Action minimizing fronts in general FPU-type chains

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Abstract

We study atomic chains with nonlinear nearest neighbour interactions and prove the existence of fronts (heteroclinic travelling waves with constant asymptotic states). Generalizing recent results of Herrmann and Rademacher we allow for non-convex interaction potentials and find fronts with non-monotone profile. These fronts minimize an action integral and can only exist if the asymptotic states fulfill the macroscopic constraints and if the interaction potential satisfies a geometric graph condition. Finally, we illustrate our findings by numerical simulations.

Keywords: Fermi-Pasta-Ulam chain, heteroclinic travelling waves, conservative shocks, least action principle

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1 Introduction

Nonlinear Hamiltonian lattices like chains of interacting atoms or coupled oscillators are ubiquitous in mathematics, physics, and material sciences. The most famous example, and most elementary model for a crystal, is a chain of identical atoms that interact by nearest neighbour forces. In reminiscence of the pioneering paper by Fermi, Pasta, and Ulam [FPU55] one usually refers to such systems as FPU or FPU-type chains.

Although FPU chains are quite simple lattice models they exhibit a rich and complicate dynamical behaviour, and we still lack a complete understanding of their dynamical properties. A mayor topic in the analysis of FPU chains is therefore the investigation of coherent structures such as travelling waves and breathers. Travelling waves are highly symmetric, exact solutions to the

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underlying lattice equation. They can be regarded as the fundamental modes of nonlinear wave propagation and provide much insight into the energy transport in discrete media. In this paper we aim in contributing to the general theory by studying fronts, i.e., heteroclinic travelling waves that connect two different constant states.

The dynamics of FPU chains is governed by the lattice equation

\[ \ddot{x}_j = \Phi'(x_{j+1} - x_j) - \Phi'(x_j - x_{j-1}). \]  

(1)

Here \( x_j = x_j(t) \) denotes the position of the \( j \)th atom at time \( t \), \( \Phi \) is the interaction potential, and the atomic mass is normalized to 1. Introducing the atomic distances \( r_j = x_{j+1} - x_j \) and velocities \( v_j = \dot{x}_j \) we can reformulate (1) as

\[ \dot{r}_j = v_{j+1} - v_j, \quad \dot{v}_j = \Phi'(r_j) - \Phi'(r_{j-1}). \]  

(2)

A travelling wave is a special solution to (2) that satisfies the ansatz

\[ r_j(t) = R(j - \sigma t), \quad v_j(t) = V(j - \sigma t). \]  

(3)

\( R \) and \( V \) are the profile functions for distances and velocities, \( \sigma \) denotes the wave speed, and \( \varphi = j - \sigma t \) is the phase variable. In dependence of the properties of \( R \) and \( V \) travelling waves come in different types. Wave trains have periodic profiles and are investigated in \[ \text{[FV99, PP00, DHM06]} \]. They describe oscillatory solutions to (1) and provide the building blocks for Whitham’s modulation theory. Another important class of travelling waves are solitons (or solitary waves), where \( R \) and \( V \) are localized over a constant background state. The existence of solitons in lattices is a nontrivial problem and has been studied intensively during the last 20 years. We refer to \[ \text{[FW94, SW97, FM02, Pan05, SZ07, Her09]} \] for variational methods, and to \[ \text{[Ioo00, IJ05]} \] for an approach via spatial dynamics and centre manifold reduction.

In this paper we study fronts which have heteroclinic shape and satisfy

\[ \lim_{\varphi \to \pm \infty} R(\varphi) = r_{\pm}, \quad \lim_{\varphi \to \pm \infty} V(\varphi) = v_{\pm} \]  

(4)

with \( (r_-, v_-) \neq (r_+, v_+) \). Fronts have attracted much less interest than solitons, maybe because they only exist if the asymptotic states satisfy some very restrictive conditions. In particular, \( \Phi' \) must have at least one turning point between \( r_- \) and \( r_+ \), and this excludes for instance the famous Toda potential. Nonetheless, fronts in FPU chains appear naturally in atomistic Riemann problems, see \[ \text{[HR10]} \] for numerical simulations, and are important in the context of phase transitions.

The first rigorous result about fronts we are aware of is the bifurcation criterion from \[ \text{[Ioo00]} \]. It implies that fronts with small jumps between the asymptotic states exist only if \( \Phi' \) has a convex-concave turning point. Recently, the existence of fronts was proven by variational methods in \[ \text{[HR09]} \]. The existence theorem therein does not require the asymptotic states to be close to each other but is restricted to convex potentials \( \Phi \). The proof relies on a Lagrangian action integral for fronts with prescribed asymptotic states and uses the direct approach to establish the existence of minimizers. A similar approach is used in \[ \text{[KZ09a, KZ09b]} \] to prove the existence of fronts for sine-Gordon chains.

In this paper we generalize the method from \[ \text{[HR09]} \] and prove the existence of fronts without convexity assumption on \( \Phi \). Our main result can be summarized as follows.

**Theorem 1.** Action minimizing front solutions to (2) exist under the following hypotheses:

(i) The asymptotic states and the front speed satisfy the macroscopic constraints, which take the form of three independent jump conditions.
The potential satisfies the graph condition with respect to the asymptotic states.

(iii) Some technical assumptions are also satisfied.

Moreover, there is no front without (i), and no action minimizing front without (ii).

The assumptions in Theorem 1 will be specified below. The macroscopic constraints, see Lemma 2, are algebraic relations and link fronts to energy conserving shocks of the p-system, which is the naive continuum limit of FPU chains. In particular, they determine the wave speed $\sigma$ and imply that the asymptotic strains $r_-$ and $r_+$ cannot be chosen independently of each other. The graph condition reformulates the area condition from [HR09] and requires that the graph of $\Phi$ is below the shock parabola associated with the asymptotic states. Both the macroscopic constraints and the graph condition appear naturally in our variational existence proof and guarantee that the action integral is well-defined and bounded from below.

Closely related to fronts are heteroclinic waves with oscillatory tails. These are travelling wave solutions to (2) which approach two different periodic waves for $\varphi \to \pm \infty$. Such oscillatory fronts are used to describe martensitic phase transitions and to derive kinetic relations in solids [BCS01a, BCS01b, AP07, Vai10]. The only available existence results, however, concern piecewise quadratic potentials, which allow for simplifying the travelling wave equation by means of Fourier transform, see [TV05, SCC05, SZ09]. It remains a challenging problem for future research to give alternative, maybe variational, existence proofs that cover more general chains.

The paper is organized as follows. In § 2 we discuss the macroscopic constraints and normalize the asymptotic states. Moreover, we reformulate the front equation as an eigenvalue problem for a nonlinear integral operator. In § 3 we set the existence problem into a variational framework and characterize fronts as minimizers of an action integral. Or main technical result is Theorem 16 and guarantees that this action integral attains its minimum on a suitable set of candidates for fronts. The proof uses separations of phases, which are introduced in § 3.4 and allow to extract convergent subsequences from action minimizing sequences. Finally, we present some numerical simulations in § 4.

