic growth conditions, then there also exists a three-parameter family of solitons. Moreover, the profile functions R and V are unimodal and even for both families.*

Closely related to this paper are the works [6, 10, 18, 19, 21], where the existence of travelling waves was likewise studied in a variational framework. We will therefore compare both our method (§ 2.2) and our results (§ 4.3) with those presented in these papers. We also refer readers to the numerical study [4], to [8] for existence

[1] The ansatz (1.3) is slightly more general than the usual one, which assumes that the atomic positions x_j depend on the phase variable φ. In fact, the ansatz $x_j(t) = X(kj + \omega t)$ is *not* invariant under Galilean transformations $x \rightsquigarrow x + v_0 t$, whereas (1.3) has this property as it respects $r \rightsquigarrow r, v \rightsquigarrow v + v_0$.

results in two-dimensional lattices and to [16], which proves the existence of small-amplitude travelling waves by means of centre-manifold reduction. Moreover, the existence of fronts is studied in [15], and [20] is concerned with oscillatory fronts in FPU chains with biharmonic potentials.

All the results presented below solely concern wavetrains and solitons in FPU chains, but the method can also be applied to other Hamiltonian lattices with convex potential energy $\mathcal{P}$, such as, for instance, Klein–Gordon chains with convex on-site potential [12] and atomic chains with next-to-nearest neighbour interactions.

We emphasize that we are unable to provide uniqueness results for travelling waves. Uniqueness of relative equilibria in Hamiltonian lattices is a notoriously difficult problem and almost nothing is known about it. The only available results concern either the near-sonic limit [9] or systems where the travelling wave equation can be solved explicitly. Examples are the Toda chain [22], the discrete nonlinear Schrödinger equation [11], the harmonic chain and the hard-sphere model [2].

1.2. Overview on the proof and organization of the paper

In a preparatory step, we reformulate the travelling wave equation (1.4) in terms of a normalized profile function $W \in \mathsf{L}^2$. More precisely, we show that (1.4) can be transformed into a nonlinear eigenvalue equation

$$\omega^2 W = \partial\mathcal{P}(W), \tag{1.5}$$

where $\mathcal{P}(W)$ is the potential energy of a travelling wave. The profile function W has no physical meaning, but determines R and V via

$$R(\varphi) = r_0 + \int_{\varphi}^{\varphi+k} W(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi} \quad \text{and} \quad V(\varphi) = v_0 + \omega W(\varphi),$$

where r_0 and v_0 are suitable normalization constants.

Our approach relies on a combination of variational and dynamical concepts, and can be summarized as follows.

(i) Equation (1.5) is the Euler–Lagrange equation for the optimization problem $\mathcal{P}(W) \to \max$ subjected to the constraint $W \in \mathcal{B}_\gamma$. Here γ is a free parameter, $\mathcal{B}_\gamma \subset \mathsf{L}^2$ denotes the ball of radius $\sqrt{2\gamma}$, and ω^2 is the Lagrangian multiplier.

(ii) There exists an improvement dynamics $W \mapsto \mathcal{T}_\gamma[W]$ on $\mathcal{B}_\gamma$ that increases the potential energy. Moreover, each stationary point of this dynamics solves (1.5) and vice versa.

(iii) There exist non-trivial cones S that are invariant under the improvement dynamics. Consequently, each maximizer of $\mathcal{P}$ in $\mathcal{S} \cap \mathcal{B}_\gamma$ is a travelling wave (see theorem 2.3).

We emphasize that the convexity of Φ is essential for this approach as it is intimately related to both the properties of $\mathcal{T}_\gamma$ and the existence of non-trivial invariant cones.

A major part of the mathematical analysis done in this paper is needed to show that there exist maximizers of $\mathcal{P}$ in $\mathcal{S}_\gamma$. In the wave-train setting we can use rather simple compactness arguments as the functional $\mathcal{P}$ is continuous with respect to the

https://doi.org/10.1017/S0308210509000146 Published online by Cambridge University Press

weak topology in L^2. In the soliton setting, however, we lack the weak compactness of $\mathcal{P}$, and the existence proof for maximizers requires more sophisticated arguments. Our main technical result in this context is lemma 4.7, which implies that (for certain S) the maximizing sequences for $\mathcal{P}$ in $\mathcal{S}_\gamma$ are *localized* and hence precompact in the strong topology.

This paper is organized as follows. In § 2.1 we derive the fixed-point equation (1.5) for both wavetrains and solitons. The details of our variational approach are presented in § 2.2, while § 2.3 is concerned with the analytical properties of the underlying functionals and operators. In § 3.1 we continue with the existence proof for wavetrains and present some numerical simulations in § 3.2. The *complete localization* of wavetrains is studied in § 3.3. The existence proof for solitons is contained in § 4.1 and relies on a natural condition for the superquadratic growth of the functional $\mathcal{P}$. In § 4.2 and § 4.3 we discuss the corresponding properties of the interaction potential Φ. Finally, inspired by the notion of Γ convergence we show in § 4.4 that wavetrains converge to solitons when the periodicity length tends to infinity.

2. Variational approach

In this section we transform the travelling wave equation into a fixed-point equation for a normalized profile function W and describe our variational approach to existence results for both wavetrains and solitons. To point out the key ideas we start with more formal considerations in § 2.1 and § 2.2 and postpone the analytical details to § 2.3.

2.1. Travelling waves as eigenfunctions of nonlinear integral equations

In what follows we assume that the periodicity length of wavetrains is given by $2L$ with $0 < L < \infty$ and we take the corresponding profile functions R and V to be defined on $[-L, L]$. Moreover, we identify the soliton case with $L = \infty$ by considering R and V as functions on $[-\infty, \infty]$, or, equivalently, as functions on the Alexandrov compactification of $\mathbb{R}$. In other words, in both cases we impose the boundary conditions $R(L) = R(-L)$ and $V(L) = V(-L)$.

In what follows we denote the Lebesgue space of all square-integrable functions on $[-L, L]$ by $\mathsf{L}^2([-L, L])$ with $L \in (0, \infty]$, and if there is no risk of confusion we write L^2 instead of $\mathsf{L}^2([-L, L])$.

Our first aim is to transform the travelling wave equations for wavetrains and solitons into eigenvalue equations for certain nonlinear integral operators defined on L^2. For this purpose we define two linear averaging operators and normalize the potential Φ. More precisely, for a given reference distance r_0 we define the potential Φ_{r_0} by

$$\Phi_{r_0}(r) = \Phi(r_0 + r) - \Phi(r_0) - \Phi'(r_0)r,$$

which is *normalized* via $\Phi_{r_0}(0) = \Phi'_{r_0}(0) = 0$ and $\Phi''_{r_0}(0) = \Phi''(r_0)$, and mention that this normalization respects the convexity of Φ. The eigenvalue equations for solitons and wavetrains involve the averaging operators

$$(\bar{\mathcal{A}}_k W)(\varphi) = \int_{\varphi - k/2}^{\varphi + k/2} W(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi}$$

and

$$\hat{\mathcal{A}}_k W = \bar{\mathcal{A}}_k W - \frac{1}{2L}\int_{-L}^{L} \bar{\mathcal{A}}_k W(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi} = \bar{\mathcal{A}}_k W - \frac{k}{2L}\int_{-L}^{L} W(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi}.$$

Note that the operator $\bar{\mathcal{A}}_k$ is well defined and symmetric on L^2 for both finite and infinite L (see lemma 2.5), whereas $\hat{\mathcal{A}}_k$ is well defined for $L < \infty$ only.

2.1.1. *Wavetrains and normalization via mean values*

In order to reformulate the travelling wave equation (1.4) for $L < \infty$ we introduce the *mean values* of wavetrains by

$$r_{\mathrm{av}} := \frac{1}{2L}\int_{-L}^{L} R(\varphi)\,\mathrm{d}\varphi, \qquad v_{\mathrm{av}} := \frac{1}{2L}\int_{-L}^{L} V(\varphi)\,\mathrm{d}\varphi.$$

Remark 2.1. With the identification

$$R(\varphi - \tfrac{1}{2}k) = r_{\mathrm{av}} + (\hat{\mathcal{A}}_k W)(\varphi), \tag{2.1 a}$$

$$V(\varphi) = v_{\mathrm{av}} + \omega W(\varphi) \tag{2.1 b}$$

for some profile function W with

$$\frac{1}{2L}\int_{-L}^{L} W(\varphi)\,\mathrm{d}\varphi = 0,$$

the integral equation

$$\omega^2 W = \hat{\mathcal{A}}_k \Phi'_{r_{\mathrm{av}}}(\hat{\mathcal{A}}_k W) \tag{2.2}$$

is equivalent to the wave train equation (1.4).

Proof. First suppose that R and V solve (1.4), and let $W = \omega^{-1}(V - v_{\mathrm{av}})$. Then (1.4 a) implies

$$\frac{\mathrm{d}}{\mathrm{d}\varphi}R(\varphi - \tfrac{1}{2}k) = W(\varphi + \tfrac{1}{2}k) - W(\varphi - \tfrac{1}{2}k) = \frac{\mathrm{d}}{\mathrm{d}\varphi}(\hat{\mathcal{A}}_k W)(\varphi),$$

and hence $R(\varphi - \frac{1}{2}k) = (\hat{\mathcal{A}}_k W)(\varphi) + c_1$ for some constant c_1. Integrating this with respect to φ, we find $r_{\mathrm{av}} = 0 + c_1$ and hence (2.1 a). Moreover, (1.4 b) provides

$$\begin{aligned}\omega^2 \frac{\mathrm{d}}{\mathrm{d}\varphi} W(\varphi) &= \Phi'(r_{\mathrm{av}} + (\hat{\mathcal{A}}_k W)(\varphi + \tfrac{1}{2}k)) - \Phi'(r_{\mathrm{av}} + (\hat{\mathcal{A}}_k W)(\varphi - \tfrac{1}{2}k)) \\ &= \Phi'_{r_{\mathrm{av}}}((\hat{\mathcal{A}}_k W)(\varphi + \tfrac{1}{2}k)) - \Phi'_{r_{\mathrm{av}}}((\hat{\mathcal{A}}_k W)(\varphi - \tfrac{1}{2}k)),\end{aligned}$$

and integration with respect to φ gives $\omega^2 W = \hat{\mathcal{A}}_k \Phi'_{r_{\mathrm{av}}}(\hat{\mathcal{A}}_k W) + c_2$ for some constant c_2. The condition

$$\frac{1}{2L}\int_{-L}^{L} W(\varphi)\,\mathrm{d}\varphi = 0$$

now implies $c_2 = 0$ and hence (2.1 b). Now let a solution W of (2.2) be given, and define both R and V as in (2.1). Then equation (1.4 a) holds by construction, and (1.4 b) follows from (2.2) by differentiation with respect to φ. □

We emphasize that the particular form of (2.2) depends on the potential Φ. For instance, in the harmonic case $\Phi(r) = \frac{1}{2}\beta r^2$ the parameter r_{av} drops out to give

$$\omega^2 W(\varphi) = \beta \int_{\varphi-k/2}^{\varphi+k/2} \int_{\tilde{\varphi}-k/2}^{\tilde{\varphi}+k/2} W(\bar{\varphi})\,\mathrm{d}\bar{\varphi}\,\mathrm{d}\tilde{\varphi},$$

and for $\Phi(r) = \exp(r)$ we find

$$\omega^2 W(\varphi) = \exp(r_{\mathrm{av}}) \int_{\varphi-k/2}^{\varphi+k/2} \exp\left(\int_{\tilde{\varphi}-k/2}^{\tilde{\varphi}+k/2} W(\bar{\varphi})\,\mathrm{d}\bar{\varphi} \right) \mathrm{d}\tilde{\varphi} - C,$$

$$C = \frac{\exp(r_{\mathrm{av}})}{2L} \int_{-L}^{+L} \exp\left(\int_{\tilde{\varphi}-k/2}^{\tilde{\varphi}+k/2} W(\bar{\varphi})\,\mathrm{d}\bar{\varphi} \right) \mathrm{d}\tilde{\varphi}.$$

Note that in both cases we have explicitly used the condition

$$\int_{-L}^{L} W(\varphi)\,\mathrm{d}\varphi = 0.$$

2.1.2. *Solitons and normalization via background states*

For solitons, it is much more convenient to base the normalization on the *background states*

$$r_{\mathrm{bg}} := \lim_{\varphi\to\pm\infty} R(\varphi), \qquad v_{\mathrm{bg}} := \lim_{\varphi\to\pm\infty} V(\varphi),$$

because then the normalized profiles are localized.

Remark 2.2. With the identification

$$R(\varphi - \tfrac{1}{2}k) = r_{\mathrm{bg}} + (\bar{\mathcal{A}}_k W)(\varphi), \qquad V(\varphi) = v_{\mathrm{bg}} + \omega W(\varphi) \tag{2.3}$$

for some profile function W with $\lim_{\varphi\to\pm\infty} W(\varphi) = 0$, the integral equation

$$\omega^2 W = \bar{\mathcal{A}}_k \Phi'_{r_{\mathrm{bg}}}(\bar{\mathcal{A}}_k W) \tag{2.4}$$

is equivalent to the soliton equation (1.4).

Proof. The proof is similar to that of remark 2.1. □

For illustration we exploit (2.4) for $\Phi(r) = \exp(r)$ and find

$$\omega^2 W(\varphi) = \exp(r_{\mathrm{bg}}) \left(-k + \int_{\varphi-k/2}^{\varphi+k/2} \exp\left(\int_{\tilde{\varphi}-k/2}^{\tilde{\varphi}+k/2} W(\bar{\varphi})\,\mathrm{d}\bar{\varphi} \right) \mathrm{d}\tilde{\varphi} \right).$$

We can also consider the integral equation (2.4) for $L < \infty$ and readily verify that each solution defines a wave train via (2.3). This normalization for wavetrains seems to be artificial because, for finite L, we have no immediate interpretation of the parameter r_{bg}. However, in § 4.4 we rely on this setting and show that the L-periodic solutions W_L to (2.4) converge to solitons as $L \to \infty$ (see corollary 4.21), and this implies $R_L(\pm L) \to r_{\mathrm{bg}}$.

