Oscillatory Waves in Discrete Scalar Conservation Laws

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Abstract

We study Hamiltonian difference schemes for scalar conservation laws with monotone flux function and establish the existence of a three-parameter family of periodic travelling waves (wavetrains). The proof is based on an integral equation for the dual wave profile and employs constrained maximization as well as the invariance properties of a gradient flow. We also discuss the approximation of wavetrains and present some numerical results.

Keywords: conservation laws, difference schemes, dispersive shocks, travelling waves, Hamiltonian lattices, variational integrators

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1 Introduction

This paper is concerned with oscillatory patterns in the nonlinear lattice equation

\[ 2 \dot{u}_j + \Phi'(u_{j+1}) - \Phi'(u_{j-1}) = 0, \quad u \in \mathbb{R}, \quad t \geq 0, \quad j \in \mathbb{Z}, \]  

which is, up to an appropriate scaling, a centred difference scheme for the scalar conservation law

\[ \partial_\tau \bar{u} + \partial_\xi \Phi'(\bar{u}) = 0, \quad \bar{u} \in \mathbb{R}, \quad \tau \geq 0, \quad \xi \in \mathbb{R}. \]  

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Although the lattice cannot be used for the approximate computation of (non-smooth) solutions of (2), there exist several reasons why it seems worth investigating the dynamical properties of (1) in greater detail. First, both the lattice and the PDE have the same Hamiltonian structure, and (1) can be regarded as a variational integrator for (2) with respect to the space discretization, see appendix A. Studying (1) therefore allows to understand in which aspects quasilinear Hamiltonian PDEs differ from their spatially discrete counterparts. Second, the lattice is, similar to Korteweg-de Vries-type (KdV) equations, a dispersive regularization of (2), and hence it generates dispersive shocks instead of Lax shocks. These dispersive shocks describe the fundamental mode of self-thermalization in dispersive Hamiltonian systems but are well understood only for systems that are completely integrable. The ODE system (1) provides a class of non-integrable examples which can be simulated effectively, for instance using variational integrators for the time discretization. Finally, discrete conservation laws provide toy models for more complicate Hamiltonian lattices. Fermi-Pasta-Ulam (FPU) chains, for instance, are equivalent to difference schemes for the so called p-system, which is a nonlinear hyperbolic system of two conservation laws.

In what follows we focus on a particular aspect of the lattice dynamics and investigate special coherent structures, namely wavetrains. These are periodic travelling wave solutions to (1) and therefore linked to nonlinear advance-delay-differential equations.

We emphasize that all subsequent considerations require a centred difference operator in (1) as only this one gives rise to a Hamiltonian lattice. Other discrete scalar conservation laws, as for instance upwind schemes, have different dynamical properties and are excluded.

1.1 Dispersive shocks and wavetrains

The relation between (1) and (2) manifests under the hyperbolic scaling

\[ \tau = \varepsilon t, \quad \xi = \varepsilon j, \quad u_j(t) = \bar{u}(\varepsilon t, \varepsilon j), \] (3)

where \(0 < \varepsilon \ll 1\) is the scaling parameter, and \(\tau\) and \(\xi\) denote the macroscopic time and particle index, respectively. On a formal level we can expand differences in powers of differential operators, i.e.,

\[ \bar{u}(\xi + \varepsilon) - \bar{u}(\xi - \varepsilon) = 2\partial_\xi \bar{u}(\xi) + \frac{1}{6}\varepsilon^2 \partial_\xi^2 \bar{u}(\xi) + O(\varepsilon^5), \]

so that, to leading order in \(\varepsilon\), the lattice dynamics is governed by the KdV-type PDE

\[ \partial_\tau \bar{u} + (\partial_\xi + \frac{1}{6}\varepsilon^2 \partial_\xi^2) \Phi'\bar{u} = 0, \]

which is in fact a dispersive regularization of (2).

As already mentioned, a key feature of all dispersive regularizations of (2) are dispersive shocks.\[^{17, 18, 20, 25}\] For illustration, and to motivate our analytical investigations, we now describe the formation of such dispersive shocks in numerical simulations of (1). For convenience we shall consider spatially periodic solutions with \(u_j = u_{j+N}\) for some \(N \gg 1\), which then defines the natural scaling parameter \(\varepsilon = 1/N\). Starting with long-wave-length initial data

\[ u_j(0) = \bar{u}_{\text{lin}}(j/N), \]
Figure 1: Numerical lattice solution with periodic boundary conditions for the data from (4): Snapshots of $u_j$ against the macroscopic particle index $j/N$ at several macroscopic times $\tau$; the vertical lines in the lower right picture mark the positions for the magnifications in Figure 2. Interpretation: Instead of Lax shocks the lattice generates dispersive shocks with strong microscopic oscillations.

Figure 2: Magnifications of the oscillations from Figure 1 in three selected points: Black points are numerical data, Grey curves represent interpolating splines and are drawn for better illustration. Interpretation: The microscopic oscillations can be described by a modulated travelling wave. In other words, the local oscillations are generated by a single wavetrain whose parameters change on the macroscopic scale.

where $\bar{u}_{ini}$ is a smooth and 1-periodic function in $\xi$, we can solve (1) numerically by using the variational integrator (28). A typical example is depicted in Figure 1 for the data

$$
\Phi(u) = \frac{1}{2} u^2 + \frac{1}{4} u^4, \quad N = 4000, \quad \bar{u}_{ini}(\xi) = 1 - \frac{13}{20} \sin (2\pi \xi).
$$

(4)