2 Preliminaries about fronts

Substituting the travelling wave ansatz (3) into (2) yields

$$\sigma \frac{d}{d\varphi} R(\varphi) + V(\varphi + 1) - V(\varphi) = 0, \quad \sigma \frac{d}{d\varphi} V(\varphi) + \Phi'(R(\varphi)) - \Phi'(R(\varphi - 1)) = 0,$$

which is a nonlinear system of advance-delay-differential equations. Moreover, combining both equations we readily verify the energy law

$$\sigma \frac{d}{d\varphi} \left( \frac{1}{2} V^2(\varphi) + \Phi(R(\varphi)) \right) + \Phi'(R(\varphi)) V(\varphi + 1) - \Phi'(R(\varphi - 1)) V(\varphi) = 0.$$

2.1 Macroscopic constraints for the asymptotic states

We now derive the macroscopic constraints that couple the front speed $\sigma$ to the asymptotic states $(r_+, v_+)$ from (1). To this end we consider continuous observables $\psi = \psi(r, v)$ and denote by

$$[\psi(r, v)] := \psi(r_+, v_+) - \psi(r_-, v_-) \quad \text{and} \quad \langle \psi(r, v) \rangle := \frac{1}{2} (\psi(r_-, v_-) + \psi(r_+, v_+)),$$

the jump and mean value, respectively.

The following result was proven in [HR09] (see also [AP07]) by integrating (4) and (6) over a finite interval $[-N, N]$ and passing to the limit $N \to \infty$. 

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Lemma 2. The asymptotic states of each front satisfy

\[ \sigma[r] + [v] = 0, \quad \sigma[v] + [\Phi'(r)] = 0, \quad \sigma[\frac{1}{2}v^2 + \Phi(r)] + [\Phi'(r)v] = 0. \]  

(7)

Heuristically, Lemma 2 reflects that fronts transform into shock waves when passing to large spatial and temporal scales. The jump conditions (7) precisely mean that the asymptotic states correspond to an energy conserving shock for the p-system and imply that each front satisfies mass, momentum, and energy. The p-system is the naïve continuum limit of FPU chains under the hyperbolic scaling and reads

\[ \partial_\tau r = \partial_y v, \quad \partial_\tau v = \partial_y \Phi'(r), \]  

(8)

where \( \tau = \varepsilon t \) and \( y = \varepsilon j \) denote the macroscopic time and space, respectively, and \( \varepsilon > 0 \) is a small scaling parameter. The conservation laws in (8) correspond to mass and momentum, and imply the conservation of energy for smooth solutions, that is

\[ \partial_\tau \left( \frac{1}{2}v^2 + \Phi(r) \right) = \partial_\tau (v\Phi'(r)). \]  

(9)

The jump conditions for (9), however, is independent of the jump conditions for (8). More details about the p-system and energy conserving shocks can be found in [HR10, HR09].

Using the discrete Leibniz rule \[ [\psi_1\psi_2] = [\psi_1]\langle \psi_2 \rangle + \langle \psi_1 \rangle[\psi_2] \] we readily verify that (7) implies

\[ [\Phi(r)] = [r]\langle \Phi'(r) \rangle, \quad \sigma^2 = \|\Phi'(r)\|/|r|. \]  

(10)

Conversely, for any \((r_-, r_+)\) with (10) there exist – up to Galilean transformations – exactly two solutions to (7) which differ in \text{sgn}\( \sigma \). We now characterize the geometric meaning of (10) and refer to Figure 1 for an illustration.

Figure 1: To each front there exists a parabola that touches the graph of \( \Phi \) in both \( r_- \) and \( r_+ \). Consequently, the signed area between the graph of \( \Phi' \) and the secant connecting \( r_- \) and \( r_+ \) vanishes the stripe \([r_-, r_+]\).

Lemma 3. The following conditions are equivalent:

(i) \((\sigma, r_-, r_+)\) fulfils (10),

(ii) there exists a parabola that touches the graph of \( \Phi \) in both \( r_- \) and \( r_+ \),

(iii) the signed area between the graph of \( \Phi' \) and the secant connecting \( r_- \) to \( r_+ \) sums up to zero in \([r_-, r_+]\).

Moreover, each condition implies that \( \Phi' \) has at least one turning point between \( r_- \) and \( r_+ \).

Proof. Consider the parabola \( f(r) = \frac{1}{2}ar^2 + br + c \). The touching conditions

\[ f(r_\pm) = \Phi(r_\pm), \quad f'(r_\pm) = \Phi'(r_\pm) \]
are equivalent to
\[
\frac{1}{2}a[r^2] + b[r] = \langle \Phi(r) \rangle, \quad \frac{1}{2}a(r^2) + b(r) + c = \langle \Phi(r) \rangle, \quad [r]a = \langle \Phi'(r) \rangle, \quad a(r) + b = \langle \Phi'(r) \rangle,
\]
and by \( \frac{1}{2}||r^2|| = \langle r \rangle[r] \) we conclude that (i) and (ii) are equivalent via
\[
a = \sigma^2, \quad b = \langle \Phi'(r) \rangle - \sigma^2 \langle r \rangle, \quad c = \langle \Phi(r) \rangle - \langle r \rangle \langle \Phi'(r) \rangle + \sigma^2 \left( \langle r \rangle^2 - \frac{1}{2} \sigma^2 \right).
\]
The equivalence of (iii) and (iv) is immediate since the secant has slope \( \sigma^2 \), and \( \Phi' \) must have a turning point because otherwise the graph of \( \Phi' \) would be either below or above the secant. \( \square \)

Condition (10) is the kinetic relation for fronts and reveals that the asymptotic states cannot be chosen arbitrarily. More precisely, for given \( r_- \) and \( r_+ \) we can choose \( \sigma \) and \( [v] \) such that the first two jump conditions in (7) (which correspond to mass and momentum) are satisfied. However, for the energy condition (7) to hold, \( r_- \) and \( r_+ \) must additionally fulfill (10). Form this we conclude that fronts do not exist if \( \Phi' \) is either convex or concave, and that in general we cannot prescribe both \( r_- \) and \( r_+ \).

We emphasize that (7) is in general not sufficient for the existence of fronts, i.e., there exist energy conserving shocks in the p-system that cannot be realized by a front in FPU. In fact, it was proven in [1000] that fronts bifurcate from convex-concave but not from concave-convex turning points of \( \Phi' \). This disproves the existence of subsonic fronts with small jump heights although there exist the corresponding energy conserving shocks.

In order to prove the existence of action minimizing fronts we shall additionally to (7) require that the graph of \( \Phi \) is below the parabola defined by the asymptotic states, see Assumption 5. In particular, our existence result provides a front for Example A from Figure 1 but does not cover Example B, see Remark 12 and the examples in [3].

2.2 Normalization and reformulation

For our analysis in [3] it is convenient to normalize the asymptotic states and to reformulate the front equation (5) as an eigenvalue problem for a nonlinear integral operator.

**Lemma 4.** Up to affine transformations we can assume that
\[
\sigma = 1, \quad r_{\pm} = \pm 1, \quad v_{\pm} = \mp 1, \quad \Phi'(\pm 1) = \pm 1, \quad \Phi(\pm 1) = \frac{1}{2}, \quad (11)
\]
Moreover, with (11) the front equation is equivalent to
\[
W = \mathcal{A}\Phi'(\mathcal{A}W), \quad \mathcal{A}W(\varphi) = \int_{\varphi - \frac{1}{2}}^{\varphi} W(\tilde{\varphi}) \, d\tilde{\varphi}, \quad (12)
\]
where \( W \) is a normalized profile with \( \lim_{\varphi \to \pm \infty} W(\varphi) = \pm 1 \).