2.1.3. *Parameter dependence of travelling waves*

The travelling wave equation (1.4) obeys a simple scaling symmetry. In fact, the solution set to (1.4) is invariant under

$$\left.\begin{array}{c} R(\varphi) \rightsquigarrow R(\lambda\varphi), \qquad V(\varphi) \rightsquigarrow V(\lambda\varphi), \\ k \rightsquigarrow \lambda^{-1}k, \qquad \omega \rightsquigarrow \lambda^{-1}\omega, \qquad L \rightsquigarrow \lambda^{-1}L, \end{array}\right\} \tag{2.5}$$

with arbitrary $\lambda > 0$, corresponding to

$$W(\varphi) \rightsquigarrow \lambda W(\lambda\varphi) \quad \text{with } r_{\mathrm{bg}} \rightsquigarrow r_{\mathrm{bg}},\ v_{\mathrm{bg}} \rightsquigarrow v_{\mathrm{bg}},\ r_{\mathrm{av}} \rightsquigarrow r_{\mathrm{av}},\ v_{\mathrm{av}} \rightsquigarrow v_{\mathrm{av}}.$$

Up to this scaling there remain four independent parameters for wavetrains. A natural choice for nonlinear potentials is to fix the length parameter L and to regard r_{av}, v_{av}, k and ω as independent parameters [2]. In this paper, however, we prefer to fix the wavenumber k so that wavetrains are parametrized by r_{av}, v_{av}, L and the *phase speed* $\sigma := \omega/k$. Accordingly, we parametrize solitons by r_{bg}, v_{bg} and σ.

Note that the velocity parameters v_{av} and v_{bg} do not appear in the travelling wave equations due to the Galilean invariance of FPU chains. However, these trivial parameters become important when studying *modulated travelling waves* [1, 2].

2.2. Variational structure for wavetrains and solitons

In view of the scaling and the reformulation results from § 2.1 we now begin to simplify our setting. In what follows we consider an arbitrary convex and smooth potential Φ normalized by $\Phi(0) = \Phi'(0) = 0$. Moreover, we restrict to $k = 1$, so the frequency ω equals the phase speed σ, and consider only the following two averaging operators:

$$(\bar{A}W)(\varphi) = \int_{\varphi-1/2}^{\varphi+1/2} W(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi}, \qquad (\hat{A}W)(\varphi) = (\bar{A}W)(\varphi) - \frac{1}{2L}\int_{-L}^{L} W(\varphi)\,\mathrm{d}\varphi. \tag{2.6}$$

Moreover, in order to point out the similarities between wavetrains and solitons we refer to an abstract averaging operator $\mathcal{A}$, which equals either $\bar{\mathcal{A}}$ or $\hat{\mathcal{A}}$, and consider the general travelling wave equation

$$\sigma^2 W = \mathcal{A}\Phi'(\mathcal{A}W) \tag{2.7}$$

with $W \in \mathsf{L}^2([-L, L])$, where L might be finite or infinite. In what follows, we call W a *travelling wave* if and only if there exist $\sigma^2 > 0$ such that (2.7) is satisfied.

The starting point for the variational formulation is the observation that (2.7) is the Euler–Lagrange equation to the action functional

$$\mathcal{L}(\sigma^2, W) = \mathcal{K}(\sigma^2, W) - \mathcal{P}(W),$$

where

$$\mathcal{K}(\sigma^2, W) = \tfrac{1}{2}\sigma^2 \int_{-L}^{L} W(\varphi)^2\,\mathrm{d}\varphi \quad \text{and} \quad \mathcal{P} = \int_{-L}^{L} \Phi((\mathcal{A}W)(\varphi))\,\mathrm{d}\varphi \tag{2.8}$$

are the *kinetic* energy and the *potential* energy, respectively.

The first rigorous existence result for wavetrains and solitons under superquadratic growth assumptions for Φ was given by Friesecke and Wattis [10]. The key idea (in our notation) is to minimize the L^2-norm of W under the constraint of prescribed potential energy, where $1/\sigma^2$ plays the role of a Lagrangian multiplier. The existence of corresponding minimizers was then established by means of Lions's concentration-compactness principle [17].

Smets and Willem [21] prove the existence of solitons by showing that, for superquadratic Φ, the functional $\mathcal{L}$ satisfies the assumptions of (a modified) mountain-pass theorem. Recently, these results were improved by Schwetlick and Zimmer in [19]. They require the superquadratic growth to hold only asymptotically, so certain double-well potentials are admissible.

Similarly to [21], Pankov and Pflüger [18] apply the mountain-pass theorem to wavetrains, and pass to the limit $L \to \infty$ by means of concentration compactness. Moreover, they present a different existence proof for solitons based on the Nehari manifold of $\mathcal{L}$.

A different idea was introduced by Filip and Venakides [6] in the context of convex potentials Φ. They proposed to maximize the potential energy $\mathcal{P}$ under the convex constraint $W \in \mathcal{B}_\gamma$ with

$$\mathcal{B}_\gamma = \{W \in L^2 \colon \tfrac{1}{2}\|W\|_2^2 \leqslant \gamma\}.$$

The first advantage of this approach is that $L < \infty$ implies the functional $\mathcal{P}$ to be continuous with respect to the weak topology in L^2, so the existence of wavetrains follows from elementary principles of infinite-dimensional convex analysis. The second advantage is that the improvement operator $\mathcal{T}_\gamma$ appears naturally in this context and allows for deriving effective approximation schemes for wavetrains (see [1, 13] and the numerical simulations below).

Our method is also based on the constrained maximization of the potential energy but yields improved results as it exploits invariance properties of $\mathcal{T}_\gamma$.

2.2.1. *Constrained maximization and the improvement operator*

In view of (2.7) we formally define the *improvement* operator $\mathcal{T}_\gamma$ as

$$\mathcal{T}_\gamma[W] := \frac{\sqrt{2\gamma}}{\|\partial\mathcal{P}[W]\|_2}\partial\mathcal{P}[W],$$

where the operator $\partial\mathcal{P}$ is the Gâteaux derivative of $\mathcal{P}$, which means that $\partial\mathcal{P}[W] = \mathcal{A}\Phi'(\mathcal{A}W)$ for all $W \in L^2$. By construction, each fixed point W of $\mathcal{T}_\gamma$ is a travelling wave with $\frac{1}{2}\|W\|_2^2 = \gamma$ and, vice versa, where the speed is given by $\sigma^2 = \|\partial\mathcal{P}[W]\|_2/\sqrt{2\gamma}$.

In § 2.3 we exploit the convexity of Φ and derive the following building blocks for the existence proof.

(i) $\partial\mathcal{P}$ respects the positive cone

$$\mathcal{U} := \{W \in L^2 \colon W(-\varphi_1) = W(\varphi_1) \geqslant W(\varphi_2) \quad \text{for almost all } 0 \leqslant \varphi_1 \leqslant \varphi_2 \leqslant L\},$$

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which consists of all functions on $[-L,-L]$ that are even and unimodal. Moreover, for $\mathcal{A}=\bar{\mathcal{A}}$ the operator $\partial\mathcal{P}$ also respects

$$\mathcal{N} := \{W \in \mathsf{L}^2 : W(\varphi) \geqslant 0 \text{ for almost all } \varphi \in [-L,-L]\},$$

which is the cone of all non-negative functions.

(ii) $\mathcal{T}_\gamma$ is well defined on $\mathcal{B}_\gamma \setminus \mathcal{M}$ and maps into $\partial\mathcal{B}_\gamma \setminus \mathcal{M}$, where

$$\mathcal{M} := \{W \in \mathsf{L}^2 : \mathcal{P}(W) = 0\}$$

is the set of all global minimizers of $\mathcal{P}$.

(iii) $\mathcal{T}_\gamma$ increases the potential energy, which means that $\mathcal{P}(\mathcal{T}_\gamma W) \geqslant \mathcal{P}(W)$ for $W \notin \mathcal{M}$, where equality holds if and only if $W = \mathcal{T}_\gamma[W]$.

We are now able to describe the key principle that provides the existence of travelling waves.

Theorem 2.3. *Let $\mathcal{S} \subset \mathsf{L}^2$ be some positive cone that is invariant under the action of the operator $\partial\mathcal{P}$. Then the set $\mathcal{S}_\gamma \setminus \mathcal{M}$ with $\mathcal{S}_\gamma = \mathcal{S} \cap \mathcal{B}_\gamma$ is invariant under the action of $\mathcal{T}_\gamma$, and each proper maximizer of $\mathcal{P}$ in $\mathcal{S}_\gamma$ is a fixed point of $\mathcal{T}_\gamma$, and hence is a travelling wave.*

Proof. The invariance of $\mathcal{S}_\gamma$ is implied by the assumption on $\mathcal{S}$ and the properties of $\mathcal{T}_\gamma$. Now let W be a proper maximizer. Then $\mathcal{P}(\mathcal{T}_\gamma[W]) = \mathcal{P}(W) > \min \mathcal{P}|_{\mathcal{S}_\gamma}$ implies both $\mathcal{T}_\gamma[W] = W$ and $W \notin \mathcal{M}$, and we conclude that W is in fact a travelling wave with $\sigma^2 > 0$. □

In what follows, the cone $\mathcal{S}$ is given by either $\mathcal{U}$ or $\mathcal{U} \cap \mathcal{N}$. Since these cones are not open in L^2, the fact that each maximizer must satisfy the Euler–Lagrange equation (2.7) with multiplier σ^2 is not clear *a priori* but is provided by the invariance of $\mathcal{S}_\gamma$ under $\mathcal{T}_\gamma$.

Theorem 2.3 yields only a sufficient condition for the existence of travelling waves. In fact, showing that $\mathcal{P}$ attains its maximum in $\mathcal{S}_\gamma$ is not trivial (at least in the soliton case), and requires a better understanding of the energy landscape in $\mathcal{S}_\gamma$. In our analysis we follow the direct approach and show that maximizing sequences for $\mathcal{P}$ are compact in some appropriate topology in L^2. More precisely, for wavetrains we use weak compactness, whereas in the soliton setting we establish the strong compactness for maximizing sequences.

2.3. Some functional analysis

Here we prove the aforementioned properties of the improvement operator $\mathcal{T}_\gamma$. To this end, we rely on the following standing assumptions on the potential Φ.

Assumption 2.4. For given $\gamma > 0$ we assume that the interaction potential Φ has the following properties on the interval $[-\sqrt{2\gamma}, \sqrt{2\gamma}]$:

- (smoothness) Φ is at least C^2;
- (convexity) $\Phi'' \geqslant 0$;

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- (normalization) $0 = \Phi(0) = \Phi'(0)$ and $\Phi''(0) = \beta \geqslant 0$;
- (non-triviality) Φ does not vanish identically.

The restriction on the interval $[-\sqrt{2\gamma}, \sqrt{2\gamma}]$ is natural in our context because $W \in \mathcal{B}_\gamma$ implies $\|\mathcal{A}W\|_\infty \leqslant \sqrt{2\gamma}$ (see lemma 2.5). As a consequence of assumption 2.4 we find

$$0 \leqslant \Phi(r) \leqslant \tfrac{1}{2}r^2(\beta + o(|r|)), \qquad \Phi'(-|r|) \leqslant 0 \leqslant \Phi'(|r|) \tag{2.9}$$

for all r with $|r| \leqslant \sqrt{2\gamma}$. Moreover, the non-triviality condition implies $\mathcal{B}_\gamma \setminus \mathcal{M} \neq \emptyset$, so each maximizer of $\mathcal{P}$ in $\mathcal{B}_\gamma$ is proper.

Within this section the parameter L can take arbitrary values in $(0, \infty]$, and L^p and $\mathsf{W}^{1,p}$ with $1 \leqslant p \leqslant \infty$ denote the usual Lebesgue and Sobolev spaces on $[-L, L]$, where

$$\langle W_1, W_2 \rangle = \int_{-L}^{L} W_1(\varphi) W_2(\varphi)\,\mathrm{d}\varphi$$

gives the inner product in L^2.

2.3.1. *Properties of the averaging operators $\bar{\mathcal{A}}$ and $\hat{\mathcal{A}}$*

We summarize some elementary properties of the averaging operators that are used in the proofs below.

LEMMA 2.5. *For any L, the operator $\bar{\mathcal{A}}$ is well defined on L^2 and has the following properties.*

(i) *$\bar{\mathcal{A}}$ maps into $\mathsf{L}^2 \cap \mathsf{L}^\infty$ with $\|\bar{\mathcal{A}}W\|_\infty \leqslant \|W\|_2$ and $\|\bar{\mathcal{A}}W\|_2 \leqslant \|W\|_2$.*

(ii) *$\bar{\mathcal{A}}$ maps into $\mathsf{W}^{1,2}$ with $(\bar{\mathcal{A}}W)'(\varphi) = W(\varphi + 1/2) - W(\varphi - 1/2)$.*

(iii) *$\bar{\mathcal{A}}$ is self-adjoint on L^2.*

(iv) *If a sequence $(W_n)_n$ converges weakly in L^2 to some limit W_∞, then $(\mathcal{A}\bar{W}_n)_n$ converges strongly in $\mathsf{L}^2([-\tilde{L}, \tilde{L}])$ for each finite $\tilde{L} < \infty$ with $\tilde{L} \leqslant L$. In particular, for $L < \infty$, the image of each bounded set in L^2 under the operator $\bar{\mathcal{A}}$ is precompact in L^2 with respect to the strong topology.*

(v) *In the wave train case ($L < \infty$) the operator $\bar{\mathcal{A}}$ is compact. Moreover, the mth eigenvalue ($m = 0, 1, 2, \dots$) is given by*

$$\varrho_m = \Theta\left(\frac{m\pi}{2L}\right), \quad \Theta(\varrho) := \varrho^{-1}\sin(\varrho),$$

and the corresponding eigenspace is spanned by

$$\cos\left(\frac{m\pi}{L}\,\cdot\right) \quad \text{and} \quad \sin\left(\frac{m\pi}{L}\,\cdot\right).$$

(vi) *In the soliton case ($L = \infty$), the operator $\bar{\mathcal{A}}$ is no longer compact, because it has continuous spectrum $\operatorname{spec}_{\mathsf{L}^2}\bar{\mathcal{A}} = \{\Theta(\varrho)\colon \varrho \in \mathbb{R}\}$. In particular,*

$$\operatorname{spec}_{\mathsf{L}^2}\bar{\mathcal{A}}^2 = [0, 1].$$

Moreover, for $L < \infty$, we have $\hat{\mathcal{A}}\colon \mathsf{L}^2 \to \mathsf{L}^2 \cap \mathsf{L}^\infty$ with $\|\hat{\mathcal{A}}W\|_\infty \leqslant \|W\|_2$ and $\|\hat{\mathcal{A}}W\|_2 \leqslant \|W\|_2$.