For small macroscopic times $\tau$, we observe that the data remain in the long-wave-length regime, so we can expect that the lattice solutions converge as $\varepsilon \to 0$ in some strong sense to a smooth solution of (2). This convergence is not surprising in view of Strang’s theorem[29], see also the discussion in Ref. [11, 17]. At time $\tau \approx 0.04$, however, the solution to the PDE (2) forms a Lax shock, which then propagates with speed $s$ according to the Rankine-Hugoniot jump condition $s [\bar{u}] = [\Phi'(\bar{u})]$. After the onset of the shock singularity, the lattice solutions do not converge anymore to a solution of (2), not even in a weak sense, but exhibit strong microscopic oscillations. These oscillations spread out in space and time, and constitute the dispersive shock. This phenomenon is fascinating from both the mathematical and the physical point of view because the formation of dispersive shocks can be regarded as a self-thermalization of the nonlinear Hamiltonian system. We refer to Ref. [4, 16] for more details including a thermodynamic discussion of dispersive FPU shocks.
The observation that certain difference schemes for hyperbolic conservation laws produce dispersive shocks is not new, see for instance Ref. [22][11], which investigate dispersive shocks in

\[ 2 \dot{v}_j + v_j(v_{j+1} - v_{j-1}) = 0. \]

This lattice also belongs to the class of equations considered here as it transforms via \( u_j = \ln v_j \) into (1) with \( \Phi' = \exp \), which is the completely integrable Kac-von Moerbeke lattice [20].

The key observation in our context is that the oscillations within a dispersive shock exhibit the typical behaviour of a modulated oscillation. As illustrated in Figure 2, the local oscillations in the vicinity of a given macroscopic point \( (\tau, \xi) \) resemble a periodic profile function, and we can expect this profile to be generated by a single wavetrain. The parameters of this wavetrain, however, depend on \( \tau \) and \( \xi \), which can be seen from the fact that each magnification in Figure 2 displays another amplitude, wave number, and average.

The goal of this paper is to prove the existence of a three-parameter family of wavetrains for a huge class of nonlinear potentials \( \Phi \). Since the only crucial assumption we have to make is strict convexity of \( \Phi \), our results cover a large number of non-integrable variants of (1). Due to rigorous results for integrable systems, such as the KdV equation [23][24] and the Toda chain [21][2], we expect the parameter modulation within a dispersive shock to be governed by a variant of Whitham’s modulation equations [30][31]. The formal derivation and investigation of this Whitham system, however, is left for future research. We also do not justify that the oscillations within dispersive shocks take in fact the form of modulated wavetrains. For a rigorous proof in non-integrable systems we still lack the analytical tools; a reliable numerical justification would be possible, and was carried out for FPU in Ref. [4], but is beyond the scope of this paper.

A travelling wave is a special solution to (1) with

\[ u_j(t) = U(kj - \omega t), \]

where \( k \) is the wave number, \( \omega \) is the frequency, and the profile \( U \) depends on the phase variable \( \varphi = kj - \omega t \). In this paper we are solely interested in wavetrains, which have periodic \( U \), but mention that one might also study solitons and fronts having homoclinic and heteroclinic profiles, respectively.

Splitting \( U \) into its constant and zero average part via \( U(\varphi) = v + V(\varphi) \), we infer from (1) that each wavetrain satisfies

\[ \omega \frac{d}{d\varphi} V = \nabla_k \Phi'(v + V), \]

where \( \nabla_k \) is defined by

\[ (\nabla_k P)(\varphi) = \frac{1}{2}(P(\varphi + k) - P(\varphi - k)). \]

1.2 Main result and organisation of the paper

Since the wavetrain equation (1) involves both advance and delay terms there is no notion of an initial value problem, and one has to use rather sophisticated methods to establish the
Figure 3: Numerical lattice solution for $N = 4000$, $\Phi'(u) = u^2$ and $\bar{u}_{ini}(\xi) = \sin(2\pi\xi)$.

**Interpretation**: If $\Phi''$ changes sign, the lattices can generate modulated binary oscillation instead of dispersive shocks.

existence of solutions. Possible candidates, which have proven to be powerful for other Hamiltonian lattices, are rigorous perturbation arguments, spatial dynamics with centre manifold reduction, critical point techniques, and constrained optimization.

Our approach also exploits the underlying variational structure and restates (6) as

$$\sigma \Psi'(Q) - \sigma \eta = BQ,$$

where $Q$ is the dual profile to be introduced in §2.2. Moreover, $B$ is a compact and symmetric integral operator, and $\Psi$ is the dual potential, i.e., the Legendre transform of $\Phi$. This formulation allows to construct wavetrains as solutions to a constrained optimization problem, where $\sigma$ and $-\sigma \eta$ play the role of Lagrangian multipliers.

The existence proof for wavetrains given below is based on a combination of variational arguments (direct method) and dynamical concepts (invariant sets of flows). These ideas can also be applied to other Hamiltonian lattices and different types of coherent structures, but discrete scalar conservation laws are special since they are first order in time and real-valued. All other Hamiltonian lattices we are aware of are either second order in time or vector-valued, and allow for a simpler variational setting for travelling waves.

Our main result guarantees the existence of a three-parameter family of wavetrains and can be summarized as follows.

**Main result.** Suppose that $\Phi$ is strictly convex and satisfies some regularity assumptions. Then, for each $k \in (0, \pi)$ there exists a two-parameter family of $2\pi$-periodic wavetrains with $v \in \mathbb{R}$ and frequency $\omega > 0$ such that the profile $V$ is even and unimodal on $[-\pi, \pi]$.

The assumptions on $\Phi$ will be specified in Assumption 2 and the precise existence result is formulated in Theorem 8. Here we proceed with some comments concerning the choice of $k$ and the convexity of $\Phi$.

1. Since (5) is invariant under $(k, \omega) \sim (-k, -\omega)$, there is a similar result for $k \in (-\pi, 0)$ with $\omega < 0$. The cases $k = 0$ and $k = \pm \pi$, however, are degenerate, see §2.1.

2. As time reversal in (1) corresponds to $(k, \omega) \sim (k, -\omega)$, the existence result can easily be adapted to the case of strictly concave $\Phi$.

3. Our proof does not cover potentials $\Phi$ that change from convex to concave or vice versa, and it is not obvious what happens near zeros of $\Phi''$. Numerical simulations as presented in Figure 3, however, indicate that then a three-parameter families of wavetrains might not exist anymore.
The paper is organized as follows. In §2 we summarize some elementary properties of wave-trains. We also derive the integral equation for the dual profile and discuss some normalization which allows to simplify the presentation. §3 is devoted to the proof of the existence result. To point out the key idea we first state an abstract result in Theorem 3 and show afterwards that the assertions we made are satisfied for wavetrains, see Theorem 8. Finally, in §4 we compute wave-trains by means of a discrete gradient flow on a constraint manifold.