**Proof.** Let \( U \) and \( W \) be two normalized profiles such that
\[
R(\varphi) = \langle r \rangle + \frac{1}{2}[r]U(\varphi + 1/2), \quad V(\varphi) = \langle v \rangle + \frac{1}{2}[v]W(\varphi).
\]
Using the first two jump conditions from (7) we readily verify that (5) transforms into
\[
\frac{d}{d\varphi} U(\varphi) = W(\varphi + 1/2) - W(\varphi - 1/2), \quad \frac{d}{d\varphi} W(\varphi) = \hat{\Phi}'(U(\varphi + 1/2)) - \hat{\Phi}'(U(\varphi - 1/2)), \quad (13)
\]
where the normalized potential
\[ \hat{\Phi}(u) = \frac{4}{\Phi'(r)[r]} \Phi\left(\langle r \rangle + \frac{1}{2}[r] u\right) - \frac{2\langle \Phi'(r) \rangle}{\Phi'(r)} u + \frac{1}{2} - \frac{4\langle \Phi(r) \rangle}{\Phi'(r)[r]} \]
satisfies \( \hat{\Phi}'(\pm 1) = \pm 1 \). Moreover, we have \( \hat{\Phi}(-1) = \hat{\Phi}(+1) = \frac{1}{2} \) if and only if the third jump condition (13) is satisfied. Towards (12) now suppose (11). Integrating (13) we find
\[ U = A W, \]
where the constant of integration vanishes due to \( U(\pm 1) = W(\pm 1) = \pm 1 \), and similarly we derive
\[ W = A \hat{\Phi}'(U) \] from (13).

The front parabola for normalized data (11) is \( r \mapsto \frac{1}{2} r^2 \) and each solution to (12) can be viewed as a perturbation of the shock profile
\[ W_{sh}(\varphi) = \text{sgn}(\varphi) = \begin{cases} +1 & \text{for } \varphi < 0, \\ 0 & \text{for } \varphi = 0, \\ -1 & \text{for } \varphi > 0. \end{cases} \] (14)

Notice that the residual of \( W_{sh} \), that is \( W_{sh} - A \Phi'(AW_{sh}) \), has compact support.

We proceed with some preliminary remarks about the action of a front. Heuristically, the action density in the normalized setting is given by
\[ \frac{1}{2} W^2 - \Phi(AW) = \frac{1}{2} W^2 - \frac{1}{2}(AW)^2 + \Psi(AW) \]
with
\[ \Psi(r) = \frac{1}{2} r^2 - \Phi(r), \] (15)
so the action integral formally reads
\[ \tilde{\mathcal{L}}(W) = \int_{\mathbb{R}} \frac{1}{2} W^2 - \frac{1}{2}(AW)^2 + \Psi(AW) \, d\varphi. \] (16)

Notice that \( \Psi \) is just the difference between the front parabola and \( \Phi \), see Figure 1 and that \( \tilde{\mathcal{L}} \) is well defined as long as \( W \) approaches its asymptotic states sufficiently fast. A further possibility for defining the action integral was introduced in [HR09] for monotone \( W \) and relies on the relative action integral
\[ \tilde{\mathcal{L}}(W) = \int_{\mathbb{R}} \left( \frac{1}{2} W^2 - \Phi(AW) \right) - \left( \frac{1}{2} W_{sh}^2 - \Phi(AW_{sh}) \right) \, d\varphi. \]

Both approaches are linked by \( \tilde{\mathcal{L}}(W) = \tilde{\mathcal{L}}(W) - \tilde{\mathcal{L}}(W_{sh}) \) and the symmetry of \( A \), compare Lemma 7 formally implies
\[ \partial \tilde{\mathcal{L}}(W) = \partial \tilde{\mathcal{L}}(W) = W - A \Phi'(AW). \]

In §3 we give a slightly different definition of \( \tilde{\mathcal{L}} \), see (18) and (23), and establish the existence of minimizers.

3 Existence of fronts

In this section we assume that the asymptotic states and the potential are normalized by (11) and show that the fixed point equation (12) has a solution in some appropriate function space.
3.1 Assumptions

We rely on the following standing assumptions on the function \( \Psi \) from \[15\]. Examples and counterexamples are given in [11].

**Assumption 5.** \( \Psi \) is continuously differentiable and satisfies the following conditions:

\( (G) \) graph condition: \( \Psi(u) \geq \Psi(\pm 1) = 0 \) for all \( u \in \mathbb{R} \),

\( (X) \) genericity: \( \Psi'(\pm 1) > 0 \) and \( \Psi(u) > 0 \) for all \( u \neq \pm 1 \),

\( (M) \) monotone asymptotic behaviour: \( \Psi(u) \) is decreasing for \( u < -1 \) and increasing for \( u > 1 \).

Condition (G) has a natural interpretation in terms of \( \Phi \) and can easily be reformulated for non-normalized data: It precisely means that the front parabola touches the graph of \( \Phi \) in both \( r^- \) and \( r^+ \) but is above this graph in all other points. Moreover, (G) is equivalent to the area condition from [HR09], which characterizes the signed area between the graph of \( \Phi' \) and the secant connecting \( r^- \) to \( r^+ \) with \( r > r^- \) and non-positive in each stripe \([r, r^+]\) with \( r < r^+ \). We refer to Figure 1 for illustration, where positive and negative area are displayed in dark and light grey colour, respectively, and recall that the signed area vanishes in the stripe \([r^-, r^+]\) due to \(10\).

We mention that (G) is truly necessary for the existence of action minimizing fronts, see Remark [12]. The conditions (M) and (X), however, are made for convenience and might be weakened for the price of more technical effort.

**Remark 6.** (X) is equivalent to

\( (S) \) supersonic front speed: \( \Phi''(\pm 1) < 1 \),

and (M) implies

\( (I) \) invariant set for \( \Phi' \): There exits a constant \( \Gamma > 1 \) such that \( \Phi' \) maps \([-\Gamma, \Gamma]\) into itself.

**Proof.** (S) follows from the definition of \( \Psi \) in \[15\]. Towards (I) we exploit (M) to choose \( \hat{\Gamma} > 1 \) such that \( \Phi'(u) > u \) for \( u < -\hat{\Gamma} \) and \( \Phi'(u) < u \) for \( u > \hat{\Gamma} \). Then we set \( \Gamma = \max\{\hat{\Gamma}, \max\{|u| \leq \hat{\Gamma} \mid \Phi'(u)|\}\} \). □

3.2 Functionals and operators

We denote by \( L^p \), \( W^{1,p} \) and \( C^k \) the usual function spaces on the real line, abbreviate the \( L^p \)-norm by \( \| \cdot \|_p \), and write

\[
\langle W_1, W_2 \rangle = \int_{\mathbb{R}} W_1(\varphi)W_2(\varphi) \, d\varphi
\]

for the dual pairing of \( W_1 \in L^p \) and \( W_2 \in L^{p'} \) with \( 1 = 1/p + 1/p' \).

**Lemma 7.** The averaging operator \( \mathcal{A} \) has the following properties:

1. \( \mathcal{A} \) maps \( L^p \) into \( L^\infty \cap W^{1,p} \subset C \) for all \( 1 \leq p \leq \infty \) with

\[
(W)(\varphi) = W(\varphi + \frac{1}{2}) - W(\varphi - \frac{1}{2})
\]

and \( \| \mathcal{A} W \|_{L^p} \leq \| W \|_{L^p} \), \( \| \mathcal{A} W \|_{L^\infty} \leq \| W \|_{L^p} \), \( \| \mathcal{A} W \|_{W^{1,p}} \leq 3 \| W \|_{L^p} \).