Proof. Definition (2.6) gives

$$\bar{\mathcal{A}}V(\varphi) = \int_{-L}^{L} \bar{\chi}(\varphi - s)V(s)\,\mathrm{d}s = \bar{\chi}(\varphi - \cdot) * V, \tag{2.10}$$

where $\bar{\chi}$ abbreviates the indicator function of the interval $[-\frac{1}{2}, \frac{1}{2}]$ and $*$ denotes the convolution operator. Hölder's inequality gives

$$|\mathcal{A}\bar{V}(\varphi)|^2 \leqslant \int_{\varphi-1/2}^{\varphi+1/2} V(s)^2\,\mathrm{d}s,$$

and from this we readily derive the first assertion. The proofs of the second and third claims are then straightforward. Now suppose $W_n \to W_\infty$ weakly in $\mathsf{L}^2([-L, L])$. Then we have $\bar{\mathcal{A}}W_n \to \bar{\mathcal{A}}W_\infty$ pointwise due to (2.10), and this implies the strong L^2 convergence on each finite interval $[-\tilde{L}, \tilde{L}]$ due to the uniform L^∞ bound.

In order to characterize the spectral properties of $\bar{\mathcal{A}}$ we study how Θ acts on plane waves. A direct calculation shows that each plane wave $E_k(\varphi) = \varphi \mapsto \mathrm{e}^{\mathrm{i}k\varphi}$ satisfies the eigenvalue equation

$$\bar{\mathcal{A}}E_k = \Theta(\tfrac{1}{2}k)E_k$$

pointwise, and this gives the fourth and the fifth assertion. Finally, for $L < \infty$ we have

$$\bar{\mathcal{A}}V(\varphi) = \hat{\chi}(\varphi - \cdot) * V, \qquad \hat{\chi}(\varphi) = \bar{\chi}(\varphi) - \frac{1}{2L}.$$

This implies

$$|\hat{\mathcal{A}}W(\varphi)|^2 \leqslant \|\hat{\chi}\|_\infty \|\bar{\chi}(\varphi - \cdot)W\|_2^2 = |\bar{\mathcal{A}}W(\varphi)|^2$$

and, in turn, the desired properties of $\hat{\mathcal{A}}$. □

As a consequence of definition (2.6) and lemma 2.5 we easily find

$$\ker_{\mathsf{L}^2} \bar{\mathcal{A}} = \left\{W \in \mathsf{L}^2\colon W(\cdot) = W(\cdot + 1),\ \int_{-1/2}^{1/2} W(\varphi)\,\mathrm{d}\varphi = 0\right\}. \tag{2.11}$$

In particular, the kernel of $\bar{\mathcal{A}}$ is trivial if either L is irrational or $L = \infty$. Moreover, for $L < \infty$ we have

$$\ker_{\mathsf{L}^2} \hat{\mathcal{A}} = \ker_{\mathsf{L}^2} \bar{\mathcal{A}} \oplus \operatorname{span}\{1\}. \tag{2.12}$$

2.3.2. *Properties of the potential energy functional $\mathcal{P}$*

We rely on assumption 2.4 and use standard methods from convex analysis to prove some properties of $\mathcal{P}$ and its derivative. All results are formulated in terms of the abstract averaging operator $\mathcal{A}$ and hold for both the wave train and the soliton case.

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Lemma 2.6. *The functional $\mathcal{P}$ is well defined, bounded, continuous and Gâteaux-differentiable on $\mathcal{B}_\gamma$, and its derivative $\partial\mathcal{P} = \mathcal{A}\circ\partial\Phi\circ\mathcal{A}$ is a monotone operator and maps $\mathcal{B}_\gamma$ continuously into L^2. Moreover, for arbitrary $W_1, W_2 \in \mathcal{B}_\gamma$ we have*

$$\mathcal{P}(W_2) - \mathcal{P}(W_1) \geqslant \tfrac{1}{2}m\|\mathcal{A}W_2 - \mathcal{A}W_1\|_2^2 + \langle\partial\mathcal{P}[W_1], W_2 - W_1\rangle \tag{2.13}$$

and

$$\langle\partial\mathcal{P}[W_2] - \partial\mathcal{P}[W_1], W_2 - W_1\rangle \geqslant m\|\mathcal{A}W_2(\varphi) - \mathcal{A}W_1(\varphi)\|_2^2, \tag{2.14}$$

where the monotonicity constant is given by $m = \inf_{|r|\leqslant\sqrt{2\gamma}} \Phi''(r) \geqslant \beta$.

Proof. For all W in $\mathcal{B}_\gamma$ we have $\|\mathcal{A}W\|_\infty \leqslant \sqrt{2\gamma}$, and assumption 2.4 implies

$$|\Phi'(r)| \leqslant C|r|, \qquad \Phi(r) \leqslant \tfrac{1}{2}Cr^2$$

for all r with $|r| \leqslant \sqrt{2\gamma}$, where $C = \sup_{|r|\leqslant\sqrt{2\gamma}} |\Phi''(r)| \geqslant \beta$. Consequently, we find

$$0 \leqslant \mathcal{P}(W) \leqslant \tfrac{1}{2}C\|\mathcal{A}W\|_2^2 \leqslant \gamma C, \qquad \|\mathcal{A}\partial\Phi[\mathcal{A}W]\|_p \leqslant C^p\|W\|_p \leqslant C^p\|W\|_p,$$

and all assertions concerning the continuity and boundedness of both $\mathcal{P}$ and $\partial\mathcal{P}$ follow immediately. Now let $W_1, W_2 \in \mathcal{B}_\gamma$ be fixed, and note that the convexity inequality $(\Phi'(r_2) - \Phi'(r_1))(r_2 - r_1) \geqslant m(r_2 - r_1)^2$ with $r_i = \mathcal{A}W_i(\varphi)$ implies (2.14) by integration with respect to φ. To prove (2.13), let $\eta \in [0, 1]$ and consider $W(\eta) := (1 - \eta)W_1 + \eta W_2 \in \mathcal{B}_\gamma$ as well as

$$p(\eta) := \mathcal{P}(W(\eta)).$$

The function p is well defined and differentiable with respect to η, and, using (2.14), we find

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\eta}p(\eta) &= \langle\partial\mathcal{P}[W(\eta)], W_2 - W_1\rangle \\
&\geqslant \eta^{-1}\langle\partial\mathcal{P}[W(\eta)] - \partial\mathcal{P}[W_1], \eta W_2 - \eta W_1\rangle + \langle\partial\mathcal{P}[W_1], W_2 - W_1\rangle \\
&= \eta^{-1}\langle\partial\mathcal{P}[W(\eta)] - \partial\mathcal{P}[W_1], W(\eta) - W_1\rangle + \langle\partial\mathcal{P}[W_1], W_2 - W_1\rangle \\
&\geqslant \eta^{-1}m\|\mathcal{A}W(\eta) - \mathcal{A}W_1\|_2^2 + \langle\partial\mathcal{P}[W_1], W_2 - W_1\rangle \\
&\geqslant \eta m\|\mathcal{A}W_2 - \mathcal{A}W_1\|_2^2 + \langle\partial\mathcal{P}[W_1], W_2 - W_1\rangle.
\end{aligned}$$

Finally, we integrate the last estimate from $\eta = 0$ to $\eta = 1$, and this gives (2.13). □

The convexity of $\mathcal{P}$ implies that each trivial travelling wave with $\sigma^2 = 0$ must belong to $\mathcal{M}$, the set of all minimizers of $\mathcal{P}$.

Remark 2.7. We have $\partial\mathcal{P}[W] \neq 0$ for all $W \in \mathcal{B}_\gamma \setminus \mathcal{M}$.

Proof. Assume that there exists some $W \in \mathcal{B}_\gamma \setminus \mathcal{M}$ with $\partial\mathcal{P}[W] = 0$. Then (2.14) with $W_2 = 0$ and $W_1 = W$ provides $\mathcal{A}W = 0$ and, hence, $\mathcal{P}(W) = 0$, which is a contradiction. □

Note that, for non-degenerate potentials Φ with $\Phi(r) > 0$ for all $r \neq 0$, we have $\mathcal{M} = \ker\mathcal{A}$, where $\ker\mathcal{A}$ is given in (2.11) and (2.12).

2.3.3. *Properties of the improvement operator* $\mathcal{T}_\gamma$

First we show that the cones $\mathcal{U}$ and $\mathcal{N}$ are invariant under the action of both $\bar{\mathcal{A}}$ and Φ'. Here again the convexity of Φ enters, as it guarantees that Φ' is increasing.

LEMMA 2.8. *The cones* $\mathcal{U}$ *and* $\mathcal{N}$ *are convex, closed under weak and strong convergence in* L^2 *and invariant under the action of* $\partial\mathcal{P}$ *and* $\bar{\mathcal{A}}$. *Moreover,* $\mathcal{U}$ *is also invariant under the action of* $\hat{\mathcal{A}}$ *(for* $L<\infty$*).*

Proof. The only non-trivial assertion is the invariance of $\mathcal{U}$ under $\bar{\mathcal{A}}$. To prove this, we fix $W\in\mathcal{U}$ and consider $Y=\mathrm{d}\bar{\mathcal{A}}W/\mathrm{d}\phi$ with $Y(\varphi)=W(\varphi+\frac{1}{2})-W(\varphi-\frac{1}{2})$ thanks to lemma 2.5. This function is odd as $W(\varphi)=W(-\varphi)$ implies

$$Y(-\varphi)=W(-\varphi+\tfrac{1}{2})-W(-\varphi-\tfrac{1}{2})=W(\varphi-\tfrac{1}{2})-W(\varphi+\tfrac{1}{2})=-Y(\varphi).$$

Hence, it remains to show that $Y(\varphi)\leqslant 0$ for all $\varphi\geqslant 0$, which is equivalent to

$$W(\varphi+\tfrac{1}{2})\leqslant W(\varphi-\tfrac{1}{2}),\quad \varphi\geqslant 0.$$

For $\frac{1}{2}\leqslant\varphi\leqslant L-\frac{1}{2}$ this estimate follows from $0\leqslant\varphi-\frac{1}{2}\leqslant\varphi+\frac{1}{2}$. Moreover, for $0\leqslant\varphi\leqslant\frac{1}{2}$ it holds thanks to $W(-\varphi+\frac{1}{2})=W(\varphi-\frac{1}{2})$ and $0\leqslant-\varphi+\frac{1}{2}\leqslant\varphi+\frac{1}{2}$, and for $L-\frac{1}{2}\leqslant\varphi\leqslant L$ it is a consequence of $W(\varphi+\frac{1}{2})=W(2L-\varphi-\frac{1}{2})$ and $2L-\varphi-\frac{1}{2}\geqslant\varphi-\frac{1}{2}$. □

LEMMA 2.9. *The operator* $\mathcal{T}_\gamma$ *maps* $\mathcal{B}_\gamma\setminus\mathcal{M}$ *continuously into* $\partial\mathcal{B}_\gamma\setminus\mathcal{M}$ *and satisfies*

$$\mathcal{P}(\mathcal{T}_\gamma[W])-\mathcal{P}(W)\geqslant\tfrac{1}{2}m\|\mathcal{A}\mathcal{T}_\gamma[W]-\mathcal{A}W\|_2^2 \tag{2.15}$$

for all $W\in\mathcal{B}_\gamma\setminus\mathcal{M}$. *Moreover, the equality sign holds if and only if* W *is a fixed point of* $\mathcal{T}_\gamma$.

Proof. Lemma 2.6 and remark 2.7 imply that $\mathcal{T}_\gamma$ is well defined and continuous on $\mathcal{B}_\gamma\setminus\mathcal{M}$. Moreover, $\|\mathcal{T}_\gamma[W_2]\|_2=\sqrt{2\gamma}$ holds by definition. Now let $W_1\in\mathcal{B}_\gamma\setminus\mathcal{M}$ be fixed and set $W_2:=\mathcal{T}_\gamma[W_1]$ and $\sigma_2^2:=\|\partial\mathcal{P}[W_1]\|_2/\sqrt{2\gamma}>0$. Hence, $\sigma_2^2W_2=\partial\mathcal{P}[W_1]$, and from (2.13) we infer that

$$\begin{aligned}\mathcal{P}(W_2)-\mathcal{P}(W_1)-\tfrac{1}{2}m\|\mathcal{A}W_2-\mathcal{A}W_1\|_2^2&\geqslant\sigma_2^{-2}\langle W_2,W_2-W_1\rangle\\&\geqslant\sigma_2^{-2}(\|W_2\|_2^2-\|W_2\|_2\|W_1\|_2),\end{aligned}$$

which gives (2.15) due to $\|W_1\|_2\leqslant\|W_2\|_2=\sqrt{2\gamma}$. Moreover, we find an equality sign in the second estimate if and only if $\|W_2\|_2^2=\|W_1\|_2^2=\langle W_1,W_2\rangle$, that is, if and only if $W_1=W_2$. □

With lemma 2.9 we have derived all the ingredients that we used in the proof of theorem 2.3.

3. Wavetrains

As a first application of theorem 2.3 we establish the existence of wavetrains in § 3.1 and proceed with some comments on the numerical computation of wavetrains in § 3.2. Afterwards we study the complete localization of wavetrains in § 3.3.

3.1. Existence results

Our first existence result concerns wavetrains that are renormalized via their mean values. This corresponds to $L < \infty$, $\mathcal{A} = \hat{\mathcal{A}}$ and $\mathcal{S} = \mathcal{U}$.