2 Preliminaries about discrete conservation laws

In this section we summarize some elementary properties of wave-trains, derive the integral equation (7) for the dual profile, and introduce some normalization.

2.1 Elementary properties and special solutions

First we observe that the wave-train equation (6) is invariant under shifts \( \varphi \mapsto \varphi_0 \), reflections \( \varphi \mapsto -\varphi \), and scalings \( k \mapsto k/s, \omega \mapsto \omega/s, V(\varphi) \mapsto V(s \varphi), v \mapsto v \) with \( s \neq 0 \). It is therefore sufficient to consider a fixed periodicity cell \( \Lambda \) and wave numbers \( k \in \Lambda \), so from now on we assume

\[ \Lambda = [-\pi, \pi]. \]

Recall that a periodic function \( V : \Lambda \to \mathbb{R} \) is even if \( V(\varphi) = V(-\varphi) \) holds for all \( \varphi \in \Lambda \), and that an even function on \( \Lambda \) is unimodal if it is monotone on \([-\pi, 0]\).

Second, we notice that (6) degenerates for both \( k = 0 \) and \( k = \pm \pi \). In fact, wave-trains for \( k = 0 \) are globally constant with \( u_j(t) \equiv u_1(0) \), while wave-trains for \( k = \pi \) are stationary binary oscillations with \( u_{2j}(t) = u_0(0) \) and \( u_{2j+1}(t) = u_1(0) \). Therefore, and since (6) is invariant under \( (k, \omega) \mapsto (-k, -\omega) \), we restrict all subsequent considerations to \( k \in (0, \pi) \).

For linear flux \( \Phi' \) we can solve (6) by Fourier transform. Specifically, linearizing (6) around \( v \) and restricting to unimodal and even profiles we find that \( \omega \) depends on \( k \) and \( v \) via the dispersion relation

\[ \omega = \Omega(k, v) = \Phi''(v) \sin k, \]

and that the unique profile is \( V(\varphi) = \alpha \cos \varphi \), where the amplitude \( \alpha \in \mathbb{R} \) is the third independent parameter. Harmonic wave-trains furthermore exemplify that simple profiles can generate rather complex patterns for the spatial oscillations in the lattice. This is illustrated in Figure 4 and in Figure 5 for the nonlinear case.

The second case in which we can solve (6) explicitly are wave-trains with wave number \( k = \pi/2 \).

**Lemma 1.** *Each wave-train for \( k = \pi/2 \) satisfies the Hamiltonian ODE*

\[
\omega \frac{d}{d\varphi} V(\varphi) = +\Phi'_{v,\text{sym}}(\tilde{V}(\varphi)), \quad \omega \frac{d}{d\varphi} \tilde{V}(\varphi) = -\Phi'_{v,\text{sym}}(V(\varphi)),
\]

(8)

6
Figure 4: Snapshots of harmonic wavetrains for several values of $k$. Although the carrier profile is always $U(\varphi) = \cos \varphi$, the plots $u_j = U(kj)$ against $j \in \mathbb{Z}$ exhibit rather different spatial patterns.

where

$$\tilde{V}(\varphi) = V(\varphi + \pi/2), \quad \Phi_{v, \text{sym}}(x) = \frac{1}{2}(\Phi(v + x) + \Phi(v - x)).$$

In particular, if $\Phi$ is smooth and convex, then for each $v$ there exists a unique one-parameter family of wavetrains with unimodal and even profiles that is parametrized by $\varphi = \Phi_{v, \text{sym}}(V(0))$.

**Proof.** By a direct computation we infer from (6) that

$$\omega \frac{d}{d\varphi} V(\varphi) = \frac{1}{2} \Phi'(v + \tilde{V}(\varphi)) - \frac{1}{2} \Phi'(v + \tilde{V}(\varphi - \pi)) = -\omega \frac{d}{d\varphi} V(\varphi + \pi).$$

Combining this with $\int_{\Lambda} V \, d\varphi = 0$ we find

$$V(\varphi + \pi) = -V(\varphi) \quad \forall \varphi \in \mathbb{R},$$

and hence (8). Finally, since (8) is a planar Hamiltonian ODE the remaining assertions follow from standard arguments.

### 2.2 Integral equation for the dual profile and normalization

We define the *dual profile* $Q$ of a wavetrain by

$$\Phi'(v + V) = q + Q, \quad q = \int_{\Lambda} \Phi'(v + V) \, d\varphi,$$

where $\bar{f}$ abbreviates the integral mean value, i.e.,

$$\int_{\Lambda} V \, d\varphi = \frac{1}{2\pi} \int_{-\pi}^{\pi} V(\varphi) \, d\varphi.$$

The key ingredient to our variational existence proof is to restate (8) as an equation for $Q$. To this end we consider the Legendre transform $\Psi$ of $\Phi$, which is well-defined and strictly convex provided that $\Phi$ is strictly convex, and satisfies

$$\Psi(\zeta) = \sup_{\nu} (\zeta \nu - \Phi(\nu)), \quad \Phi' \circ \Psi' = \Psi' \circ \Phi' = \text{id}.$$
Using $\Psi$ and (9) we now find that (6) is equivalent to
\[ \omega \frac{d}{d\varphi} \Psi'(q + Q) = \nabla_k Q, \]
and integration with respect to $\varphi$ yields
\[ \omega (\Psi'(q + Q) - v) = A_k Q, \quad v = \int_A \Psi'(q + Q) \, d\varphi. \tag{10} \]
Here, $v$ appears as a constant of integration and the integral operator $A_k$ is defined by
\[ (A_k Q)(\varphi) = \frac{1}{2} \int_{\varphi-k}^{\varphi+k} Q(\tilde{\varphi}) \, d\tilde{\varphi}. \tag{11} \]
With (10) we have derived the dual formulation of (6); the main mathematical difference between both formulations will be discussed at the end of §3.1.