2. \( \mathcal{A} \) is symmetric in the sense that \( \langle \mathcal{A} W_1, W_2 \rangle = \langle W_1, \mathcal{A} W_2 \rangle \) holds for all \( W_1 \in L^p \) and \( W_2 \in L^{p'} \).
3. $\mathcal{A}$ is self-adjoint in $L^2$ with spectrum $\text{spec}\mathcal{A} = \{\varrho(k) : k \in \mathbb{R}\}$ where $\varrho(k) = \frac{2}{k^2} \sin \left(\frac{k}{2}\right)$.

**Proof.** The first two statements are straightforward. The third one follows since $\mathcal{A}$ diagonalizes in Fourier space via $\mathcal{A} e^{ik\phi} = \varrho(k) e^{ik\phi}$.

We now introduce the affine space
\[
\mathcal{H} = \{W : W - W_{sh} \in L^2\},
\]
where $W_{sh}$ is the shock profile from (14). Exploiting Lemma 7, the Taylor expansion of $\Phi'$ around $\pm 1$, and the properties of $W_{sh}$ we then find
\[
\mathcal{A}W, \Phi'(\mathcal{A}W), \mathcal{A}\Phi'(\mathcal{A}W) \in \mathcal{H}, \quad W - \mathcal{A}W, W - \mathcal{A}^2 W \in L^2.
\]
(17)

for all $W \in \mathcal{H}$. In view of the action integral (16) we also define a functional $\mathcal{M}$ on $L^2$ by
\[
\mathcal{M}(V) = \frac{1}{2} \int_{\mathbb{R}} V^2 - (\mathcal{A}V)^2 \, d\phi = \frac{1}{2} \int_{\mathbb{R}} (V - \mathcal{A}^2 V) V \, d\phi,
\]
and a functional $\mathcal{N}$ on $\mathcal{H}$ by
\[
\mathcal{N}(W) = \mathcal{M}(W - W_{sh}) + \frac{1}{2} \int_{\mathbb{R}} W_{sh}^2 - (AW_{sh})^2 \, d\phi + \int_{\mathbb{R}} (W - W_{sh})(W_{sh} - \mathcal{A}^2 W_{sh}) \, d\phi.
\]
(18)

Notice that $\mathcal{N}(W)$ is well defined on $\mathcal{H}$ as both $W_{sh}^2 - (AW_{sh})^2$ and $W_{sh} - \mathcal{A}^2 W_{sh}$ have compact support. Moreover, if $W - W_{sh}$ decays sufficiently fast for $\phi \to \pm \infty$ (say $W - W_{sh} \in L^1$), then we have
\[
\mathcal{N}(W) = \frac{1}{2} \int_{\mathbb{R}} W^2 - (\mathcal{A}W)^2 \, d\phi = \frac{1}{2} \int_{\mathbb{R}} (W - \mathcal{A}^2 W) W \, d\phi.
\]
(19)

**Lemma 8.** The functional $\mathcal{M}$ is non-negative and weakly lower semi-continuous on $L^2$.

**Proof.** Denoting the Fourier transform of $V$ by $\hat{V}$ we find
\[
\mathcal{M}(V) = \int_{\mathbb{R}} (1 - \varrho(k)^2) \hat{V}(k)^2 \, dk = \|\sqrt{1 - \varrho^2} \hat{V}\|_2^2
\]
with $\varrho$ as in Lemma 7. This gives the desired result as $V_n \rightharpoonup V_\infty$ implies $\hat{V}_n \rightharpoonup \hat{V}_\infty$ and hence $\sqrt{1 - \varrho^2} \hat{V}_n \rightharpoonup \sqrt{1 - \varrho^2} \hat{V}_\infty$.

**Lemma 9.** The functional $\mathcal{N}$ is Gâteaux differentiable on $\mathcal{H}$ with derivative
\[
\partial \mathcal{N}(W) = W - \mathcal{A}^2 W \in L^2.
\]
(20)

Moreover, $\mathcal{N}$ is invariant under shifts in $\phi$-direction, and satisfies
\[
\mathcal{N}(W_2) = \mathcal{N}(W_1) + \mathcal{M}(W_2 - W_1) + \langle W_2 - W_1, W_1 - \mathcal{A}^2 W_1 \rangle
\]
(21)

for all $W_1, W_2 \in \mathcal{H}$.
Proof. A direct computation with \( W \in H \) and \( \delta W \in L^2 \) shows
\[
\langle \partial N(W), \delta W \rangle = \langle W - W_{sh}, \delta W \rangle - \langle AW - AW_{sh}, A\delta W \rangle + \langle W_{sh} - A^2 W_{sh}, \delta W \rangle
\]
and this gives (20). Towards the shift invariance we approximate \( W \) by \( W_n = \chi_{[-n, n]}(W - W_{sh}) + W_{sh} \) where \( \chi_{[-n, n]} \) is the indicator function of the interval \([-n, n]\). Then we use (19) for \( W_n \) to find \( \mathcal{L}(W_n) = \mathcal{L}(W_n(\cdot + \bar{\varphi})) \) for all shifts \( \bar{\varphi} \), and passing to the limit \( n \to \infty \) gives the desired result.

Finally, by definition we have
\[
\mathcal{N}(W_2) - \mathcal{N}(W_1) = \mathcal{M}(W_2 - W_{sh}) - \mathcal{M}(W_1 - W_{sh}) + \langle W_2 - W_1, W_{sh} - A^2 W_{sh} \rangle
\]
and
\[
\mathcal{M}(W_2 - W_{sh}) - \mathcal{M}(W_1 - W_{sh}) = \mathcal{M}(W_2 - W_1) + \langle W_2 - W_1, W_1 - W_{sh} - A^2 W_1 + A^2 W_{sh} \rangle,
\]
so (24) follows from adding both identities.

To conclude this section we consider the functional
\[
\mathcal{P}(W) = \int_{\mathbb{R}} \Psi(AW) \, d\varphi,
\]
which gives the non-quadratic part of the action integral (16).

**Lemma 10.** \( \mathcal{P} \) is well defined on \( \mathcal{H} \) with
\[
\underline{c} \|AW - \text{sgn}(AW)\|_2 \leq \mathcal{P}(W) \leq \overline{c} \|AW - \text{sgn}(AW)\|_2
\]
for some constants \( \underline{c} \) and \( \overline{c} \) that depend only on \( \|AW\|_\infty \). Moreover, \( \mathcal{P} \) is Gâteaux differentiable on \( \mathcal{H} \) with derivative \( \partial \mathcal{P}(W) = A^2 W - A \Phi'(AW) \).

**Proof.** Let \( W \in \mathcal{H} \) be given and recall that \( U = AW \) satisfies \( U \in \mathcal{H} \cap L^\infty \) due to Lemma 7.

Condition (X) provides two constants \( \underline{c} \) and \( \overline{c} \) such that
\[
\underline{c}(u - \text{sgn}u)^2 \leq \Psi(u) \leq \overline{c}(u - \text{sgn}u)^2
\]
holds for all \( |u| \leq \|U\|_\infty \), and we conclude that \( \mathcal{P} \) is well defined and satisfies (22). Finally, (17) provides \( A^2 W - A \Phi'(AW) \in L^2 \), so both the existence of and the formula for \( \partial \mathcal{P} \) follow from a direct calculation.