THEOREM 3.1. *For each $L < \infty$ and $\gamma > 0$ there exists a unimodal and even wave train W such that $\frac{1}{2}\|W\|_2^2 = \gamma$ and $\sigma^2 W = \hat{\mathcal{A}}\Phi'(\hat{\mathcal{A}}W)$ for some $\sigma^2 > 0$.*

Proof. With respect to the weak topology in L^2, the functional $\mathcal{P}$ is continuous and the set $\mathcal{S}_\gamma = \mathcal{U} \cap \mathcal{B}_\gamma$ is compact. Therefore, and since Φ is convex, there exists a proper maximiser W with $\sup \mathcal{P}|_{\mathcal{S}_\gamma} = \mathcal{P}(W) > 0 = \min \mathcal{P}|_{\mathcal{S}_\gamma}$. The desired result now follows from theorem 2.3. □

In view of remark 2.1 and the scaling (2.5) we infer that theorem 3.1 implies the existence of a four-parameter family of solutions (R, V) to the original travelling wave equation (1.4) with fixed L. This family is parametrized by r_{av}, v_{av}, k and γ, and for nonlinear potentials we can expect (at least locally) that γ can be replaced by ω.

Similar existence results for wavetrains in convex FPU chains are proven in [2,6], but provide only $\mathcal{W} \in \partial\mathcal{B}_\gamma$. Our method improves these results as it establishes the existence of wavetrains with the additional property $W \in \mathcal{U}$, which in turn implies $R \in \mathcal{U}$ and $\sigma V \in \mathcal{U}$. This sheds light on some observations from [1, 14]: the traces of travelling waves found in the numerical simulations of initial-value problems for (1.1) typically encircle convex sets in the (r, v)-plane (see part (e) of figure 1). In particular, these curves have exactly two extrema in both the r-direction and the v-direction, and hence they correspond to unimodal profile functions R and V.

We proceed with some remarks concerning the uniqueness of wavetrains. The norm constraint $\frac{1}{2}\|W\|_2^2 = \gamma$ alone is not sufficient for uniqueness as the travelling wave equation is invariant under shifts in φ. Moreover, since the set of all $2\tilde{L}$-periodic functions with $m\tilde{L} = L$ for some $m \in \mathbb{N}$ is invariant under the action of $\mathcal{T}_\gamma$, we can construct a whole family of wavetrains satisfying the norm constraint.

From these considerations we conclude that any uniqueness result for wavetrains must prescribe further properties of the profile function W. Motivated by numerical simulations, we conjecture that for each γ there exists exactly one travelling wave with $W \in \mathcal{U}$ and $\frac{1}{2}\|W\|_2^2 = \gamma$, but we are not able to prove this conjecture.

Finally, using similar arguments to those in the proof of theorem 3.1 we can derive an existence result for wavetrains in the setting $L < \infty$, $\mathcal{A} = \bar{\mathcal{A}}$ and $\mathcal{S} = \mathcal{U} \cap \mathcal{N}$.

LEMMA 3.2. *For each $L < \infty$ and $\gamma > 0$ there exist a wave train $W \in \mathcal{U} \cap \mathcal{N} \cap \partial\mathcal{B}_\gamma$ such that $\sigma^2 W = \bar{\mathcal{A}}\Phi'(\bar{\mathcal{A}}W)$ for some $\sigma^2 > 0$.*

3.2. Numerical computation of wavetrains

It is natural to use the improvement dynamics

$$W \in \mathcal{S}_\gamma \mapsto \mathcal{T}_\gamma[W] \in \mathcal{S}_\gamma \tag{3.1}$$

for the approximation of wavetrains, and a corresponding discrete scheme is readily derived and implemented. It was proven in [13] that the orbits generated by (3.1) are compact in the strong L^2 topology, but from a theoretical point of view this

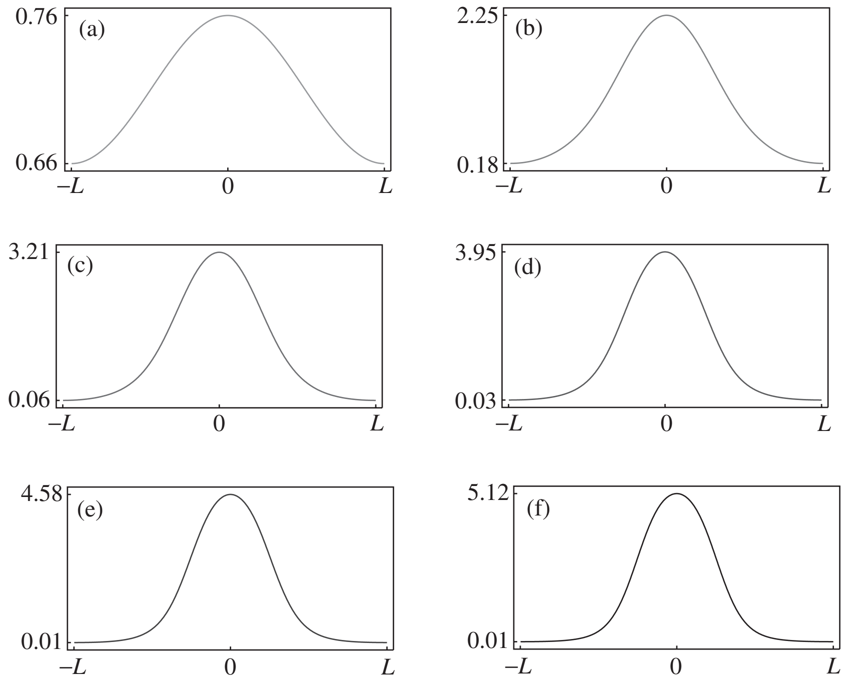

Figure 2. Profile functions W for several values of γ with $L = 2$ and Φ as in (3.2). (a) $\gamma = 1$, (b) $\gamma = 3$, (c) $\gamma = 5$, (d) $\gamma = 7$, (e) $\gamma = 9$, (f) $\gamma = 11$.

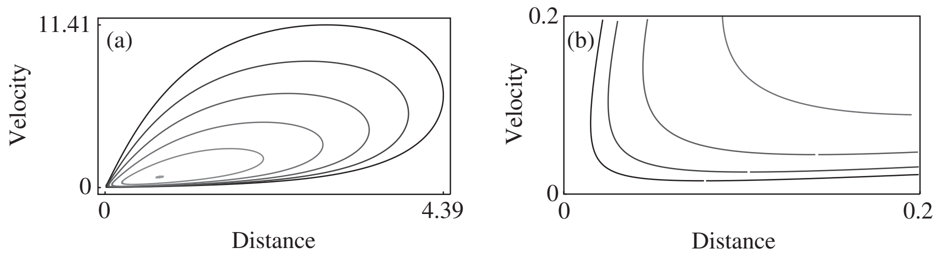

Figure 3. Traces for the wavetrains from figure 2.

result remains unsatisfactory due to the lack of uniqueness. So it is clear neither that maximizers of $\mathcal{P}$ in $\mathcal{S}_\gamma$ are unique, nor that all fixed points of $\mathcal{T}_\gamma$ are (global) maximizers.

In numerical simulations, however, we found (3.1) to have good properties. For a wide class of potentials we observed rapid convergence to a unique limit independent of the chosen initial data. In figure 2 we present the numerically computed profiles W for different values of γ with $\mathcal{A} = \bar{\mathcal{A}}$ and

$$\Phi(r) = \cosh(r) - 1. \tag{3.2}$$

For small γ we can approximate Φ by $\Phi_{\mathrm{harm}}(r) = \Phi''(0)r^2$, and hence the profile W is close to a rescaled plane wave. For increasing γ, however, the nonlinearity dominates and the profile function becomes tighter. Figure 3 shows the corresponding *traces*

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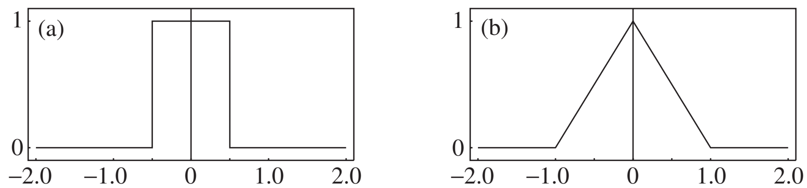

Figure 4. The functions W_{CL} and $\bar{\mathcal{A}}W_{\mathrm{CL}}$: (a) W_{CL} versus φ; (b) $\bar{\mathcal{A}}W_{\mathrm{CL}}$ versus φ.

in the (r, v)-plane: these are the curves

$$\varphi \mapsto (\bar{\mathcal{A}}W(\varphi), \sigma W(\varphi)) \cong (R(\varphi), V(\varphi)),$$

(see remark 2.2). Surprisingly, we find a nested family of curves that mean the traces for different values of γ do not intersect but fill out a convex region. We are not able to prove this observation but mention that a similar phenomenon occurs when FPU chains generate dispersive shocks [3, 14].

3.3. Complete localization of wavetrains

It is well known for strongly nonlinear potentials that in certain limits the wavetrains (and even the solitons) localize completely in the sense that, under a suitable rescaling, the profile functions W converge to the indicator function of an interval plus a constant background state. Such profile functions are, up to renormalization, equal to the profile functions of travelling waves in the hard-sphere model for the atomic chain, in which all atomic interactions are described by elastic collisions. Thus, the effect of localization can often be linked in a natural way to the high energy limit of travelling waves. For more details we refer the reader to [2, 7, 13, 22].

In this section we discuss the localization phenomenon in our context, and aim at deriving a localization criterion for wavetrains. To keep the presentation simple we consider only non-negative and unimodal profile functions, that is, we investigate the localization of solutions to (2.7) with $L < \infty$, $\mathcal{A} = \bar{\mathcal{A}}$ and $\mathcal{S} = \mathcal{U} \cap \mathcal{N}$. Moreover, for our purposes it is sufficient to assume that the localized limit profile is given by

$$W_{\mathrm{CL}}(\varphi) = \chi_{[-1/2,1/2]}(\varphi) = \begin{cases} 1 & \text{if } |\varphi| \leqslant \frac{1}{2}, \\ 0 & \text{if } |\varphi| > \frac{1}{2}, \end{cases} \tag{3.3}$$

(see figure 4). It is easy to check that this profile satisfies

$$\|W_{\mathrm{CL}}\|_2 = 1, \qquad (\bar{\mathcal{A}}W_{\mathrm{CL}})(\varphi) = \max\{1 - |\varphi|, 0\}, \qquad \mathcal{P}(W_{\mathrm{CL}}) = 2\int_0^1 \Phi(s)\,\mathrm{d}s. \tag{3.4}$$

In what follows we consider sequences $(\Phi_n)_n$ of rescaled potentials, where each $\Phi_n \colon [0, 1] \to \mathbb{R}$ satisfies assumption 2.4. Moreover, we refer to a sequence of profile functions $W_n \subset \mathsf{L}^2$ as a *corresponding sequence of maximizers*, if W_n is a maximizer of $\mathcal{P}_n$ in $\mathcal{S}_{1/2}$ for each n, where $\mathcal{P}_n$ is the potential energy functional (2.8) corresponding to Φ_n.

We say that a sequence of such potentials $(\Phi_n)_n$ has the *complete localization property on* $[0, 1]$ if any corresponding sequence of maximizers converges strongly in L^2 to $W_{\rm CL}$. Our main result in this section is a necessary condition for the complete localization of wavetrains and is implied by the following observation.

LEMMA 3.3. *We have* $\|\bar{A}W\|_\infty < \|\bar{A}W_{\rm CL}\|_\infty = 1$ *for any* $W \in \mathcal{S}_{1/2}$ *with* $W \neq W_{\rm CL}$.

Proof. $W \in \mathcal{U}\cap\mathcal{N}$ implies $\|\bar{A}W\|_\infty = (\bar{A}W)(0)$, and Hölder's inequality provides

$$(\bar{A}W)^2(0) = \biggl(\int_{-1/2}^{1/2} W(\varphi)\,\mathrm{d}\varphi\biggr)^2 = \biggl(\int_{-1/2}^{1/2} W_{\rm CL}(\varphi)W(\varphi)\,\mathrm{d}\varphi\biggr)^2$$

$$\leqslant \biggl(\int_{-1/2}^{1/2} W_{\rm CL}(\varphi)^2\,\mathrm{d}\varphi\biggr)\biggl(\int_{-1/2}^{1/2} W(\varphi)^2\,\mathrm{d}\varphi\biggr) = \int_{-1/2}^{1/2} W(\varphi)^2\,\mathrm{d}\varphi \tag{3.5}$$

$$\leqslant 1 = (\bar{A}W_{\rm CL})^2(0). \tag{3.6}$$

Moreover, the estimate in (3.5) is strict unless there exists a constant c such that

$$W(\varphi) = cW_{\rm CL}(\varphi) \quad \text{for almost all } \varphi \in [-\tfrac{1}{2}, \tfrac{1}{2}], \tag{3.7}$$

whereas the estimate in (3.6) is strict except for

$$\int_{-1/2}^{1/2} W(\varphi)^2\,\mathrm{d}\varphi = 1. \tag{3.8}$$

Now suppose that both (3.7) and (3.8) are satisfied. Then we have $c = 1$, and the norm constraint $\|W\|_2^2 \leqslant 1$ implies $W(\varphi) = 0 = W_{\rm CL}(\varphi)$ for almost all $\varphi \notin [-\frac{1}{2}, \frac{1}{2}]$, and hence $W = W_{\rm CL}$. □

LEMMA 3.4. *The sequence* $(\Phi_n)_n$ *has the complete localization property on* $[0, 1]$ *provided that the following two conditions are satisfied.*

(i) $\mathcal{P}_n(W_{\rm CL}) = 1$ *for all* n.

(ii) Φ_n *converges uniformly and essentially monotonically to* 0 *on each interval* $[0, r_0]$ *with* $0 < r_0 < 1$. *That means for any* r_0 *we have* $\sup_{0\leqslant r\leqslant r_0} \Phi_n(r) \to 0$ *as* $n \to \infty$, *and there exists* $n_0(r_0)$ *such that*

$$0 \leqslant \Phi_{n_2}(r) \leqslant \Phi_{n_1}(r)$$

for all $n_2 > n_1 > n_0(r_0)$ *and all* $0 \leqslant r \leqslant r_0$.