For the existence proof in §3 it is convenient to normalize (10) in two steps. At first we incorporate the parameter $q$ into the nonlinearity by considering the normalized dual potential
\[ \Psi_q(\zeta) = \Psi(q + \zeta) - \Psi(q) - \Psi'(q) \zeta, \tag{12} \]
which satisfies
\[ \Psi''_q(\zeta) = \Psi''(q + \zeta), \quad \Psi'_q(0) = \Psi_q(0) = 0. \]
This transforms (10) into
\[ \omega (\Psi'_q(Q) - \eta) = A_k Q, \quad \eta = v - \Psi'(q) = \int_A \Psi'_q(Q) \, d\varphi. \]
The second normalization step is motivated by the harmonic case and the observation that the formula for the phase speed $\sigma$ depends on the value of $k$. In fact, the linearization of (10) around $q$ gives the dispersion relation
\[ Q(\varphi) = \alpha \cos \varphi, \quad \omega = \Omega(q, k) = \frac{\sin(k)}{\Psi''(q)}, \quad v = \Psi'(q), \]
and we conclude that $\sigma = \omega/k$ for $0 < k \leq \pi/2$ but $\sigma = \omega/(\pi - k)$ for $\pi/2 < k < \pi$, see Figure 5. We also notice that $A_k$ has slightly different properties for $0 < k \leq \pi/2$ and $\pi/2 < k < \pi$. In particular, by (11) we have
\[ A_{\pi-k} Q = -A_k T Q \tag{13} \]
for all $Q$ with $\int_A Q \, d\varphi = 0$, where $T$ denotes the shift operator
\[ T Q = Q(\cdot + \pi). \]
To complete the normalization we now replace $\omega$ by $\sigma$, and $A_k$ by either $\hat{B}_k$ or $\tilde{B}_{\pi-k}$, which are defined for $0 < \kappa \leq \pi/2$ by
\[ \hat{B}_{\kappa} = \kappa^{-1} A_{\kappa}, \quad \tilde{B}_{\kappa} = \kappa^{-1} A_{\pi-\kappa} = -\kappa^{-1} A_{\kappa} T. \]
Specifically, for $0 < k \leq \pi/2$ we restate the dual wavetrain equation (10) as

$$\sigma (\Psi_q'(Q) - \eta) = \hat{B}_\kappa Q, \quad \kappa = k, \quad \sigma = \omega / k,$$

(14)

whereas for $\pi/2 \leq k < \pi$ we write

$$\sigma (\Psi_q'(Q) - \eta) = \tilde{B}_\kappa Q, \quad \kappa = \pi - k, \quad \sigma = \omega / (\pi - k).$$

(15)

Notice that for $k = \pi/2$ both formulations agree and encode the ODE solution from Lemma 1. In particular, in this case we have the further symmetry $Q = -T Q$.

3 Variational existence proof for wavetrains

In this section we prove the existence of a three-parameter family of wavetrains by showing that the dual integral equations (14) and (15) possess corresponding three-parameter families of solutions. To elucidate the key ideas we start with an abstract existence result in §3.1 and check the validity of its assumptions in §3.2.

From now on we rely on the following standing assumption.

**Assumption 2.** $\Psi$ is twice continuously differentiable and strictly convex with

$$0 < \underline{c} \leq \Psi''(\zeta) \leq \bar{c} < \infty$$

for all $\zeta \in \mathbb{R}$ and some constants $\underline{c}$, $\bar{c}$.

We remark that Assumption (2) holds if and only if $\Phi$, the Legendre transform of $\Psi$, is twice continuously differentiable and strictly convex with $1/\bar{c} \leq \Phi'' \leq 1/\underline{c}$. This follows from basic properties of the Legendre transform [3].

Throughout the remainder of this paper, $L^2$ denotes the usual Hilbert space of square-integrable and periodic functions on the periodicity cell $\Lambda$, where the dual pairing and the integral norm are normalized via

$$\langle Q_1, Q_2 \rangle = \int_\Lambda Q_1 Q_2 \, d\varphi, \quad \|Q\|_2^2 = \int_\Lambda Q^2 \, d\varphi.$$
Moreover, we define
\[ \mathcal{H} = \left\{ Q \in L^2 : \int_A Q \, d\varphi = 0 \right\}. \]

### 3.1 Variational approach and abstract existence result

We now prove the existence of a one-parameter family of solutions \((Q, \sigma, \eta) \in \mathcal{H} \times \mathbb{R}_+ \times \mathbb{R}\) to the abstract wavetrain equation (7). To this end we assume that the operator \(B : \mathcal{H} \to \mathcal{H}\) is compact and symmetric, and that \(\Psi\) is normalized by
\[ \Psi(0) = \Psi'(0) = 0. \] (16)

Our variational approach to (7) is based on the functionals
\[ F(Q) = \frac{1}{2} \int_A Q B Q \, d\varphi = \frac{1}{2} \langle Q, B Q \rangle, \quad W(Q) = \int_A \Psi(Q) \, d\varphi, \] (17)
and the constrained optimization problem
\[ \text{maximize } F \text{ on } N_\gamma = \{ Q \in \mathcal{H} : W(Q) \leq \gamma \}, \] (18)
where \(\gamma > 0\) is a free parameter. We readily justify that (7) is the corresponding Euler-Lagrange equation for a maximizer \(Q \in L^2\), where \(\sigma\) and \(\mu = -\sigma \eta\) are Lagrangian multipliers for the constraints \(W(Q) \leq \gamma\) and \(\int_A Q \, d\varphi = 0\), respectively.