### 3.3 Variational setting

We now introduce the action functional on \( \mathcal{H} \) by
\[
\mathcal{L}(W) = \mathcal{N}(W) + \mathcal{P}(W).
\]
In virtue of Lemma 8 and Lemma 10 the functional \( \mathcal{L} \) is well defined, shift invariant, and Gâteaux differentiable with derivative
\[
\partial \mathcal{L}(W) = A^2 W - A \Phi'(AW) \in L^2,
\]
and we conclude that each minimizer of \( \mathcal{L} \) in \( \mathcal{H} \) must solve the front equation \([12]\). However, proving the existence of minimizers in \( \mathcal{H} \) turns out to be difficult and therefore we restrict \( \mathcal{L} \) to the convex subset

\[
\mathcal{C} = \left\{ W \in \mathcal{H} \cap W^{1,\infty} : \|W\|_\infty \leq \Gamma, \quad \|W\|_\infty \leq 2\Gamma \right\}.
\]

Notice that the ansatz \( W \in \mathcal{C} \) is reasonable due to condition \( (I) \) and since the front equation \([12]\) combined with Lemma \([7]\) implies \( W \in \mathcal{H} \cap W^{1,\infty} \).

In order to link fronts to minimizers of \( \mathcal{L} \) in \( \mathcal{C} \) we observe that the properties of \( \Phi' \) and \( A \) guarantee \( \mathcal{C} \) to be invariant under the \( L^2 \)-gradient flow of \( \mathcal{L} \). To see this we consider the explicit Euler scheme

\[
W \mapsto T_\lambda(W) = W - \lambda \partial \mathcal{L}(W) = (1 - \lambda)W + \lambda A\Phi'(AW)
\]

with small step size \( \lambda \).

**Lemma 11.** The set \( \mathcal{C} \) is invariant under the action of \( T_\lambda \) for \( 0 < \lambda < 1 \). Consequently, each minimizer of \( \mathcal{L} \) in \( \mathcal{C} \) solves the front equation \([12]\).

**Proof.** For \( W \in \mathcal{C} \) let \( P = \Phi'(AW) \) and recall that \( AW, P, AP \in \mathcal{H} \) according to \([17]\). Combining \( (I) \) with \( \|AW\|_\infty \leq \Gamma \) and \( \|AP\|_\infty \) gives

\[
\|P\|_\infty, \quad \|AP\|_\infty \leq \Gamma, \quad \|\Phi'(AW)\|_\infty \leq 2\Gamma,
\]

and hence \( AP \in \mathcal{C} \). Since \( \mathcal{C} \) is convex we also have \( T_\lambda(W) \in \mathcal{C} \) for all \( 0 < \lambda < 1 \), and passing to the limit \( \lambda \to 0 \) we then establish the invariance of \( \mathcal{C} \) under the \( L^2 \)-gradient flow of \( \mathcal{L} \). In particular, each minimizer of \( \mathcal{L} \) in \( \mathcal{C} \) must be a stationary point for the gradient flow of \( \mathcal{L} \) and hence a solution to the front equation.

To complete the existence proof for fronts it remains to show that \( \mathcal{L} \) attains its minimum in \( \mathcal{C} \). We prove this in the next section by using the direct approach, that means we construct minimizers as limits of minimizing sequences.

A particular problem we have to overcome in the subsequent analysis is that \( \mathcal{L} \) is not coercive on \( \mathcal{H} \). In fact, as illustrated in Figure \([2]\) there exist sequences \( (W_n)_n \subset \mathcal{C} \) with extending plateaus at \(-1\) or \(+1\). These plateaus contribute neither to \( \mathcal{N} \) nor \( \mathcal{P} \) but may imply

\[
\|W_n - W_{sh}(\varphi_n + \cdot)\|_2 \xrightarrow{n \to \infty} \infty
\]

for all choices of the relative shifts \( \varphi_n \). Heuristically it is clear that the cartoon from Figure \([2]\) cannot be prototypical for action minimizing sequences, but in order to proof this we need a better understanding of sequences with bounded action.

We conclude with a remark about the necessity of the graph condition \( (G) \) and refer to \([4]\) for numerical examples.

**Remark 12.** Suppose that \( \Psi \) satisfies \( (M) \), \( (X) \), and \( \Psi(\pm 1) = 0 \), but violates \( (G) \) because there is some \( u_\ast \) with \( |u_\ast| < \Gamma \) and \( \Psi(u_\ast) < 0 \). Then \( \mathcal{L} \) is unbounded from below.

**Proof.** We define a sequence \( (W_n)_n \subset \mathcal{H} \) of piecewise linear profiles by \( W_n(\varphi) = u_\ast \) for \( |\varphi| \leq n \) and \( W_n(\varphi) = \text{sgn} \varphi \) for \( |\varphi| \geq n + 1/\Gamma \). By construction, \( W_n - A^2W_n \) is supported in \( I_n \cup (-I_n) \) with \( I_n = [n - 1, n + 1 + \Gamma] \), and a direct calculation shows

\[
\mathcal{L}(W_n) \leq C + 2(n - 1)\Psi(u_\ast) \xrightarrow{n \to \infty} -\infty,
\]

where \( C \) is some constant independent of \( n \). \( \square \)
Figure 2: Sketch of a sequence with bounded action and two extending plateaus at ±1: graphs of $W_n$ and $U_n = AW_n$ in Black in Gray, respectively. The shaded areas indicate corresponding separations of phases with $I_{n,j} = \varphi_{n,j} + J_j$ as in Lemma 15.

3.4 Separation of phases for sequences with bounded $P$

To characterize the qualitative properties of a profile $U = AW$ with $W \in C$ we interpret $U < \frac{1}{2}$ and $U > \frac{1}{2}$ as negative phase and positive phase, respectively, and regard intervals in which $U$ takes intermediate values as transition layers. Obviously, adjacent plateaus of different height are separated by a transition layer and each $U$ must exhibit at least one transition layer as it connects $-1$ to $+1$.

We next exploit the uniform $L^\infty$-bound for $W \in C$ to derive a lower bound for the $P$-contribution of each transition layer. To this end we introduce

$$Z_U = \{ \bar{\varphi} : |U(\bar{\varphi})| \leq \frac{1}{2} \}.$$

which is nonempty, closed and bounded as $U \in C$ is continuous with $U(\varphi) \to \pm 1$ as $\varphi \to \pm \infty$.

**Remark 13.** There exist constants $\bar{\eta} > 0$ and $\bar{\mu} > 0$ such that

$$\int_{\bar{\varphi} - \bar{\eta}}^{\bar{\varphi} + \bar{\eta}} \Psi(U(\varphi)) \, d\varphi > \bar{\mu}$$

for each $U \in C$ and $\bar{\varphi} \in Z_U$.

**Proof.** This follows since $U \in C$ implies $|U(\varphi_2) - U(\varphi_1)| \leq \int_{\varphi_2}^{\varphi_1} |U'(\varphi)| \, d\varphi \leq 2\Gamma|\varphi_2 - \varphi_1|$. In particular, we have $|U(\varphi)| \leq 3/4$ for all $|\varphi - \bar{\varphi}| \leq \bar{\eta} = 1/(8\Gamma)$ and the claim follows with $\bar{\mu} = \bar{\sigma}/(2\bar{\eta})$ and $\bar{\sigma} = \sup_{|u| \leq 3/4} \Psi(u) > 0$.