Proof. First we additionally assume that $W_n \to W_\infty$ weakly in L^2, and suppose for contradiction that $W_\infty \neq W_{\rm CL}$. Then, $\|\bar{A}W_\infty\|_\infty < 1$ thanks to lemma 3.3, and since $\bar{A}W_n \to \bar{A}W_\infty$ pointwise and $\|\bar{A}W_n\|_\infty = (\bar{A}W_n)(0)$ we find some $0 < r_0 < 1$ such that $\|\bar{A}W_n\|_\infty \leqslant r_0$ for almost all n. Therefore, $\mathcal{P}_{n_1}(W_{n_2}) \geqslant \mathcal{P}_{n_2}(W_{n_2})$ holds for all $n_2 \geqslant n_1$ and all sufficiently large n_1, and since each W_n is a maximizer for $\mathcal{P}_n$, we also have $\mathcal{P}_{n_2}(W_{n_2}) \geqslant \mathcal{P}_{n_2}(W_{\rm CL}) \geqslant 1$. We conclude that $\mathcal{P}_{n_1}(W_{n_2}) \geqslant 1$ and, passing to the limits $n_2 \to \infty$ and $n_1 \to \infty$, we obtain $\liminf_{n\to\infty} \mathcal{P}_n(W_\infty) \geqslant 1$. However, $\|\bar{A}W_\infty\|_\infty \leqslant r_0 < 1$ implies $\lim_{n\to\infty} \mathcal{P}_n(W_\infty) = 0$, which is the desired contradiction. The result obtained so far implies that $W_{\rm CL}$ is the unique accumulation point of a maximizing sequence, and this yields the weak convergence to $W_{\rm CL}$ for any maximizing sequence. Finally, the strong convergence follows from $1 = \|W_{\rm CL}\|_2 = \|W_n\|_2$ for all n. □

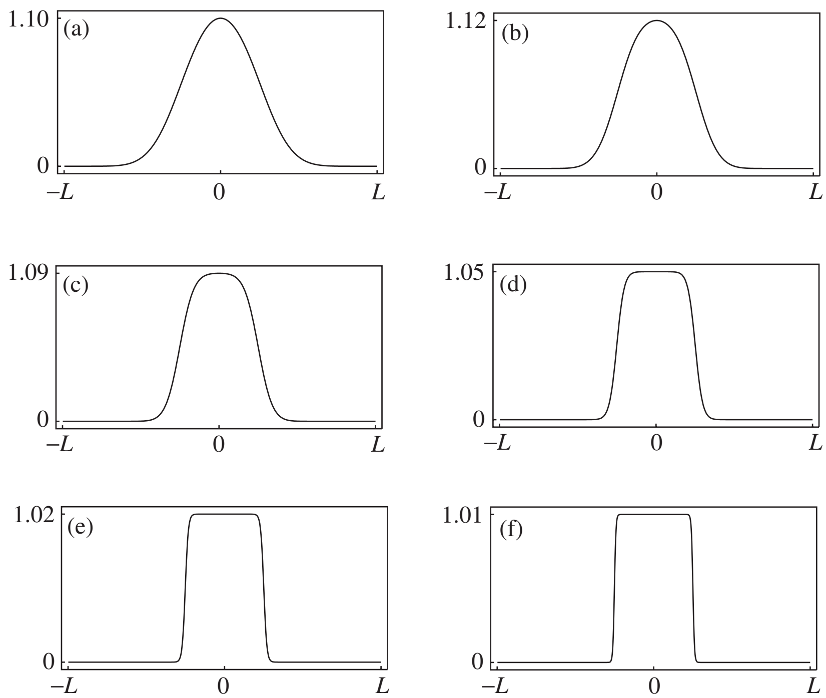

Figure 5. Profile functions W with $\gamma = \frac{1}{2}$, $L = 2$ and potentials Φ_q as in remark 3.5. This example describes the wavetrains for homogeneous potentials in the limit of increasing degree: (a) $q = 4$; (b) $q = 6$; (c) $q = 10$; (d) $q = 20$; (e) $q = 50$; (f) $q = 100$.

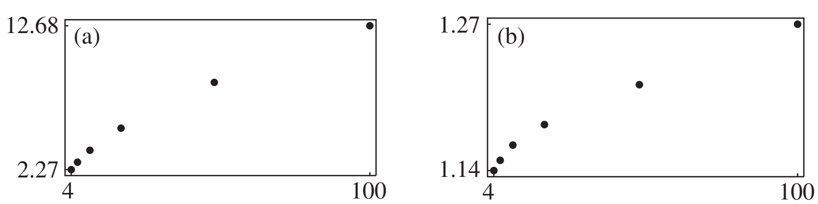

Figure 6. (a) Speed σ and (b) potential energy $\mathcal{P}(W)$ versus q for the wavetrains from figure 5.

Note that the two conditions from lemma 3.4 imply $\Phi_n(r) \to 0$ for all $0 \leqslant r < 1$, but $\Phi_n(1) \to \infty$ as $n \to \infty$, and for this reason it is not clear whether or not the complete localization (convergence of maximizers) implies the convergence of maxima. The simulations from figure 6, however, provide evidence for

$$\liminf_{n\to\infty} \mathcal{P}_n(W_n) > 1 = \lim_{n\to\infty} \mathcal{P}_n(W_{\mathrm{CL}}).$$

Our first application concerns the maximizer for homogeneous potentials of large degree. For an illustration we refer the reader to the numerical results in figures 5 and 6.

Example 3.5. The family of potentials $\Phi_q(r) = \frac{1}{2}(q+1)r^q$ with $c > 0$ and $q > 2$ has the complete localization property on $[0, 1]$ for $q \to \infty$.

Proof. $\mathcal{P}_q(W_{\mathrm{CL}}) = 1$ follows from (3.4) by a direct computation and, for fixed $0 < r_0 < 1$, we choose q_0 such that $1 + (q_0 + 1)\ln r_0 < 0$. Then we find

$$\partial_q(\tfrac{1}{2}(q+1)r^q) = \tfrac{1}{2}r^q(1 + (q+1)\ln r) < 0 \quad \text{for all } 0 \leqslant r < r_0 \text{ and } q > q_0.$$

□

The second candidate for the complete localization property is related to the limit $\gamma \to \infty$ for fixed potential Φ. We consider the rescaled potentials

$$\Phi_\gamma(r) := \frac{\Phi(\sqrt{2\gamma}r)}{2\int_0^1 \Phi(\sqrt{2\gamma}s)\,\mathrm{d}s} \tag{3.9}$$

with corresponding energy functionals $\mathcal{P}_\gamma$, and note that the two optimization problems

$$\mathcal{P} \to \max \text{ on } \mathcal{S}_\gamma \quad \text{and} \quad \mathcal{P}_\gamma \to \max \text{ on } \mathcal{S}_{1/2}$$

are equivalent due to $W \in \mathcal{S}_\gamma \Leftrightarrow W/\sqrt{2\gamma} \in \mathcal{S}_{1/2}$.

Example 3.6. For Φ as in (3.2) the rescaled potentials Φ_γ from (3.9) have the complete localization property on $[0, 1]$ for $\gamma \to \infty$.

Proof. $\mathcal{P}_\gamma(W_{\mathrm{CL}}) = 1$ holds by construction, and for each $0 < r_0 < 1$ we can find γ_0 such that $\partial_\gamma \Phi_\gamma(r) < 0$ for all $0 \geqslant r \geqslant r_0$ and $\gamma \geqslant \gamma_0$. □

More generally, the family $(\Phi_\gamma)_\gamma$ can be expected to have the complete localization property for $\gamma \to \infty$ provided that Φ grows faster than every polynomial. The super-polynomial growth condition is necessary as, for every homogeneous potential of degree q, we have $\Phi_\gamma \equiv \Phi_1$. This reflects the scaling

$$W \rightsquigarrow \lambda W, \qquad \sigma^2 \rightsquigarrow \lambda^{q-2}\sigma^2$$

and shows that the wavetrains for homogeneous or polynomial potentials do not localize in the limit $\gamma \to \infty$.

4. Solitons

In this section we study soliton solutions to (2.7). We set

$$L = \infty, \qquad \mathcal{A} = \bar{A}, \qquad \mathcal{S} = \mathcal{U} \cap \mathcal{N}.$$

Moreover, we assume that the potential energy $\mathcal{P}$ is genuinely superquadratic (see definition 4.4) and show that, for each $\gamma > 0$, there exists a maximizer of $\mathcal{P}$ in $\mathcal{S}_\gamma = \mathcal{U} \cap \mathcal{N} \cap \mathcal{B}_\gamma$, which is a soliton according to theorem 2.3.

In what follows, we set

$$P(\gamma) := \sup_{W \in \mathcal{S}_\gamma} \mathcal{P}(W),$$

and for comparison with the harmonic case we introduce

$$P_{\mathrm{harm}}(\gamma) := \sup_{W \in \mathcal{S}_\gamma} \mathcal{P}_{\mathrm{harm}}(W), \tag{4.1}$$

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with

$$\mathcal{P}_{\text{harm}}(W) = \int_{-L}^{L} \Phi_{\text{harm}}((\mathcal{A}W)(\varphi))\,\mathrm{d}\varphi = \tfrac{1}{2}\beta\|\mathcal{A}W\|_2^2$$

being the energy functional corresponding to $\Phi_{\text{harm}}(r) = \frac{1}{2}\beta r^2$. Next we show $P_{\text{harm}}(\gamma) = \beta\gamma$ by studying the maximizing sequence $(U_n)_n \subset \mathcal{S}_\gamma$ defined as

$$U_n(\varphi) = \begin{cases} \dfrac{\sqrt{2\gamma}}{\sqrt{n}} \cos\left(\dfrac{\pi}{2n}\varphi\right) & \text{for } |\varphi| \leqslant n, \\ 0 & \text{for } |\varphi| \geqslant n. \end{cases} \tag{4.2}$$

LEMMA 4.1. *We have $\beta\gamma \geqslant \mathcal{P}_{\text{harm}}(U_n) \geqslant \beta\gamma(1 - O(n^{-2}))$ for all n, and hence*

$$P_{\text{harm}} = \sup \mathcal{P}_{\text{harm}}|_{\mathcal{S}_\gamma} = \sup \mathcal{P}_{\text{harm}}|_{\mathcal{B}_\gamma} = \beta\gamma.$$

Proof. A direct calculation shows $\frac{1}{2}\|U_n\|_2^2 = \gamma$ as well as

$$(\mathcal{A}U_n)(\varphi) = \begin{cases} \Theta\left(\dfrac{\pi}{4n}\right)U_n(\varphi) & \text{for } |\varphi| \leqslant n - \frac{1}{2}, \\ 0 & \text{for } |\varphi| \geqslant n + \frac{1}{2} \end{cases}$$

and

$$0 \leqslant (\mathcal{A}U_n)(\varphi) = O(n^{-3/2}) \quad \text{for } ||\varphi| - n| \leqslant \tfrac{1}{2},$$

where we used the identity $U_n(n - \frac{1}{2}) = (\sqrt{2\gamma}/\sqrt{n})\cos(\frac{1}{2}\pi(1 - 1/2n))$. Moreover, we have

$$\mathcal{P}_{\text{harm}}(U_n) \geqslant \beta\gamma\Theta\left(\frac{\pi}{4n}\right)^2 \int_{-1+1/2n}^{1-1/2n} \cos\left(\frac{\pi}{2}\varphi\right)^2 \mathrm{d}\varphi \geqslant \beta\gamma(1 - O(n^{-2})),$$

and this implies $\mathcal{P}_{\text{harm}}(U_n) \to \beta\gamma$ as $n \to \infty$. Finally, due to lemma 2.5 we find

$$\mathcal{P}_{\text{harm}}(W) = \tfrac{1}{2}\beta \int_{\mathbb{R}} |(\mathcal{A}W)(\varphi)|^2\,\mathrm{d}\varphi = \beta\tfrac{1}{2}\|\mathcal{A}W\|_2^2 \leqslant \tfrac{1}{2}\beta\|W\|_2^2$$

for all $W \in \mathcal{B}_\gamma$, and the proof is complete. □

COROLLARY 4.2. *We have $P(\gamma) \geqslant \beta\gamma = P_{\text{harm}}(\gamma)$ for all $\gamma \geqslant 0$.*

Proof. Since the case $\beta = 0$ is trivial we suppose that $\beta > 0$. Some elementary analysis shows that the sequence $(U_n)_n$ from (4.2) satisfies

$$\begin{aligned} \mathcal{P}(U_n) &\approx \int_{|\varphi| \leqslant n-1/2} \Phi\left(\Theta\left(\frac{\pi}{4n}\right)U_n(\varphi)\right) \mathrm{d}\varphi \\ &\approx \frac{1}{2} \int_{|\varphi| \leqslant n-1/2} U_n(\varphi)^2 \left(\beta + o\left(\frac{1}{\sqrt{n}}\right)\right) \mathrm{d}\varphi \\ &\approx \beta\gamma, \end{aligned}$$

where all approximation errors tend to 0 as $n \to \infty$. □

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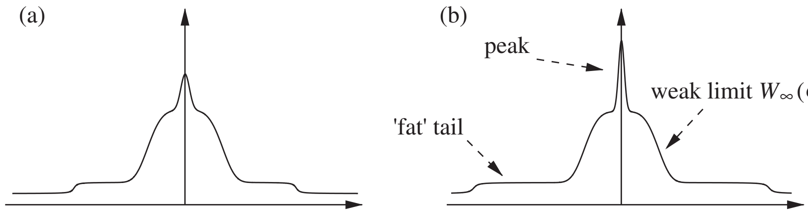

Figure 7. On the weak convergence in $\mathcal{U} \cap \mathcal{N} \cap \mathcal{B}_\gamma$: (a) $W_n(\varphi)$ versus φ; (b) $W_{n+m}(\varphi)$ versus φ. A weakly convergent sequence may fail to converge strongly due to the formation of a peak at the origin and/or a 'fat' tail.

As mentioned in the introduction, solitons are genuinely nonlinear phenomena. In particular, the harmonic chain does not allow for solitons, and thus the supremum in (4.1) cannot be attained.

REMARK 4.3. For $\beta > 0$ there is no maximizer for $\mathcal{P}_{\text{harm}}$.