The existence of maximizers \(Q \in \mathcal{H}\) can be proven by the direct method using weak compactness arguments, see the first part in the proof of Theorem 3. However, in order to gain more qualitative information about shape of the profile function \(Q\) we refine the optimization problem (18). For this purpose we introduce the corresponding (negative) gradient flow, that is the \(\mathcal{H}\)-valued ODE
\[ \frac{d}{d\tau} Q = B Q - \sigma(Q) \mathcal{P}(Q), \quad \mathcal{P}(Q) = \Psi'(Q) - \eta(Q). \] (19)
Here \(\tau > 0\) is the flow time, and
\[ \eta(Q) = \int_A \Psi(Q) \, d\varphi, \quad \sigma(Q) = \frac{\langle \mathcal{P}(Q), B Q \rangle}{\|\mathcal{P}(Q)\|^2} \]
are two dynamical multipliers which guarantee that \(\int_A Q \, d\varphi = 0\) and \(W(Q) = \text{const}\) hold along each trajectory of (19). Notice that, by construction, each stationary point of (19) solves (7) with \(\sigma = \sigma(Q)\) and \(\eta = \eta(Q)\), and vice versa. For later use we also mention that the explicit Euler scheme to (19) with time step \(\tau > 0\) is given by the mapping
\[ Q \mapsto \mathcal{I}_\tau(Q) = (1 - \tau)Q + \tau B Q - \tau \sigma(Q) \mathcal{P}(Q). \] (20)

We are now able to formulate the refined existence result.

**Theorem 3.** Let \(\mathcal{C} \subset \mathcal{H}\) be any positive cone that

1. is convex and closed,
2. invariant under the gradient flow (19),
3. satisfies \( \sup_{Q \in C} F(Q) > 0 \).

Then, for each \( \gamma > 0 \) the functional \( F \) attains its maximum on \( C \cap N_\gamma \) and each maximizer \( Q \) solves (7) with multipliers \( \eta = \eta(Q) \) and \( \sigma = \sigma(Q) \). Moreover, each maximizer \( Q \) satisfies \( \sigma(Q) > 0 \) and \( W(Q) = \gamma \).

In preparation for the proof of Theorem 3 we draw the following conclusions from Assumption 2, the normalization condition (16), and the postulated properties of \( B \).

**Lemma 4.** The following assertions are satisfied.
1. \( F : L^2 \to \mathbb{R} \) is well defined and weakly continuous,
2. \( W : L^2 \to \mathbb{R} \) is well defined, convex, continuous, and Gâteaux-differentiable with derivative \( \partial W(Q) = \Psi'(Q) \). We also have
   \[
   \frac{1}{2}c\|Q\|_2^2 \leq W(Q) \leq \frac{1}{2}7\|Q\|_2^2, \quad \langle \Psi'(Q), Q \rangle > 0 \quad (21)
   \]
   for all \( 0 \neq Q \in L^2 \).
3. For each \( \gamma > 0 \), the set \( N_\gamma \subset H \) is convex and weakly compact in \( L^2 \). It is also star-shaped in the sense that for each \( 0 \neq Q \in H \) there exists a unique \( \lambda_\gamma(Q) > 0 \) such that \( \lambda Q \in N_\gamma \) for all \( 0 \leq \lambda \leq \lambda_\gamma(Q) \).

**Proof.** All assertions follow immediately from the definitions of \( F, W, \) and \( N_\gamma \), see (17) and (18).

**Lemma 5.** The gradient flow (19) is well defined on \( H \setminus \{0\} \) and conserves \( W \). Moreover, \( F \) increases strictly on each non-stationary trajectory.

**Proof.** Suppose that \( Q \) is given with \( P(Q) = 0 \), that means \( \Psi'(Q) = \text{const} \). The strict convexity of \( \Psi \) implies \( Q = \text{const} \) and \( Q \in H \) gives \( Q = 0 \). From this we infer that \( \sigma(Q) \) is well defined for \( Q \neq 0 \). Consequently, and since the right hand side in (19) is locally Lipschitz in \( Q \), the ODE (19) is well posed in \( H \setminus \{0\} \). By straightforward computations we now verify
\[
\frac{d}{dt} W(Q) = 0 \quad \text{and} \quad \frac{d}{dt} F(Q) = \langle BQ - \sigma(Q)P(Q), BQ \rangle = \|BQ\|^2_2 - \frac{\langle P Q, B Q \rangle}{\|P(Q)\|^2} \geq 0.
\]
In particular, we have \( \frac{d}{dt} F(Q) = 0 \) if and only if \( BQ \) and \( P(Q) \) are collinear, i.e., if and only if \( Q \) is a stationary point of (19).

We now finish the proof of the abstract existence result.

**Proof of Theorem 3.** With respect to the weak topology in \( L^2 \), the objective functional \( F \) is continuous and the constraint set \( C \cap N_\gamma \) is compact. The existence of a maximizer \( Q \) thus follows from basic topological principles, and by assumption we have \( F(Q) > 0 \). By Lemma 4 we find
\[
\lambda_\gamma(Q)^2 F(Q) = F(\lambda_\gamma(Q)Q) \leq F(Q),
\]
which implies $\lambda_\gamma(Q) \leq 1$. On the other hand, $Q \in \mathcal{N}_\gamma$ yields $\lambda_\gamma(Q) \geq 1$, and thus we find $\lambda_\gamma(Q) = 1$, which means $Q \in \partial \mathcal{N}_\gamma$. Moreover, Lemma 5 ensures that $Q$ is stationary under the gradient flow (11), and hence a solution to (1). Finally, testing (7) with $Q$ we find
\[ 2\mathcal{F}(Q) = \sigma \langle \Psi'(Q), Q \rangle, \]
and $\mathcal{F}(Q) > 0$ combined with (21) implies $\sigma > 0$.