In order to show that each function $U$ possesses a finite number of transition layers we introduce the following definition. A *separation of phases* for a given profile $U \in C$ is a finite collection of closed intervals (transition layers) $I_1, \ldots, I_m, m \geq 1$, such that

1. the intervals are disjoint and ordered, i.e.,

$$\min I_1 < \max I_1 < \min I_2 < \ldots < \max I_{m-1} < \min I_m < \max I_m,$$

2. $Z_U$ is contained in $I_1 \cup \ldots \cup I_m$. 

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3. for each interval $I_j$ there exists $\bar{\varphi}_j \in \mathbb{Z}_U$ such that with $[\bar{\varphi}_j - \bar{\eta}, \bar{\varphi}_j + \bar{\eta}] \subset I_j$,

**Lemma 14.** Let $W \in \mathcal{C}$ be given and set $U = AW$. Then there exists a separation of phases $I_1, ..., I_m$ for $U$ with

$$m \leq \text{floor}(\mathcal{P}(W)/\bar{\mu}) \quad \text{and} \quad 2\bar{\eta} \leq |I_j| \leq 4\mathcal{P}(W)\bar{\eta}/\bar{\mu}$$

for all $j = 1, ..., m$.

**Proof.** We define a finite number of points $\bar{\varphi}_j \in \mathbb{Z}_U$ and intervals $I_j = (\bar{\varphi}_j - 2\bar{\eta}, \bar{\varphi}_j + 2\bar{\eta})$ iteratively as follows: $\bar{\varphi}_1$ is the smallest element of $\mathbb{Z}_U$, i.e., $U(\varphi) < -\frac{1}{2}$ for all $\varphi < \bar{\varphi}_1$. If $\mathbb{Z}_U \setminus I_1$ is empty we stop the iteration; otherwise we choose $\bar{\varphi}_2$ to be the smallest zero of $\mathbb{Z}_U$ outside of $I_1$. Then we have $\bar{\varphi}_2 - \bar{\varphi}_1 \geq 2\bar{\eta}$, so Remark 13 yields

$$\mathcal{P}(W) \geq \int_{\bar{\varphi}_1 - \bar{\eta}}^{\bar{\varphi}_1 + \bar{\eta}} \Psi(U(\varphi)) \, d\varphi + \int_{\bar{\varphi}_2 - \bar{\eta}}^{\bar{\varphi}_2 + \bar{\eta}} \Psi(U(\varphi)) \, d\varphi \geq 2\bar{\mu}.$$ 

If possible, we now define $\bar{\varphi}_3$ as the minimum of $\mathbb{Z}_U \setminus (I_1 \cup I_2)$ and proceed iteratively until the iteration stops after $m \leq \text{floor}(\mathcal{P}(W)/\bar{\mu})$ steps. By construction, we have $\mathbb{Z}_U \subset \bigcup_{j=1}^{m} I_j$ and $|I_j| \leq 4\bar{\eta}$ for all $j$ but the intervals $I_j$ may overlap. Finally, we obtain the desired separation of phases by merging overlapping intervals. \qed

Our main result in this section concerns sequences $(W_n)_n \in \mathcal{C}$ with bounded $\mathcal{P}(W_n)$. It guarantees, roughly speaking, the existence of compatible transitions layers which (i) have the same length, (ii) separate the same phases, and (iii) depart from each other. For an illustration we refer to Figure 2.

**Lemma 15.** Let $(W_n)_n \subset \mathcal{C}$ be a sequence with $\limsup_{n \to \infty} \mathcal{P}(W_n) < \infty$. Then there exists a not relabelled subsequence along with a finite number of intervals $J_1, ..., J_m$ with the following properties:

1. Each interval $J_j$ is centred around zero, i.e., $J_j = [-\eta_j, \eta_j]$ for some $0 < \eta_j < \infty$.
2. For each $n$ there exist shifts $\varphi_{n,1} < ... < \varphi_{n,m}$ such that
   
   (a) $\varphi_{n,1} + J_1, ..., \varphi_{n,m} + J_m$ is a separation of phases for $U_n = AW_n$,
   
   (b) $\varphi_{n,j+1} - \varphi_{n,j} \to \infty$ as $n \to \infty$ for all $j = 1, ..., m - 1$.
3. There exists a choice of signs $s_0, ..., s_m$ with $s_0 = -1, s_m = 1$, and $s_j \in \{-1, +1\}$ such that

   $$\begin{align*}
   \text{sgn}(U_n(\varphi)) &= s_0 \quad \text{for} \quad \varphi < \varphi_{n,1} - \eta_1 \\
   \text{sgn}(U_n(\varphi)) &= s_1 \quad \text{for} \quad \varphi_{n,1} + \eta_1 < \varphi < \varphi_{n,2} - \eta_2 \\
   \text{...} \\
   \text{sgn}(U_n(\varphi)) &= s_{m-1} \quad \text{for} \quad \varphi_{n,m-1} + \eta_{m-1} < \varphi < \varphi_{n,m} - \eta_m \\
   \text{sgn}(U_n(\varphi)) &= s_{m+1} \quad \text{for} \quad \varphi_{n,m} + \eta_m < \varphi
   \end{align*}$$

   hold for all $n$.

**Proof.** Thanks to Lemma 14 we can extract a subsequence such that each $U_n$ has a separation of phases that consists of $m$ intervals $I_{n,1}, ..., I_{n,m}$ where $m$ is independent of $n$. We denote the centre of $I_{n,j}$ by $\bar{\varphi}_{n,j}$, set $J_{n,j} = I_{n,j} - \varphi_{n,j}$, and notice that $\xi \leq |J_{n,j}| \leq \overline{\tau}$ and $\varphi_{n,j+1} - \varphi_{n,j} > \xi$ for some constants $\overline{\tau} > \xi > 0$ independent of $n$ and $j$. In particular, the intervals $J_j = \bigcup_{n} J_{n,j}$ have finite length $\overline{\tau} \leq |J_j| \leq \overline{\tau}$.

Our strategy for the proof is to refine $m$, the subsequence $(W_n)_n$, the phase shifts $\varphi_{n,j}$, and the intervals $J_j$ in several steps. To this end we start the following algorithm at level 1.
Level $k$

If $m = k$, then we stop the algorithm.

If $\varphi_{n,k+1} - \varphi_{n,k} \to \infty$ as $n \to \infty$ along a subsequence, then we extract this subsequence and jump to level $k + 1$.

If $m < k$ and $0 < \sup_n (\varphi_{n,k+1} - \varphi_{n,k}) < \infty$, then we merge $J_k$ and $J_{k+1}$ as follows: At first we choose $\tilde{J}_k$ sufficiently large such that

$$\tilde{J}_k \supseteq J_k \cup \bigcup_n (\varphi_{n,k+1} - \varphi_{n,k} + J_{k+1}).$$

Secondly we define $\tilde{\varphi}_{n,k} = \varphi_{n,k}$, $\tilde{m} = m - 1$ and

$$\tilde{J}_j = J_j \quad \text{and} \quad \tilde{\varphi}_{n,j} = \varphi_{n,j} \quad \text{for} \quad j < k,$$

$$\tilde{J}_j = J_{j+1} \quad \text{and} \quad \tilde{\varphi}_{n,j} = \varphi_{n,j+1} \quad \text{for} \quad j > k.$$

Finally we restart level $k$ with $\tilde{m}$, $\tilde{\varphi}_{n,j}$, and $\tilde{J}_j$ instead of $m$, $\varphi_{n,j}$, and $J_j$.