Proof. Suppose, for contradiction, the existence of a maximizer $W_{\max}$ for $\mathcal{P}_{\text{harm}}$ in $\mathcal{B}_\gamma$. Then the Lagrangian multiplier rule implies that there exists a (non-negative) Lagrangian multiplier σ^2 such that

$$\sigma^2 W_{\max} = \partial\mathcal{P}[W_{\max}] = \beta\bar{\mathcal{A}}^2 W_{\max}.$$

In particular, $W_{\max}$ is an L^2-eigenfunction to $\bar{\mathcal{A}}^2$ with corresponding eigenvalue σ^2/β. This is the desired contradiction because the point spectrum of $\bar{\mathcal{A}}^2$ is empty due to lemma 2.5. □

4.0.1. *On the weak convergence of unimodal, even and non-negative functions*

For the sake of clarity we proceed with some remarks on the strong compactness of weakly convergent sequences from $\mathcal{U} \cap \mathcal{N} \cap L^2$ as this problem becomes relevant in our existence proof for solitons. Strong compactness criteria are, in principle, provided by the concentration compactness method from [17], but since we consider only functions from $\mathcal{U} \cap \mathcal{N}$ here, the arguments are simplified.

Consider a sequence $(W_n)_n \subset \mathcal{S}_\gamma = \mathcal{U} \cap \mathcal{N} \cap \mathcal{B}_\gamma$ that converges weakly in L^2 to some limit $W_\infty \in \mathcal{S}_\gamma$. Passing to a subsequence, we can always assume that $\gamma_n = \frac{1}{2}\|W_n\|_2^2 \to \bar{\gamma}_\infty$ for some $\bar{\gamma}_\infty$ with $\gamma_\infty \leqslant \bar{\gamma}_\infty \leqslant \gamma$, where $\gamma_\infty = \frac{1}{2}\|W_\infty\|_2^2$. For $\gamma_\infty = \bar{\gamma}_\infty$ the convergence of norms forces the convergence $W_n \to W_\infty$ to be strong in L^2, and we are done in this case.

In the case where $\bar{\gamma}_\infty > \gamma_\infty$ the convergence cannot be strong as some amount of the 'mass' of the measures $\mu_n = W_n(\varphi)^2\,\mathrm{d}\varphi$ disappears when passing to $\mu_\infty = W_\infty(\varphi)^2\,\mathrm{d}\varphi$. However, since all functions are non-negative, unimodal and even, the annihilation of mass is governed by only two elementary processes (see figure 7). The weakly convergent sequence can form a *peak at the origin* and/or a *'fat' tail*, where 'fat' means

$$\lim_{L\to\infty}\lim_{n\to\infty}\int_{-\infty}^{-L} W_n^2(\varphi)\,\mathrm{d}\varphi + \int_L^\infty W_n^2(\varphi)\,\mathrm{d}\varphi > 0,$$

so that some non-negligible amount of the norm is transferred to infinity.

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The first observation is that a peak does not contribute to the potential energy $\mathcal{P}$. In fact, if the height of the peak is of order $1/\varepsilon$ with $\varepsilon \ll 1$, then the norm constraint $\frac{1}{2}\|W\|_2 \leqslant \gamma$ implies that the width of the peak is of order ε^2, and thus the peak disappears after applying the averaging operator $\mathcal{A}$. More rigorously, lemma 2.5 guarantees that $\mathcal{A}W_n$ converges strongly to $\mathcal{A}W_\infty$ on each compact subset of $\mathbb{R}$. Consequently, if the strong convergence fails due only to the formation of a peak, we still have $\mathcal{P}(W_n) \to \mathcal{P}(W_\infty)$.

The formation of a tail, however, is much more crucial as this, in general, implies $\mathcal{P}(W_n) \nrightarrow \mathcal{P}(W_\infty)$. Recall the maximizing sequence U_n for $\mathcal{P}_{\text{harm}}$ from (4.2) having the property that all mass of the measures $U_n(\varphi)^2\,\mathrm{d}\varphi$ is contained in a fat 'tail' with increasing support and decreasing height, so that the weak limit is zero. Even worse, since the spectrum of $\mathcal{A}^2 = \beta^{-1}\partial\mathcal{P}_{\text{harm}}$ is continuous, *each* maximizing sequence for $\mathcal{P}_{\text{harm}}$ is expected to have this property, so we conclude that the formation of tails is directly related to the non-existence of solitons for the harmonic chain.

Our strategy to prove the existence of solitons for nonlinear potentials is to show that each sequence that maximizes $\mathcal{P}$ in $\mathcal{S}_\gamma$ is *localized*, so a 'fat' tail cannot be formed. To this end we restrict our considerations to superquadratic potentials and derive suitable tightness results.

4.1. Existence of solitons for genuinely superquadratic $\mathcal{P}$

For the remainder of this section we require superquadratic growth conditions. We start with the assumptions concerning the energy functional $\mathcal{P}$ as they appear naturally in our existence proof. In §§ 4.2 and 4.3 we discuss the corresponding properties of the atomic interaction potential Φ.

Definition 4.4. The functional $\mathcal{P}$ is called *superquadratic* on $\mathcal{S}_\gamma$ with $\gamma > 0$ if

$$\mathcal{P}(sW) \geqslant s^2\mathcal{P}(W) \quad \text{for all } W \in \mathcal{S}_\gamma \text{ and all } 1 \leqslant s \leqslant \frac{\sqrt{2\gamma}}{\|W\|_2}. \tag{4.3}$$

Moreover, $\mathcal{P}$ is called *genuinely superquadratic* on $\mathcal{S}_\gamma$ if, in addition,

$$P(\gamma) > P_{\text{harm}}(\gamma) = \beta\gamma.$$

Note that, for each $\gamma > 0$, the harmonic functional $\mathcal{P}_{\text{harm}}$ is superquadratic, but not genuinely superquadratic in $\mathcal{S}_\gamma$.

Remark 4.5. Let $\mathcal{P}$ be superquadratic on $\mathcal{S}_\gamma$. Then it is superquadratic on $\mathcal{S}_{\tilde{\gamma}}$ for all $0 \leqslant \tilde{\gamma} \leqslant \gamma$, and we have

$$\frac{P(\gamma_2)}{\gamma_2} \geqslant \frac{P(\gamma_1)}{\gamma_1} \geqslant \beta$$

for all $0 \leqslant \gamma_1 \leqslant \gamma_2 \leqslant \gamma$. In particular, if $\mathcal{P}$ is genuinely superquadratic for $\gamma_1 \leqslant \gamma$, so it is for every γ_2 with $\gamma_1 \leqslant \gamma_2 \leqslant \gamma$.

Remark 4.6. Let $\mathcal{P}$ be a superquadratic on $\mathcal{S}_\gamma$. Then we have

$$\langle \partial\mathcal{P}[W], W\rangle \geqslant 2\mathcal{P}(W) \tag{4.4}$$

for all $W \in \mathcal{S}_\gamma$.

Proof. In view of the continuity properties of $\mathcal{P}$ and $\partial\mathcal{P}$ it is sufficient to consider the case $\|W\|_2 < \gamma$. For sufficiently small ε, (4.3) implies

$$\varepsilon^{-1}(\mathcal{P}((1+\varepsilon)W) - \mathcal{P}(W)) \geqslant \varepsilon^{-1}((1+\varepsilon^2)-1)\mathcal{P}(W) = (2+\varepsilon)\mathcal{P}(W),$$

and the limit $\varepsilon \to 0$ gives (4.4). □

We now formulate our main technical result concerning the tightness of maximizing sequences. Roughly speaking, 'fat' tails are not energetically optimal as their contributions to $\mathcal{P}$ and $\mathcal{P}_{\text{harm}}$ are comparable, and peaks are not optimal as they do not contribute to the potential energy at all. These naive explanations can be stated rigorously as follows.

Lemma 4.7. *For any* $\delta > 0$, *the set*

$$\mathcal{S}_{\gamma,\delta} = \{W \in \mathcal{S}_\gamma : \mathcal{P}(W) - \beta\tfrac{1}{2}\|W\|_2^2 \geqslant \delta\}$$

is closed under weak convergence.

Proof. Let $(W_n)_n \subset \mathcal{S}_\gamma$ be a given sequence such that $W_n \to W_\infty$ as $n \to \infty$ weakly in L^2, and $\mathcal{P}(W_n) \geqslant \beta\gamma_n + \delta$ with $\gamma_n = \frac{1}{2}\|W_n\|_2^2$. Without loss of generality, we can assume that $\frac{1}{2}\|W_n\|_2^2 \to \bar{\gamma}_\infty$ for some $\bar{\gamma}_\infty$ with $\gamma_\infty \leqslant \bar{\gamma}_\infty \leqslant \gamma$ and $\gamma_\infty = \frac{1}{2}\|W_\infty\|_2^2$. It remains to show that $\mathcal{P}(W_\infty) \geqslant \beta\gamma_\infty + \delta$. For $n \in \mathbb{N} \cup \{\infty\}$ we set

$$\tilde{W}_n := W_n|_{[-m,+m]}, \qquad \hat{W}_n := W_n - \tilde{W}_n, \tag{4.5}$$

where $m > 0$ is some constant to be chosen below, and this definition implies

$$\|W_n\|_2^2 = \|\tilde{W}_n\|_2^2 + \|\hat{W}_n\|_2^2. \tag{4.6}$$

Our strategy for this proof is to establish the approximations

$$\mathcal{P}(W_n) \approx \mathcal{P}(\tilde{W}_n) + \mathcal{P}(\hat{W}_n), \qquad \mathcal{P}(\hat{W}_n) \approx \mathcal{P}_{\text{harm}}(\hat{W}_n),$$

where the approximation error becomes arbitrarily small if both m and n are sufficiently large. To show this, we fix $\varepsilon > 0$ and suppose m to be sufficiently large such that

$$\tfrac{1}{2}\|\hat{W}_\infty\|_2^2 + |\mathcal{P}(W_\infty) - \mathcal{P}(\tilde{W}_\infty)| + \int_{m-1}^{m} W_\infty(\varphi)\,\mathrm{d}\varphi \leqslant \varepsilon. \tag{4.7}$$

Such a choice for m exists as $\tilde{W}_\infty \to W_\infty$ strongly in L^2 as $m \to \infty$. Since m is finite lemma 2.5 provides $\mathcal{A}\tilde{W}_n \to \mathcal{A}\tilde{W}_\infty$ strongly in L^2 as $n \to \infty$, and thus we find

$$|\|\tilde{W}_\infty\|_2^2 - \|\tilde{W}_n\|_2^2| + |\mathcal{P}(\tilde{W}_\infty) - \mathcal{P}(\tilde{W}_n)| + \left|\int_{m-1}^{m} W_\infty(\varphi) - W_n(\varphi)\,\mathrm{d}\varphi\right| \leqslant \varepsilon \tag{4.8}$$

for all sufficiently large n. Moreover, combining $\frac{1}{2}\|\hat{W}_\infty\|_2^2 \leqslant \varepsilon$ and $|\|\tilde{W}_\infty\|_2^2 - \|\tilde{W}_n\|_2^2| \leqslant \varepsilon$ with (4.6) and $\gamma_n \to \bar{\gamma}_\infty$ shows

$$\tfrac{1}{2}\|\hat{W}_n\|_2^2 = \gamma_n - \tfrac{1}{2}\|\tilde{W}_n\|_2^2 \leqslant \bar{\gamma}_\infty - \tfrac{1}{2}\|\tilde{W}_\infty\|_2^2 + C\varepsilon \leqslant \bar{\gamma}_\infty - \gamma_\infty + C\varepsilon \tag{4.9}$$

with C being independent of n and ε. In virtue of

$$\int_{m-1}^{m} W_\infty(\varphi)\,\mathrm{d}\varphi \leqslant \varepsilon \quad \text{and} \quad \left|\int_{m-1}^{m} W_\infty(\varphi) - W_n(\varphi)\,\mathrm{d}\varphi\right| \leqslant \varepsilon,$$

and since all functions W_n are unimodal, non-negative and even, we also obtain

$$0 \leqslant (\mathcal{A}\hat{W}_n)(\varphi) \leqslant (\mathcal{A}W_n)(\varphi) \leqslant (\mathcal{A}W_n)(m - \tfrac{1}{2}) \leqslant \int_{m-1}^{m} W_n(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi} \leqslant 2\varepsilon$$

for large n and all φ with $|\varphi| \geqslant m - \frac{1}{2}$. This provides

$$\|\mathcal{A}\hat{W}_n\|_\infty \leqslant C\varepsilon, \qquad \int_{||\varphi|-m|\leqslant 1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi \leqslant C\varepsilon \tag{4.10}$$

and, exploiting the expansion of $\Phi(r)$ for small r from (2.9), we find

$$\begin{aligned}\mathcal{P}(\hat{W}_n) &\leqslant \tfrac{1}{2}(\beta + o(\varepsilon)) \int_{\mathbb{R}} (\mathcal{A}\hat{W}_n)(\varphi)^2\,\mathrm{d}\varphi \\ &\leqslant \tfrac{1}{2}(\beta + o(\varepsilon))\|\hat{W}_n\|_2^2 \\ &\leqslant \beta(\bar{\gamma}_\infty - \gamma_\infty) + C\varepsilon \end{aligned} \tag{4.11}$$

due to (4.9). Finally, by (4.5), we have

$$\begin{aligned}\mathcal{P}(W_n) &= \int_{|\varphi|\leqslant m-1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi + \int_{||\varphi|-m|\leqslant 1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi \\ &\quad + \int_{|\varphi|\geqslant m+1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi \\ &= \int_{|\varphi|\leqslant m-1/2} \Phi(\mathcal{A}\tilde{W}_n)\,\mathrm{d}\varphi + \int_{||\varphi|-m|\leqslant 1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi \\ &\quad + \int_{|\varphi|\geqslant m+1/2} \Phi(\mathcal{A}\hat{W}_n)\,\mathrm{d}\varphi \\ &\leqslant \mathcal{P}(\tilde{W}_n) + \int_{||\varphi|-m|\leqslant 1/2} \Phi(\mathcal{A}W_n)\,\mathrm{d}\varphi + \mathcal{P}(\hat{W}_n), \end{aligned}$$

and $|\mathcal{P}(W_\infty) - \mathcal{P}(\tilde{W}_\infty)| \leqslant \varepsilon$ and $|\mathcal{P}(\tilde{W}_\infty) - \mathcal{P}(\tilde{W}_n)| \leqslant \varepsilon$ combined with (4.10) and (4.11) imply

$$\mathcal{P}(W_n) \leqslant \mathcal{P}(\tilde{W}_\infty) + \mathcal{P}(\hat{W}_n) + C\varepsilon \leqslant \mathcal{P}(W_\infty) + \beta(\bar{\gamma}_\infty - \gamma_\infty) + C\varepsilon.$$

Using $W_n \in \mathcal{S}_{\gamma,\delta}$ we conclude that $\mathcal{P}(W_\infty) \geqslant \gamma_\infty + \delta - C\varepsilon$, and this completes the proof because ε was chosen arbitrarily. □

As a direct consequence of lemma 4.7 we find in the genuinely superquadratic case that each maximizing sequence must be localized and hence contain a strongly convergent subsequence.