To conclude this section we mention that there also exist variational characterizations of solutions $V$ to (9), but these are less feasible than the integral equation for the dual profile. The analogue to (7) is
\[ \sigma \mathcal{B}^{-1}V = \Phi'(v + V) - \theta, \quad \theta = \int \Phi'(v + V) \, d\varphi, \]
which has a variational structure, but a direct treatment is difficult as $\mathcal{B}^{-1}$ is not continuous. One can get rid off $\mathcal{B}^{-1}$ by making the ansatz $V = BS$ with $S \in \mathcal{H}$ and working with the functionals
\[ \mathcal{X}(S) = \frac{1}{2} \int_{\Lambda} SBS \, d\varphi, \quad \mathcal{Y}(S) = \int_{\Lambda} \Phi(v + BS) \, d\varphi. \]
However, the level sets of neither $\mathcal{X}$ nor $\mathcal{Y}$ are weakly compact, and therefore it is not obvious how to set up a variational framework that allows to prove the existence of solutions. Finally, one might think about solving the equation $V = \mathcal{B}(\Phi'(v + V) - \theta)/\sigma$ by fixed point arguments, but then one has find a way to exclude the trivial solution $V \equiv 0$.

3.2 Proof of the main result

Here we apply the abstract result from the previous section and prove the existence of a three-parameter family of wavetrains as claimed in the introduction. We therefore define $\mathcal{C}$ to be the positive cone of all $L^2$-functions on $\Lambda$ that are even, unimodal, and have zero average. This reads
\[ \mathcal{C} = \left\{ Q \in \mathcal{H} : Q(-\varphi_2) = Q(\varphi_2) \leq Q(\varphi_1) \text{ for almost all } 0 \leq \varphi_1 \leq \varphi_2 \leq \pi \right\}. \quad (22) \]
We next summarize some properties of the averaging operator $A_k$.

**Lemma 6.** For all $0 < k < \pi$ the operator $A_k$ maps $\mathcal{H}$ into itself and is symmetric and compact. Moreover, it maps $\mathcal{C}$ into $\mathcal{C}$.

**Proof.** The first three assertions follow directly from (11). It remains to prove that $\mathcal{C}$ is invariant under $A_k$ for $0 < k \leq \pi/2$; the claim for $\pi/2 \leq k < \pi$ then follows from (13) and the fact that $T : \mathcal{C} \to -\mathcal{C}$. Let $Q \in \mathcal{C}$ be given, and notice that $A_kQ \in \mathcal{H}$ is even with weak derivative $P = \nabla_k Q \in L^2$. For $\varphi \in [-\pi, -\pi + k]$, the periodicity and the evenness of $Q$ imply $Q(\varphi - k) = Q(2\pi + \varphi - k) = Q(-2\pi - \varphi + k)$ where $-\pi \leq -2\pi - \varphi + k \leq \varphi + k$, so the monotonicity of $Q$ in $[-\pi/2, 0]$ gives $2P(\varphi) = Q(\varphi + k) - Q(\varphi - k) = Q(\varphi + k) - Q(-2\pi - \varphi + k)$. Similarly, for $\varphi \in [-\pi + k, -k]$ and $\varphi \in [-k, 0]$ we have $2P(\varphi) = Q(\varphi + k) - Q(\varphi - k) \geq 0$ and $2P(\varphi) = Q(\varphi + k) - Q(\varphi - k) \geq 0$, respectively. In summary, $A_kQ$ is increasing on $[-\pi/2, 0]$, and since it is also even, the proof is complete. \(\square\)
Lemma 6 guarantees that both $\hat{B}_{\kappa}$ and $\tilde{B}_{\kappa}$ are symmetric and compact, and map $\mathcal{H} \to \mathcal{H}$ and $C \to C$.

**Lemma 7.** For given $q \in \mathbb{R}$ and $0 < \kappa \leq \pi/2$, Theorem 3 holds with $\Psi_q$ instead of $\Psi$ if $C$ is given by (22), and if $B$ is replaced by either $\hat{B}_{\kappa}$ or $\tilde{B}_{\kappa}$.

**Proof.** The cone $C$ is convex and closed, and we have $\cos \in C$ with $\langle \cos, \hat{B}_{\kappa}\cos \rangle = \langle \cos, \tilde{B}_{\kappa}\cos \rangle = \frac{1}{2} \kappa^{-1} \sin \kappa > 0$. Therefore, it remains to show that $C$ is invariant under the gradient flow (19). To this end we remark that $C$ is invariant under the action of the operator $Q \mapsto \mathcal{L}_\tau(Q) = G_{\tau, \sigma(Q), \eta(Q)}(Q) + \tau B Q$, where the family of nonlinear functions $G_{\tau, \sigma, \eta}: \mathbb{R} \to \mathbb{R}$ is given by $G_{\tau, \sigma, \eta}(\zeta) = \zeta - \tau \zeta - \tau \sigma \Psi'(\zeta) + \tau \sigma \eta$. Thanks to Assumption 2, for each bounded set $U \subset \mathbb{R}^2$ there exists $\bar{\tau} > 0$ such that $\frac{d}{d\kappa} G_{\tau, \sigma, \eta}(\zeta) \geq 0$ holds true for all $0 < \tau \leq \bar{\tau}$, all $\zeta \in \mathbb{R}$, and all $(\sigma, \eta) \in U$. From this, the invariance of $C$ under the action of $\tau B$, and the continuous dependence of $\sigma$ and $\eta$ on $Q \neq 0$, we conclude that for each ball $B \subset L^2 \setminus \{0\}$ there exists $\bar{\tau} > 0$ such that $\mathcal{L}_\tau$ maps $B \cap C$ into $C$ for all $0 < \tau \leq \bar{\tau}$. The claimed invariance of the gradient flow now follows by passing to the limit $\tau \to 0$. We are now able to concretize the informal existence result from the introduction as follows.