This algorithm stops after a finite number of steps when $m - k = 0$. It provides intervals $J_j$ and phase shifts $\varphi_{n,j}$ for $j = 1..m$ and $n \in N$ with $\lim_{n \to \infty} \varphi_{n,j+1} - \varphi_{n,j} = \infty$ for all $j$. By extracting subsequences we can also ensure that, for each $n$, the intervals $\varphi_{n,j} + J_{n,j}$ are pairwise disjoint and provide therefore a separation of phases for $U_n$. Finally, by extracting further subsequences if necessary we guarantee the existence of a choice of signs.

3.5 Existence of minimizers for $\mathcal{L}$

We now finish the existence proof for fronts.

**Theorem 16.** $\mathcal{L}$ attains its minimum on $\mathcal{C}$ and each minimizer is a front.

**Proof.** Step 0. We start with some notations. For a given minimizing sequence $(W_n)_n \subset \mathcal{C}$ we define

$$U_n = AW_n, \quad S_n = \text{sgn}U_n,$$

and for each $K > 0$ we introduce the operator

$$E_K : \mathcal{C} \to \mathcal{C}, \quad E_K W = \chi_{[-K,K]}(W - W_{sh}) + W_{sh}.$$ 

Here $\chi_{[-K,K]}$ denotes the usual indicator function, so we have $\|E_K W - W\|_2 \to 0$ as $K \to \infty$ for each $W \in \mathcal{C}$. Finally, within this proof $C$ always denotes a positive constant that is independent of $n$ and $K$, but the value of $C$ may change from line to line.

Step 1. By assumption and $\mathcal{M}(W_n - W_{sh}) \geq 0$ we have

$$\mathcal{P}(W_n) = \mathcal{L}(W_n) - \mathcal{N}(W_n) \leq C + \|W - W_{sh}\|_\infty \|W_{sh} - \mathcal{A}^2 W_{sh}\|_1 \leq C. \quad (25)$$

Therefore we can extract (a not relabelled) subsequence for which Lemma 15 provides a finite number of intervals $J_1...J_m$, sequences of phase shifts $(\varphi_{n,j})_n$ and a choice of signs $(s_{n,j})_n$. There exits at least one $1 \leq j_* \leq m$ such that $s_{j_*-1} = -1$ and $s_{j_*} = +1$, and since $\mathcal{L}$ is invariant under shifts we can assume that $\varphi_{n,j_*} = 0$. With $J_{j_*} = [-\eta_{j_*}, \eta_{j_*}]$ and due to $\lim_{n \to \infty} \varphi_{n,j_*+1} - \varphi_{n,j_*} = \infty$ we then have

$$\lim_{n \to \infty} \sup U_n(\varphi) \leq -\frac{1}{2} \quad \text{for} \quad \varphi < -\eta_{j_*}, \quad \lim_{n \to \infty} \inf U_n(\varphi) \geq \frac{1}{2} \quad \text{for} \quad \varphi > \eta_{j_*}.$$
By compactness we can extract a further subsequence such that \( W_n \to W_\infty \) weakly* in \( W^{1, \infty} \). In particular, \( W_n \) converges to \( W_\infty \) uniformly on each compact interval, and hence

\[
E_K W_n \xrightarrow{n \to \infty} E_K W_\infty, \quad E_K U_n \xrightarrow{n \to \infty} E_K U_\infty \quad \text{strongly in } L^2 \text{ for all } K.
\] (26)

**Step 2.** Towards \( W_\infty \in \mathcal{C} \) we show that \( W_n - S_n \) is uniformly bounded in \( L^2 \). The first observation is that (25) combined with (22) implies

\[
\| U_n - S_n \|_2 \leq C. \tag{27}
\]

The second observation is that both \( S_n - \mathcal{A} S_n \) and \( S_n - \mathcal{A}^2 S_n \) are supported in the 1-neighbourhood of \( I_n = \bigcup_{j=1}^n (J_j + \varphi_{n,j}) \). Therefore, \( |I_n| \leq \sum_{j=1}^n |J_j| \leq C \) yields

\[
\| S_n - \mathcal{A} S_n \|_2 \leq C, \quad \| S_n - \mathcal{A}^2 S_n \|_1 \leq C, \quad |\mathcal{N}(S_n)| = |\langle S_n - \mathcal{A}^2 S_n, S_n \rangle| \leq C,
\]

and by (27) we find

\[
\| U_n - \mathcal{A} S_n \|_2 \leq \| U_n - S_n \|_2 + \| S_n - \mathcal{A} S_n \|_2 \leq C. \tag{28}
\]

Exploiting (21) for \( W_2 = W_n \) and \( W_1 = S_n \) gives

\[
\mathcal{M}(W_n - S_n) = \mathcal{N}(W_n) - \mathcal{N}(S_n) - \langle W_n - S_n, S_n - \mathcal{A}^2 S_n \rangle \\
\leq \mathcal{L}(W_n) + |\mathcal{N}(S_n)| + (\| W_n \|_\infty + \| S_n \|_\infty) \| S_n - \mathcal{A}^2 S_n \|_1 \leq C,
\]

and with (28) we obtain

\[
\| W_n - S_n \|_2^2 = \mathcal{M}(W_n - S_n) + \| U_n - \mathcal{A} S_n \|_2^2 \leq C. \tag{29}
\]

Now we are able to show \( W_\infty \in \mathcal{C} \). From (29) we infer that

\[
\| E_K W_n - W_{sh} \|_2 \leq \| E_K W_n - E_K S_n \|_2 + \| E_K S_n - E_K W_{sh} \|_2 \leq C + \| E_K S_n - E_K W_{sh} \|_2,
\]

and with \( S_n(\varphi) \to W_{sh}(\varphi) \) as \( n \to \infty \) for all \( \varphi \neq J_j \), we find

\[
\| E_K W_\infty - W_{sh} \|_2 \leq C.
\]

Passing to the limit \( K \to \infty \) now gives \( W \in \mathcal{H} \), and \( W \in \mathcal{C} \) follows because \( W_\infty \) was defined as weak* limit in \( W^{1, \infty} \).