Corollary 4.8. *Let $\mathcal{P}$ be genuinely superquadratic on $\mathcal{S}_\gamma$, and suppose that the sequence $(W_n)_n \subset \mathcal{S}_\gamma$ is a maximizing sequence for $\mathcal{P}$ on S_γ, which means that*

$$\lim_{n\to\infty} \mathcal{P}(W_n) = P(\gamma) = \beta\gamma + \delta > P_{\mathrm{harm}}(\gamma)$$

for some $\delta > 0$. Then there exists a subsequence, still denoted by $(W_n)_n$, and $W_\infty \in \partial\mathcal{S}_\gamma$ such that $W_n \to W_\infty$ strongly in L^2, and hence $\mathcal{P}(W_\infty) = P(\gamma)$.

Proof. We choose the subsequence and $W_\infty \in \mathcal{S}_\gamma$ such that $W_n \to W_\infty$ weakly in L^2. Thanks to (4.3) we know that $\mathcal{P}(sW_n) \geqslant s^2\mathcal{P}(W_n)$ for all $s > 1$, and this implies $\gamma_n = \frac{1}{2}\|W_n\|_2^2 \to \gamma$ as $n \to \infty$, because otherwise the sequence $(W_n)_n$ could not be maximizing. Therefore, with

$$\tilde{W}_n = \frac{\sqrt{2\gamma}}{\sqrt{2\gamma_n}} W_n \in \partial\mathcal{S}_\gamma$$

we find $\mathcal{P}(\tilde{W}_n) \to \beta\gamma + \delta$ and $\tilde{W}_n \to W_\infty$ weakly in $\mathcal{S}_\gamma$, and lemma 4.7 provides

$$\mathcal{P}(W_\infty) \geqslant \beta\gamma_\infty + \delta$$

with $\gamma_\infty = \frac{1}{2}\|W_\infty\|_2^2 \leqslant \gamma$. In order to show $W_\infty \in \partial\mathcal{S}_\gamma$ we again use (4.3) and find

$$\beta\gamma + \delta = P(\gamma) \geqslant \mathcal{P}\left(\sqrt{\frac{\gamma}{\gamma_\infty}} W_\infty\right) \geqslant \frac{\gamma}{\gamma_\infty}\mathcal{P}(W_\infty) \geqslant \frac{\gamma}{\gamma_\infty}(\beta\gamma_\infty + \delta) \geqslant \beta\gamma + \frac{\gamma}{\gamma_\infty}\delta.$$

Since $\delta > 0$ we conclude that $\gamma_\infty = \gamma$, which means $\|W_n\|_2 \to \|W_\infty\|_2$, and this implies that the convergence $W_n \to W_\infty$ is strong in L^2. □

The combination of theorem 2.3 and corollary 4.8 immediately provides the desired existence result for non-negative and unimodal solitons.

Corollary 4.9. *If $\mathcal{P}$ is genuinely superquadratic on $\mathcal{S}_\gamma$, then there exists a maximizer W of $\mathcal{P}$ in $\mathcal{S}_\gamma$. This maximizer is a non-negative and unimodal soliton with $\frac{1}{2}\|W\|_2^2 = \gamma$.*

Finally, we characterize the soliton speed of maximizers of $\mathcal{P}$.

Remark 4.10. The soliton from corollary 4.9 is supersonic, which means that $\sigma^2 > \beta$.

Proof. Testing (2.7) with W, and using (4.4), we find $\sigma^2\|W\|_2^2 \geqslant 2\mathcal{P}(W) > 2\beta\gamma$. □

4.2. Criteria for superquadratic $\mathcal{P}$

Definition 4.11. The potential Φ is called superquadratic on the interval $[0, \sqrt{2\gamma}]$ if

$$\Phi(sr) \geqslant s^2\Phi(r)$$

holds for all $r \geqslant 0$ and all $s \geqslant 1$ with $rs \in [0, \sqrt{2\gamma}]$.

Remark 4.12. If the potential Φ is superquadratic on the interval $[0, \sqrt{2\gamma}]$, then $\mathcal{P}$ is superquadratic on $\mathcal{S}_\gamma$.

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Proof. Let $W \in \mathcal{S}_\gamma$ be fixed, and let s be arbitrary with $1 \leqslant s \leqslant \sqrt{2\gamma}/\|W\|_2$. For all $r = (\mathcal{A}W)(\varphi) \leqslant \sqrt{\|W\|_2}$ we have $rs \leqslant \sqrt{2\gamma}$, and hence $\Phi(s(\mathcal{A}W)(\varphi)) \geqslant s^2\Phi((\mathcal{A}W)(\varphi))$ for (almost) all $\varphi \in \mathbb{R}$. Finally, integration with respect to φ yields the desired result. □

Definition 4.11 implies that Φ is superquadratic on the interval $[0, \sqrt{2\gamma}]$ if and only if the function

$$\beta_\Phi(r) := 2\frac{\Phi(r)}{r^2} \tag{4.12}$$

is non-decreasing on $[0, \sqrt{2\gamma}]$ (note that $\beta_\Phi(0) = \beta$ in the sense of assumption 2.4). To obtain further characterizations of superquadratic growth we consider the following differential inequalities:

(C1) $\Phi'(r)r - 2\Phi(r) \geqslant 0$ for all $r \in [0, \sqrt{2\gamma}]$;

(C2) $\Phi''(r)r - \Phi'(r) \geqslant 0$ for all $r \in [0, \sqrt{2\gamma}]$;

(C3) $\Phi'''(r) \geqslant 0$ for all $r \in [0, \sqrt{2\gamma}]$.

Remark 4.13. For all $\gamma > 0$ and all sufficiently smooth potentials Φ with $\Phi(0) = \Phi'(0) = 0$, we have

$$\text{(C3)} \implies \text{(C2)} \implies \text{(C1)},$$

where (C1) holds if and only if Φ is superquadratic on $[0, \sqrt{2\gamma}]$.

Proof. (C3) is equivalent to $\mathrm{d}(\Phi''(r)r - \Phi'(r))/\mathrm{d}r \geqslant 0$, and in view of $\Phi''(0)0 - \Phi'(0) = 0$ we find (C3) ⇒ (C2). Moreover, the implication (C2) ⇒ (C1) can be proven similarly, and (C1) is equivalent to $\mathrm{d}\beta_\Phi(r)/\mathrm{d}r \geqslant 0$. □

We proceed with a remark concerning the relation between superquadratic growth and the convexity of Φ. In our context, of course, non-convex superquadratic potentials are forbidden, but solitons can still be shown to exist for such potentials (see [10] and our comments below).

Remark 4.14. (C2) implies the convexity of Φ (on the interval $[0, \sqrt{2\gamma}]$), but there exist non-convex potentials satisfying (C1).

Proof. Suppose that Φ satisfies (C2). Then, the comparison principle for ordinary differential equations gives $\Phi'(r) \geqslant \beta r$ for some $\beta \geqslant 0$, and (C2) implies $\Phi''(r) \geqslant \beta$ for all $r > 0$. Now let $\eta > 0$ be arbitrary, and consider the potential

$$\Phi_\eta(r) = r^2(1 + 2\pi^{-1}\arctan(\eta(r-1))),$$

which is superquadratic on $[0, \infty)$ as the function β_{Φ_η} is strictly increasing by construction. A direct calculation yields

$$\Phi''_\eta(1 + \eta^{-1}) = \pi^{-1}(3 + 3\pi + 2\eta - \eta^2),$$

hence Φ_η is not convex for large η. □

Another remark concerns the convexity of forces, which become important in the context of atomistic Riemann problems [14].

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REMARK 4.15. (C3) implies the convexity of Φ' (on the interval $[0,\sqrt{2\gamma}]$), but there exist potentials Φ that satisfy (C2) with non-convex derivative.

Proof. The first statement is obvious, and to obtain the second claim we argue as follows. We choose a non-negative, but not monotonically increasing, function h with $h(0)=0$, and compute Φ' as solution to the ordinary differential equation $h(r)=\Phi''(r)r-\Phi'(r)$. Then each local extremum of h for $r>0$ is a turning point of Φ', and vice versa. □

4.3. Criteria for genuinely superquadratic $\mathcal{P}$

In order to complete the existence proof for solitons we must show that, for a given superquadratic potential Φ, the corresponding energy functional $\mathcal{P}$ is in fact genuinely superquadratic on $\mathcal{S}_\gamma$. In the simplest case there is no harmonic contribution to $\mathcal{P}$, and then there exist solitons with arbitrary small γ. This holds in particular for all homogenous potentials $\Phi(r)=cr^\alpha$ with $c>0$ and $\alpha>2$.

REMARK 4.16. Let Φ be superquadratic on $[0,\infty)$ with $\beta=\Phi''(0)=0$ and $\Phi(r)>0$ for all $r>0$. Then $\mathcal{P}$ is genuinely superquadratic on $\mathcal{S}_\gamma$ for all $\gamma>0$.

The case when $\beta>0$ is more involved and needs a better understanding of the balance between the harmonic and anharmonic contributions to $\mathcal{P}$. Our strategy in this case is to find a particular function W_0 such that $\mathcal{P}(W_0)>\frac{1}{2}\beta\|W_0\|_2^2$, and this in turn implies the existence of solitons for all $\gamma\geqslant\frac{1}{2}\|W_0\|_2^2$.

LEMMA 4.17. *Suppose that Φ is superquadratic on $[0,\infty)$ and that the function β_Φ from (4.12) satisfies $\lim_{r\to\infty}\beta_\phi(r)>\frac{3}{2}\beta=\frac{3}{2}\beta_\Phi(0)$. Then $\mathcal{P}$ is genuinely superquadratic on $\mathcal{S}_\gamma$ for all sufficiently large γ.*

Proof. For fixed $0<\varepsilon<1$ and $W=\sqrt{2\gamma}W_{\mathrm{CL}}$ with W_{CL} as in (3.3) we find

$$\begin{aligned}
\mathcal{P}(W) &= 2\int_0^1 \Phi(\sqrt{2\gamma}s)\,\mathrm{d}s\\
&\geqslant 2\gamma\int_0^1 \beta_\Phi(\sqrt{2\gamma}s)s^2\,\mathrm{d}s\\
&\geqslant 2\gamma\beta_\Phi(0)\int_0^\varepsilon s^2\,\mathrm{d}s 2\gamma\beta_\Phi(\varepsilon\sqrt{2\gamma})\int_\varepsilon^1 s^2\,\mathrm{d}s\\
&= \tfrac{2}{3}\beta\gamma\biggl(\varepsilon^3+\frac{\beta_\Phi(\sqrt{2\gamma}\varepsilon)}{\beta}(1-\varepsilon^3)\biggr),
\end{aligned}$$

and conclude that $\mathcal{P}(W)>\beta\gamma$ for all sufficiently large γ. □

Lemma 4.17 implies the existence of solitons for weakly superquadratic potentials as for instance

$$\Phi(r)=\tfrac{1}{2}\beta r^2(1+c\ln(1+r)),\qquad \Phi(r)=\tfrac{1}{2}\beta r^2(1+d\arctan(r))$$

with $\beta\geqslant 0$, $c>0$ arbitrary and $d>0$ sufficiently large.

Next we evaluate the sequence $(U_n)_n$ from (4.2) and find an existence criterion for solitons that is very close to that given in [10].

Lemma 4.18. *Let Φ be superquadratic on $[0,\infty)$, and suppose*

$$\Phi(r) \geqslant \tfrac{1}{2}\beta r^2 + \varepsilon r^p$$

for all $r \geqslant 0$ with two constants $\varepsilon > 0$ and $p > 2$. Then there exists $\gamma_0 > 0$ such that $\mathcal{P}$ is genuinely superquadratic on $\mathcal{S}_\gamma$ for all $\gamma > \gamma_0$. Moreover, $\beta = 0$ or $2 < p < 6$ implies $\gamma_0 = 0$.

Proof. Let $\gamma > 0$ be arbitrary and consider the sequence $(U_n)_n$ from (4.2). Then,

$$\mathcal{P}(U_n) - \mathcal{P}_{\mathrm{harm}}(U_n) \geqslant \varepsilon\mathcal{P}_{\mathrm{nl}}(U_n)$$

with

$$\begin{aligned}\mathcal{P}_{\mathrm{nl}}(U_n) &= \int_{\mathbb{R}} (\mathcal{A}U_n)^p \,\mathrm{d}\varphi \\ &\geqslant \int_{|\varphi|\leqslant n-1/2} \left(\Theta\left(\frac{\pi}{4n}\right)U_n\right)^p \mathrm{d}\varphi \\ &\geqslant \left(\Theta\left(\frac{\pi}{4n}\right)\right)^p \left(\frac{2\gamma}{n}\right)^{p/2} n \int_{-1+1/2n}^{1-1/2n} (\cos(\tfrac{1}{2}\pi\varphi))^p \,\mathrm{d}\varphi \\ &\geqslant cn^{1-p/2}.\end{aligned}$$

We conclude that

$$\mathcal{P}(U_n) \geqslant \mathcal{P}_{\mathrm{harm}}(U_n) + c\gamma^{p/2}n^{1-p/2} > 0$$

for some positive constant $c > 0$, and according to lemma 4.1 there exists a constant $\tilde{c} > 0$ such that

$$\mathcal{P}(U_n) \geqslant c\gamma^{p/2}n^{1-p/2} + \beta\gamma(1 - \tilde{c}n^{-2}).$$

Finally, for $\beta = 0$, or sufficiently large γ, or $-1 + \frac{1}{2}p < 2$ and n large, we find $\mathcal{P}(U_n) > \beta\gamma$. □

As an application of lemma 4.18 we find the following existence result for unimodal solitons with non-negative W. Let Φ be analytic with non-negative coefficients, i.e.

$$\Phi(r) = \tfrac{1}{2}\beta r^2 + \sum_{i=3}^{\infty} \kappa_i r^i$$

with $\kappa_i \geqslant 0$ for all $i \geqslant 3$. Then Φ is superquadratic on $[0,\infty)$ and genuinely superquadratic for large γ. Moreover, if at least one of the coefficients κ_3, κ_4 and κ_5 is positive, then Φ is genuinely superquadratic for all $\gamma > 0$.