**Theorem 8.** Let $0 < \kappa \leq \pi/2$, $q \in \mathbb{R}$, and $\gamma > 0$ be given. Then, there exist profiles $\hat{Q}, \tilde{Q} \in C$ along with multipliers $\hat{\sigma}, \tilde{\sigma} > 0$ and $\hat{\eta}, \tilde{\eta}$ such that

$$
\hat{\sigma}(\Psi_q'(\hat{Q}) - \hat{\eta}) = \hat{B}_{\kappa}\hat{Q}, \quad \tilde{\sigma}(\Psi_q'(\tilde{Q}) - \tilde{\eta}) = \tilde{B}_{\kappa}\tilde{Q}.
$$

In particular, the profile $\hat{\tilde{V}} = \Psi_q'(\hat{Q}) - \hat{\eta} \in C$ solves

$$
\hat{\omega} \frac{d}{d\varphi} \hat{\tilde{V}} = \nabla_{\kappa} \Psi'(\hat{\varphi} + \hat{\tilde{V}})
$$

with $\hat{\omega} = \kappa \hat{\sigma} > 0$ and $\hat{\varphi} = \hat{\eta} + \Psi'(q)$, whereas $\tilde{\tilde{V}} = \Psi_q'(\tilde{Q}) - \tilde{\eta} \in C$ solves

$$
\tilde{\omega} \frac{d}{d\varphi} \tilde{\tilde{V}} = \nabla_{\pi - \kappa} \Psi'(\tilde{\varphi} + \tilde{\tilde{V}})
$$

with $\tilde{\omega} = \kappa \tilde{\sigma} > 0$ and $\tilde{\varphi} = \tilde{\eta} + \Psi'(q)$.

**Proof.** The existence of both $\hat{Q}$ and $\tilde{Q}$ is a consequence of Lemma 7 and Theorem 3. The remaining assertions then follow by straightforward computations.

We conclude this section with some remarks concerning the assumptions and assertions of Theorems 3 and 8.
1. The strict convexity of $\Psi$ (or equivalently, of $\Phi$) is crucial for our existence proof. In fact, it is truly necessary for relating the integral equations (14) and (15) to the wavetrain equation (6). It also plays an important role in the proof of Theorem 3 as it guarantees the weak compactness of $N_\gamma$. The assumptions about upper and lower bounds for $\Psi''$, however, are made for convenience and might be weakened for the price of more technical effort.

2. It would be highly desirable to give uniqueness results that classify wavetrains up to phase shifts and scalings of the periodic cell. In analogy to the harmonic case, we conjecture that the three-parameter family from Theorem (8) contains all wavetrains which satisfy the profile constraint $V \in C$, but we are not able to prove this. Another open problem is the stability of wavetrains.

3. Obviously, in Theorem 3 we can choose $C = H$ to obtain solutions $Q \in N_\gamma$ to the original optimization problem (18). In this case, (7) is provided by the Lagrangian multiplier rule. If $C$, however, is a proper subset of $H$ then the validity of (7) does not follow from the multiplier rule but is a consequence of the invariance properties of $C$. We also remark that numerical simulations indicate that each maximizer of $F$ in $N_\gamma$ is (up to phase shifts) unimodal and even, and hence contained in $C$. We therefore conjecture that (18) and its refined variant from Theorem 3 have the same solutions, but a rigorous proof is not available.

4 Numerical simulations

In this section we illustrate our analytical findings by numerical simulations, which are computed by the following implementation of the discrete gradient flow (20) with $\Psi_q$ instead of $\Psi$, see (12), and $B = \bar{B}_k$ and $B = \tilde{B}_k$ for $k \in [0, \pi/2]$ and $k \in [\pi/2, \pi]$, respectively:

1. We sample the periodicity cell $[-\pi, \pi]$ by grid points $\varphi_m = -\pi + 2\pi m/M$ with $m = 1, ..., M$. 

Figure 6: Numerical simulations for example (23) with several values of $k$. The plots show the graph of the dual profile, i.e., $Q(\varphi)$ against $\varphi \in \Lambda$. The lower right picture sketches the graphs of $\Psi''$ (Black), $\Phi'$ (Dark Grey), and $\Phi$ (Light Grey).
2. We approximate $Q$ by $Q_m = Q(\varphi_m)$ and replace all integrals with respect to $\varphi$ by Riemann sums.

3. After each update step according to (20), we enforce the conservation of $\mathcal{W}(Q)$ by a scaling $Q_m \mapsto \lambda Q_m$, where the factor $\lambda$ is computed by a single Newton step.

4. For given $k$ and $q$, we initialize the scheme with $Q_m = \alpha \cos \varphi_m$, where the amplitude $\alpha$ determines $\gamma$ via $\gamma = \int_\Lambda \Psi_q(\alpha \cos \varphi) \, d\varphi$.

Although this numerical scheme is rather simple it shows good convergence properties, provided that $M$ is sufficiently large and the time step $\tau$ is sufficiently small. All simulation presented below are performed with $\tau = 0.1$ and $M = 200$.

The first example concerns the data

$$
\Psi''(\zeta) = \frac{1}{2} + \frac{1}{2} \exp(-\zeta^2), \quad \alpha = 5, \quad q = 0,
$$

where $\gamma$ is determined by $\alpha$ as described above. The numerical results are presented in Figure 7, which shows the dual profile $Q$ as function of $\varphi$ for several values of $k$. We also refer to Figure 9, which illustrates how the wavetrains appear in snapshots $u_j = \Psi'(q + Q(kj - \omega t))$.
Figure 9: Snapshots of $u_j$ against $j = 1...50$ for the simulations from Figure 6–8 at a randomly chosen time $t$. Black points and grey curves represent the data on the lattice $\mathbb{Z}$ and the continuous carrier profiles $U = v + V$, respectively. Under the evolution all points move with constant speed along the grey curves.

against $j \in \mathbb{Z}$. A special feature of this example is that $\Psi_q$ is even for $q = 0$, and this implies that (7) is invariant under $Q \sim -TQ$. We therefore find that the profiles are the same for $k$ and $\pi - k$, and exhibit the further symmetry $Q(\varphi + \pi) = -Q(\varphi)$.

The second example is computed with

$$\Psi''(\zeta) = 1 - \frac{1}{\pi} \arctan (2\zeta), \quad \alpha = 3, \quad q = 0,$$

and illustrates the generic case that $\Psi_q$ is not even. In Figure 7 we therefore observe that the profiles do not satisfy $Q = -TQ$ anymore, and are no longer the same for $k$ and $\pi - k$. 