**Step 3.** There remains to show that \( W_\infty \) minimizes \( \mathcal{L} \). From (21) we infer that

\[
\mathcal{N}(W_n) = \mathcal{N}(E_K W_n) + \mathcal{M}(W_n - E_K W_n) + \langle W_n - E_K W_n, E_K W_n - \mathcal{A}^2(E_K W_n) \rangle \tag{30}
\]

and

\[
|\mathcal{N}(E_K W_n) - \mathcal{N}(E_K W_\infty)| \leq \mathcal{M}(E_K W_n - E_K W_\infty) + \| E_K W_n - E_K W_\infty \|_2 \| E_K W_\infty - \mathcal{A}^2(E_K W_\infty) \|_2 \tag{31}
\]

hold for all \( K \) and \( n \in \mathbb{N} \cup \{ \infty \} \). Combining (31) with (20) gives

\[
\mathcal{N}(E_K W_n) \xrightarrow{n \to \infty} \mathcal{N}(E_K W_\infty).
\]

Moreover, since \( E_K W_n - \mathcal{A}^2(E_K W_n) \) is supported in \([-K - 1, K + 1]\) for all \( n \), we also have

\[
\langle W_n - E_K W_n, E_K W_n - \mathcal{A}^2(E_K W_n) \rangle \xrightarrow{n \to \infty} \langle W_\infty - E_K W_\infty, E_K W_\infty - \mathcal{A}^2(E_K W_\infty) \rangle,
\]

and

\[
\| E_K W_n - E_K W_{sh} \|_2 \leq C.
\]

The first observation follows because

\[
\| E_K W_n - E_K W_{sh} \|_2 \leq \| E_K W_n - E_K S_n \|_2 + \| E_K S_n - E_K W_{sh} \|_2 \leq C + \| E_K S_n - E_K W_{sh} \|_2.
\]

and with \( S_n(\varphi) \to W_{sh}(\varphi) \) as \( n \to \infty \) for all \( \varphi \neq J_j \), we find

\[
\| E_K W_\infty - W_{sh} \|_2 \leq C.
\]
and passing to the limit \( n \to \infty \) in (30) provides

\[
\liminf_{n \to \infty} \mathcal{N}(W_n) \geq \mathcal{N}(E_K W_\infty) + \langle W_\infty - E_K W_\infty, E_K W_\infty - \mathcal{A}^2(E_K W_\infty) \rangle,
\]

where we used that \( \mathcal{M}(W_n - E_K W_n) \geq 0 \) according to Lemma 8. On the other hand, evaluating (30) for \( n = \infty \) gives

\[
\mathcal{N}(W_\infty) = \mathcal{N}(E_K W_\infty) + \mathcal{M}(W_\infty - E_K W_\infty) + \langle W_\infty - E_K W_\infty, E_K W_\infty - \mathcal{A}^2(E_K W_\infty) \rangle
\]

and due to \( \mathcal{M}(W_\infty - E_K W_\infty) \to 0 \) as \( K \to \infty \) we find

\[
\mathcal{N}(E_K W_\infty) + \langle W_\infty - E_K W_\infty, E_K W_\infty - \mathcal{A}^2(E_K W_\infty) \rangle \xrightarrow{K \to \infty} \mathcal{N}(W_\infty).
\]

The combination of (32) and (33) reveals

\[
\liminf_{n \to \infty} \mathcal{N}(W_n) \geq \mathcal{N}(W_\infty),
\]

and Fatou’s Lemma provides

\[
\liminf_{n \to \infty} \mathcal{P}(W_n) \geq \mathcal{P}(W_\infty)
\]

due to \( \Psi \geq 0 \) and since \( W_n \) converges to \( W_\infty \) pointwise. Adding (34) and (35) we conclude that \( W_\infty \) is in fact a minimizer of \( \mathcal{L} \), and Lemma 11 guarantees that \( W_\infty \) solves the front equation (12).

We conclude with some remarks.

1. Theorem 1 follows by combining Lemma 2, Lemma 4, Lemma 11, Remark 12, and Theorem 16.

2. The assertions of Theorem 16 can be sharpened as follows. For each minimizing sequence \( (W_n)_n \) we have equality signs in both (34) and (35), and hence

\[
\lim_{K \to \infty} \lim_{n \to \infty} \mathcal{M}(W_n - E_K W_n) = 0.
\]

This implies that there is only one interval \( J_1 = J_{j_*} \) and in turn that \( W_n - W_\infty \to 0 \) strongly in \( L^2 \). In this sense each minimizing sequence obeys exactly one transition from negative phase to positive phase.

3. If \( \Phi' \) is increasing in \([-1, +1]\) we can improve the existence result for fronts as follows. We choose \( \Gamma = 1 \) in (I) and consider the set

\[
\tilde{C} = \{ W \in C : W' \geq 0 \}.
\]

Then \( \tilde{C} \) is an invariant set for the gradient flow of \( \mathcal{L} \) and again one can show that \( \mathcal{L} \) restricted to \( \tilde{C} \) attains its minimum (a proof tailored to monotone profiles is given in [HR09]). In particular, in this case there exist action minimizing fronts with monotone profile \( W \).
4 Approximation of fronts

In this section we illustrate the analytical results from §3 by some numerical simulations. To this end we discretize the Euler scheme for the gradient flow of $L$, see (24), as follows:

1. Fix a finite interval $[-L, +L]$ and introduce equidistant grid points by $\varphi_k = -L + 2kL/D$, where $k = 0, \ldots, D$ and $D \in \mathbb{N}$ is large.

2. Approximate each profile $W \in C$ by the discrete vector $W_i = W(\varphi_i)$ and impose the boundary conditions $W_i = -1$ and $W_i = +1$ for $i < 0$ and $i > D$, respectively.

3. Replace the integrals in the definition of $A$ by Riemann sums with respect to the $\varphi_i$'s.

4. Choose $\lambda$ sufficiently small and initialize the iteration (24) with shock initial data $W_i = \text{sgn} \varphi_i$.

Figure 3: Three examples with admissible potential as in Assumption 5 where $\Phi'$ is plotted in the invariant interval. During the iteration the profiles $W$ converge to a front.

Figure 4: Potentials $\Phi$ with front parabolas for the examples from Figure 3 (top row) and 5 (bottom row).
Figure 5: Three counterexamples for the existence of action minimizing fronts. The first two examples satisfy the macroscopic constraints but violate the graph condition (G), so the iteration minimizes the action via an extending plateau. The third example violates the constraint $\Phi(+1) = \Phi(-1)$, so the profiles converge to one of the asymptotic states.

In numerical simulations, the resulting iteration scheme has good convergence properties and decreases the action provided that $\lambda$ is sufficiently small and $L$ is sufficiently large. Three examples with normalized front data and $\Phi$ as in Assumption 5 are shown in Figure 3, where $\Phi'$ is always plotted over the invariant interval $[-\Gamma, \Gamma]$. For plots of $\Phi$ see Figure 4. In the first example $\Phi'$ is increasing in $[-1, 1]$ and the front profile $W$ turns out to be monotone. We refer to the remark at the end of §3 for an explanation, and to [HR09] for more examples. The other two examples in Figure 3 illustrate that the front profiles for non-convex $\Phi$ are in general non-monotone.

In order to illustrate the necessity of the graph condition (G) we present in Figure 5 simulations for potentials that violate this condition. In the first example the interval $[-1, 1]$ is invariant under $\Phi'$ but $\Psi$ is negative in this interval. After some initial iterations the profiles exhibit an extending plateau at $-1 < w_* < 1$, where $w_*$ is the minimizer of $\Psi$ in $[-1, 1]$ and satisfies $w_* = \Phi'(w_*)$. The onset of the extending plateau is a direct consequence of the energy landscape of $L$, see Remark 12. The second simulation provides another counterexample for the existence of action minimizing fronts. Here $\Psi$ has the correct sign close to $\pm1$ but attains again a negative minimum in $-1 < w_* < 1$. As before, the profiles minimize their action by converging to the ‘global minimizer’ $W \equiv w_*$. Finally, the third example illustrates what happens if the asymptotic states violate the macroscopic constraints. More precisely, here we violate (10) due to $\Phi(+1) > \Phi(-1)$, and observe that the profiles converge to the global minimizer $W \equiv +1$. 
Acknowledgements

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