Since the travelling wave equation (2.7) is invariant under the reflection symmetry

$$W \rightsquigarrow -W, \qquad \Phi(r) \rightsquigarrow \Phi(-r),$$

we also find existence results for solitons with nonpositive W. For instance, the Toda potential $\Phi_{\mathrm{Toda}}(r) = \mathrm{e}^{-r} + r - 1$ is not superquadratic for $r \geqslant 0$ but the reflected potential $\tilde{\Phi}_{\mathrm{Toda}}(r) = \mathrm{e}^{r} - r - 1$ has solitons with arbitrary small γ (see lemma 4.18). Consequently, the Toda chain allows for solitons with $W \leqslant 0$.

Finally, we summarize some other superquadratic growth conditions for Φ under which the existence of solitons was proven by other authors.

(i) $\Phi'(r)r > 2\Phi(r)$: Friesecke and Wattis [10] prove the existence of supersonic solitons with prescribed potential energy $\mathcal{P} \geqslant P_0$ above some critical value $P_0 \geqslant 0$. Moreover, $\Phi(r) = \frac{1}{2}\beta r^2 + \varepsilon r^p(1 + o(r))$ with $\varepsilon > 0$ and p as in lemma 4.18 implies $P_0 = 0$.

(ii) $\Phi(r) = \frac{1}{2}\beta r^2 + \Phi_{\mathrm{nl}}(r)$ and $\Phi'_{\mathrm{nl}}(r)r \geqslant \alpha\Phi_{\mathrm{nl}}(r)$ for all $r \geqslant 0$ and some $\alpha > 2$: Smets and Willem [21] establish the existence of solitons with prescribed supersonic speed $\sigma^2 > \beta = \Phi''(0)$.

(iii) $\Phi'_{\mathrm{nl}}(r)r \geqslant \alpha\Phi_{\mathrm{nl}}(r)$ for all $r \geqslant 0$ and some $\alpha > 2$, or $\Phi''_{\mathrm{nl}}(r)r \geqslant \tilde{\alpha}\Phi'_{\mathrm{nl}}(r)$ for all $r \geqslant 0$ and some $\tilde{\alpha} > 1$: Pankov and Pflüger [18] prove under both assumptions the existence of a family of solitons parametrized by $\sigma^2 > \beta = \Phi''(0)$.

(iv) $\Phi'(r) \geqslant 0$ for all $r \geqslant 0$ and $\liminf_{r\to\infty} r^{-\alpha}(\Phi'(r)r - \alpha\Phi(r)) > 0$ and some $\alpha > 2$: Schwetlick and Zimmer [19] show that for each supersonic speed $\sigma^2 > \sigma_{\mathrm{crit}} \geqslant \beta = \Phi''(0)$ there exists a soliton.

All these existence results imply that the soliton profile W belongs to $\mathcal{N}$, but since they do not require the convexity of Φ, they do not provide $W \in \mathcal{U}$.

4.4. Solitons as limits of wavetrains

It is natural to investigate whether wavetrains converge to solitons when the periodicity length L tends to ∞. In this section we establish such a convergence result for unimodal and non-negative wavetrains. To this end we allow for arbitrary values of $L \in (0, \infty]$ and write $\mathcal{A}_L$ for the operator $\mathcal{A}$ acting on $L^2([-L, L])$. Consequently, we introduce

$$\mathcal{S}_{L,\gamma} := \mathcal{U} \cap \mathcal{N} \cap \mathcal{B}_{L,\gamma},$$

where $\mathcal{B}_{L,\gamma}$ denotes the ball of radius $\sqrt{2\gamma}$ in $L^2([-L, L])$, and consider

$$P_L := \sup_{W\in\mathcal{S}_{L,\gamma}} \int_{-L}^{L} \Phi((\mathcal{A}_L W)(\varphi))\,\mathrm{d}\varphi.$$

Moreover, we define an *embedding* operator $E_L : \mathcal{S}_{L,\gamma} \to \mathcal{S}_{\infty,\gamma}$ by

$$(E_L W_L)(\varphi) = \begin{cases} W_L(\varphi) & \text{for } |\varphi| \geqslant L, \\ 0 & \text{otherwise.} \end{cases}$$

Inspired by the notion of Γ-convergence we show that the energy of each periodic profile can be approximated by localized profiles and prove that each localized profile can be recovered by periodic profiles.

LEMMA 4.19. *For each $\gamma > 0$ and $L < \infty$ there exists a constant $C_{L,\gamma}$ of order $o(\sqrt{\gamma/L})$ such that*

$$\mathcal{P}_\infty(E_L W_L) + C_{L,\gamma} \geqslant \mathcal{P}_L(W_L) \geqslant \mathcal{P}_\infty(E_L W_L) \tag{4.13}$$

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holds for all $W_L \in \mathcal{S}_{L,\gamma}$*. Moreover, for any* $W_\infty \in \mathcal{S}_{\infty,\gamma}$ *there exists a family of functions* $(W_L)_{L<\infty}$ *such that*

$$\mathcal{P}_L(W_L) \xrightarrow{L\to\infty} \mathcal{P}_\infty(W_\infty). \tag{4.14}$$

Proof. First let $W_L \in \mathcal{S}_{L,\gamma}$ be fixed, and note that

$$(\mathcal{A}_\infty E_L W_L)(\varphi) = (E_L \mathcal{A}_L W_L)(\varphi), \quad ||\varphi| - L| \geqslant \tfrac{1}{2}, \tag{4.15}$$

hold by construction. For $||\varphi| - L| \leqslant \frac{1}{2}$ we have $0 \leqslant W_L(\varphi) \leqslant W_L(L-1)$ due to $W_L \in \mathcal{U} \cap \mathcal{N}$, and hence

$$0 \leqslant (\mathcal{A}_\infty E_L W_L)(\varphi) \leqslant (E_L \mathcal{A}_L W_L)(\varphi) \leqslant \int_{\varphi-1/2}^{\varphi+1/2} W_L(\tilde{\varphi})\,\mathrm{d}\tilde{\varphi} = W_L(L-1).$$

Moreover, $W_L \in \mathcal{U} \cap \mathcal{N}$ gives $(\mathcal{A}_\infty E_L W_L)(\varphi) \leqslant (E_L \mathcal{A}_L W_L)(\varphi)$ and

$$2\gamma \geqslant \int_{-L+1}^{L-1} W_L(\varphi)^2\,\mathrm{d}\varphi \geqslant 2(L-1)(W_L(L-1))^2,$$

and we therefore have

$$0 \leqslant (\mathcal{A}_\infty E_L W_L)(\varphi) \leqslant (E_L \mathcal{A}_L W_L)(\varphi) \leqslant \varepsilon := \sqrt{\frac{\gamma}{L-1}}, \quad ||\varphi| - L| \leqslant \tfrac{1}{2}. \tag{4.16}$$

The estimate (4.13) now follows from (4.15) and (4.16) via

$$\begin{aligned}
0 &\leqslant \mathcal{P}_L(W_L) - \mathcal{P}_\infty(E_L W_L) \\
&\leqslant \int_{-\infty}^{\infty} \Phi((E_L \mathcal{A}_L W_L)(\varphi)) - \Phi((\mathcal{A}_\infty E_L W_L)(\varphi))\,\mathrm{d}\varphi \\
&\leqslant \int_{||\varphi|-L|\leqslant 1/2} \Phi((E_L \mathcal{A}_L W_L)(\varphi)) - \Phi((\mathcal{A}_\infty E_L W_L)(\varphi))\,\mathrm{d}\varphi \\
&\leqslant f(\varepsilon),
\end{aligned}$$

where $f(\varepsilon) = 2\varepsilon \sup_{0\leqslant r\leqslant\varepsilon} \Phi'(r) = o(\varepsilon)$. Now let $W_\infty \in \mathcal{S}_{\infty,\gamma}$ be fixed, and define $W_L \in \mathcal{S}_{L,\gamma}$ by

$$(W_L)(\varphi) = W_\infty(\varphi) \quad \text{for } |\varphi| \leqslant L.$$

Then, in general we have $W_\infty(\varphi) \neq (E_L W)_L(\varphi) = 0$ for $\varphi > L$ but always $E_L W_L \to W_\infty$ strongly in $\mathsf{L}^2(\mathbb{R})$ as $L \to \infty$. This implies $\mathcal{P}_\infty(E_L W_L) - \mathcal{P}_\infty(W_\infty) \to 0$, and due to (4.13) we find (4.14). □

Lemma 4.19 now provides the convergence of suprema.

Corollary 4.20. *We have* $P_L(\gamma) \xrightarrow{L\to\infty} P_\infty(\gamma)$.

Proof. For given $L < \infty$, let $\overline{W}_L$ be a maximizer of $\mathcal{P}$ on $\mathcal{S}_{L,\gamma}$. Then (4.13) implies

$$P_L(\gamma) \leqslant \mathcal{P}_\infty(E_L \overline{W}_L) + o\biggl(\sqrt{\frac{\gamma}{L}}\biggr) \leqslant P_\infty(\gamma) + o\biggl(\sqrt{\frac{\gamma}{L}}\biggr),$$

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and hence $\limsup_{L\to\infty} P_L(\gamma) \leqslant P_\infty(\gamma)$. Moreover, in view of (4.14) we have

$$\mathcal{P}_\infty(W_\infty) \leqslant \liminf_{L\to\infty} P_L(\gamma)$$

for all W_∞, and this shows $P_\infty(\gamma) \leqslant \liminf_{L\to\infty} P_L(\gamma)$. □

We finally show that solitons can be constructed as limits of wavetrains. More precisely, corollary 4.20 combined with corollary 4.8 provides the following convergence result for maximizers.

COROLLARY 4.21. *Let $\mathcal{P}$ be genuinely superquadratic on $\mathcal{S}_\gamma$, and, for each $L < \infty$, let $\overline{W}_L$ be a maximizer of $\mathcal{P}$ in $\mathcal{S}_{L,\gamma}$. Then, for any sequence $(L_n)_n$ with $L_n \to \infty$ there exist a subsequence, still denoted by L_n, and a maximizer $\overline{W}_\infty \in \mathcal{S}_{\infty,\gamma}$, such that $E_{L_n}\overline{W}_{L_n} \to \overline{W}_\infty$ strongly in $\mathsf{L}^2(\mathbb{R})$.*

Acknowledgements

The author is grateful to Jens D. M. Rademacher for several stimulating discussions, and to Michael Helmers for providing the example of remark 4.14.

References

1 W. Dreyer and M. Herrmann. Numerical experiments on the modulation theory for the nonlinear atomic chain. *Physica* D **237** (2008), 255–282.
2 W. Dreyer, M. Herrmann and A. Mielke. Micro–macro transition for the atomic chain via Whitham's modulation equation. *Nonlinearity* **19** (2006), 471–500.
3 W. Dreyer, M. Herrmann and J. Rademacher. Pulses, traveling waves and modulational theory in oscillator chains. In *Analysis, modeling and simulation of multiscale problems* (Springer, 2006).
4 D. B. Duncan, J. C. Eilbeck, H. Feddersen and J. A. D. Wattis. Solitons on lattices. *Physica* D **68** (1993), 1–11.
5 E. Fermi, J. Pasta and S. Ulam. *The many body problem* (World Scientific, 1993).
6 A.-M. Filip and S. Venakides. Existence and modulation of traveling waves in particle chains. *Commun. Pure Appl. Math.* **51** (1999), 693–735.
7 G. Friesecke and K. Matthies. Atomic-scale localization of high-energy solitary waves on lattices. *Physica* D **171** (2002), 211–220.
8 G. Friesecke and K. Matthies. Geometric solitary waves in a 2D mass spring lattice. *Discrete Contin. Dynam. Syst.* B **3** (2003), 105–114.
9 G. Friesecke and R. L. Pego. Solitary waves on FPU lattices. I. Qualitative properties, renormalization and continuum limit. *Nonlinearity* **12** (1999), 1601–1627.
10 G. Friesecke and J. A. D. Wattis. Existence theorem for solitary waves on lattices. *Commun. Math. Phys.* **161** (1994), 391–418.
11 M. H. Hays, C. D. Levermore and P. D. Miller. Macroscopic lattice dynamics. *Physica* D **79** (1994), 1–15.
12 M. Herrmann. Periodic travelling waves in convex Klein–Gordon chains. *Nonlin. Analysis TMA* **71** (2009), 5501–5508.
13 M. Herrmann. Ein Mikro-Makro-Übergang für die nichtlineare atomare Kette mit Temperatur. PhD Thesis, Humboldt-Universität zu Berlin, 2005.
14 M. Herrmann and J. Rademacher. Riemann solvers and undercompressive shocks of convex FPU chains. *Nonlinearity* **23** (2010), 277–304.
15 M. Herrmann and J. Rademacher. Heteroclinic travelling waves in convex FPU-type chains. *SIAM J. Math. Analysis* **42** (2010), 1483–1504.
16 G. Iooss. Travelling waves in the Fermi–Pasta–Ulam lattice. *Nonlinearity* **13** (2000), 849–866.

17 P.-L. Lions. The concentration-compactness principle in the calculus of variations. The locally compact case. I. *Annales Inst. H. Poincaré Analyse Non Linéaire* **1** (1984), 109–145.

18 A. Pankov and K. Pflüger. Traveling waves in lattice dynamical systems. *Math. Meth. Appl. Sci.* **23** (2000), 1223–1235.

19 H. Schwetlick and J. Zimmer. Solitary waves for nonconvex FPU lattices. *J. Nonlin. Sci.* **17** (2007), 1–12.

20 H. Schwetlick and J. Zimmer. Existence of dynamic phase transitions in a one-dimensional lattice model with piecewise quadratic interaction potential. *SIAM J. Math. Analysis* **41** (2009), 1231–1271.

21 D. Smets and M. Willem. Solitary waves with prescribed speed on infinite lattices. *J. Funct. Analysis* **149** (1997), 266–275.

22 M. Toda. *Theory of nonlinear lattices*, Springer Series in Solid-State Sciences, vol. 20 (Springer, 1981).

(*Issued 6 August 2010*)