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Finally, the third example uses
\[
\Psi''(\zeta) = \frac{1}{4} \exp(2\zeta) - \frac{1}{2} \zeta - \frac{1}{4}, \quad \alpha = 2, \quad q = 0,
\]
and is shown in Figure 7. Here \( \Psi \) is still convex but does not satisfy Assumption 2 due to \( \Psi''(0) = 0 \). Nevertheless, the numerical scheme works very well and provides wavetrains for all values of \( k \).

### A Lagrangian and Hamiltonian structures for scalar conservation laws

For the readers convenience we summarize some basic facts about the Lagrangian and Hamiltonian structures of discrete scalar conservation laws. Both structures are very similar to the respective structures for the KdV equation, compare for instance [1], and originate from the skew-symmetry of centred difference operators. Specifically, for \( \nabla \) with \( \nabla y_j = \frac{1}{2} (y_{j+1} - y_{j-1}) \) the identity
\[
\sum_{j \in \mathbb{Z}} y_j \nabla y_j = -\sum_{j \in \mathbb{Z}} \tilde{y}_j \nabla y_j
\]
holds for all sequences \( y, \tilde{y} \) for which the series are well-defined. Notice that the one-sided difference operators \( \nabla^{\pm} \) with \( \nabla^{\pm} y_j = \pm y_{j \pm 1} \mp y_j \) are not skew-symmetric but satisfy \( (\nabla^{\pm})^* = -\nabla^{\mp} \).

To derive the Lagrangian structure we assume that there exists \( y = y_i(t) \) such that \( u_j = \nabla y_j \). This transform (1) into
\[
\nabla \dot{y} + \nabla \Phi'(\nabla y) = 0,
\]
and reveals that the action integral is given by
\[
L(\dot{y}, y) = -\frac{1}{2} \int_0^{t_{\text{fin}}} \sum_{j \in \mathbb{Z}} \dot{y}_j \nabla y_j \, dt - \int_0^{t_{\text{fin}}} \sum_{j \in \mathbb{Z}} \Phi(\nabla y_j) \, dt,
\]
where \( t_{\text{fin}} \) is a given final time. In fact, computing the variational derivatives \( \partial_y L = -\frac{1}{2} \nabla \dot{y} \) and \( \partial_y L = \frac{1}{2} \nabla \dot{y} + \nabla \Phi'((\nabla y) \) we easily check that (26) is just the Euler-Lagrange equation
\[
-\frac{d}{dt} \partial_y L + \partial_y L = 0.
\]

A special feature of \( L \) is that the canonical momenta \( \partial_y L \) do not depend on \( \dot{y} \), and therefore we cannot apply the standard procedure to derive the Hamiltonian structure. There is, however, a non-canonical Hamiltonian structure. Using the Hamiltonian
\[
H(y) = \sum_{j \in \mathbb{Z}} \Phi(\nabla y_j),
\]
the discrete scalar conservation law (11) can be written as
\[
\nabla \dot{y} = \partial_y H.
\]
This is indeed a Hamiltonian equation, where $\nabla$ acts as non-canonical symplectic operator that corresponds to the symplectic product

$$\langle \dot{y}, y' \rangle_{\text{sympl}} = -\sum_{j \in \mathbb{Z}} \dot{y}_j \nabla y'_j = \sum_{j \in \mathbb{Z}} y'_j \nabla \dot{y}_j.$$

The PDE (2) has the same Lagrangian and Hamiltonian structures in the sense that all formulas from above remain valid provided that we (i) apply the scaling (3), (ii) replace sums over $j$ by integrals with respect to $\xi$, and (iii) employ the differential operator $D = \partial_\xi$ instead of $\nabla$. In other words, the scalar conservation law (2) is the Euler-Lagrange equation to the action integral

$$L(\partial \tilde{y}, \tilde{y}) = \frac{1}{2} \int_0^{\tau_{\text{fin}}} \int_\mathbb{R} \partial_\tau \tilde{y} D\tilde{y} \, d\xi \, d\tau - \int_0^{\tau_{\text{fin}}} \int_\mathbb{R} \Phi(D\tilde{y}) \, d\xi \, d\tau.$$

It is moreover equivalent to

$$\partial_\tau D\tilde{y} + D\Phi'(D\tilde{y}) = 0, \quad \bar{u} = D\tilde{y},$$

which has Hamiltonian $H(\tilde{y}) = \int_\mathbb{R} \Phi(D\tilde{y}) \, d\xi$ and symplectic product $\langle \dot{y}, y' \rangle_{\text{sympl}} = \int_\mathbb{R} y' D\dot{y} \, d\xi$. The analogies between the structures of lattice and PDE are – in view of the skew-symmetry of both $\nabla$ and $D$ – not surprising and exemplify the more general principles laid out in [10]. Moreover, if we replace $D$ by the macroscopic difference operator

$$D_\varepsilon \tilde{y}(\xi) = \frac{\tilde{y}(\xi + \varepsilon) - \tilde{y}(\xi - \varepsilon)}{2\varepsilon},$$

we easily recover the scaled version of (1). In this sense the lattice (1) is just a variational integrator of the scalar conservation law (2), i.e., a semi-discrete scheme that respects the underlying variational and symplectic structures.

The very same idea also allows to derive variational integrators for the time discretization. If we replace the continuous time derivative in (27) by $\frac{1}{2}h^{-1}(y_{k+1,j} - y_{k-1,j})$, where $h$ is the time step size and the index $k$ refers to the $k^{\text{th}}$ time step, we obtain the discrete action integral

$$L = -\frac{1}{8h} \sum_{k,j} (y_{k+1,j} - y_{k-1,j})(y_{k,j+1} - y_{k,j-1}) - \sum_{k,j} \Phi\left(\frac{1}{2}(y_{k,j+1} - y_{k,j-1})\right),$$

which depends on all the $y_{k,j}$’s. Evaluating the Euler-Lagrange equation $\partial_{y_{k,j}} L = 0$, and replacing $y$ by $u$, yields the fully discrete scheme

$$u_{k+1,j} = u_{k-1,j} - h\Phi'(u_{k,j+1}) + h\Phi'(u_{k,j-1}), \quad (28)$$

which also served to compute the numerical examples from [11].

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