Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Wave trains, solitons and modulation theory in FPU chains

Wolfgang Dreyer[1], Michael Herrmann[2], and Jens D.M. Rademacher[1]

submitted: 11th May 2006

[1] Weierstraß–Institut
für Angewandte Analysis
und Stochastik
Mohrenstraße 39
10117 Berlin
E-Mail: dreyer@wias-berlin.de
rademach@wias-berlin.de

[2] Humboldt-Universität zu Berlin
Institut für Mathematik,
Unter den Linden 6
10099 Berlin
michaelherrmann@mathematik.hu-berlin.de

No. 1132
Berlin 2006

2000 *Mathematics Subject Classification.* 34E13, 37K60, 70F45, 70K70, 82C21.

Key words and phrases. FPU chain, traveling waves, multiscale ansatz, modulation theory, dispersive shocks.

M. Herrmann and J. Rademacher were supported by the Deutsche Forschungsgemeinschaft (DFG) within the Priority Programme SPP 1095 *Analysis, Modeling and Simulation of Multiscale Problems*, see `http://www.mathematik.uni-stuttgart.de/~mehrskalen`.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We present an overview of recent results concerning wave trains, solitons and their modulation in FPU chains. We take a thermodynamic perspective and use hyperbolic scaling of particle index and time in order to pass to a macroscopic continuum limit. While strong convergence yields the well-known p-system of mass and momentum conservation, we generally obtain a weak form of it in terms of Young measures. The modulation approach accounts for microscopic oscillations, which we interpret as temperature, causing convergence only in a weak, average sense. We present the arising Whitham modulation equations in a thermodynamic form, as well as analytic and numerical tools for the resolution of the modulated wave trains. As a prototype for the occurrence of temperature from oscillation-free initial data, we discuss various Riemann problems, and the arising dispersive shock fans, which replace Lax-shocks. We predict scaling and jump conditions assuming a generic soliton at the shock front.

1 Introduction

We consider chains of N identical particles as plotted in Figure 1.1, nearest neighbor coupled in a nonlinear potential $\Phi : \mathbb{R} \to \mathbb{R}$ by Newton's equations

$$\ddot{x}_\alpha = \Phi'(x_{\alpha+1} - x_\alpha) - \Phi'(x_\alpha - x_{\alpha-1}), \tag{1.1}$$

where $\dot{} = \frac{\mathrm{d}}{\mathrm{d}t}$ is the time derivative, $x_\alpha(t)$ the atomic position, and $\alpha = 1, \dots, N$ the particle index. Since the work of Fermi, Pasta and Ulam [FPU55] one usually refers to (1.1) as FPU chains.

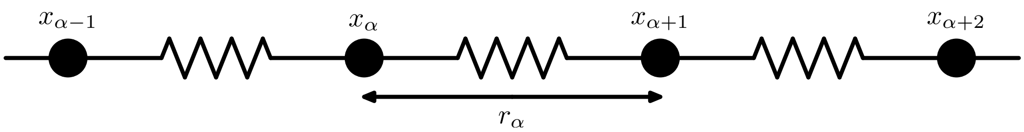

Figure 1.1: The atomic chain with nearest neighbour interaction.

We mainly consider general, convex potentials Φ. While our focus lies on nonlinear Φ', the harmonic potential with linear forces is an instructive, completely integrable example. A nonlinear example, but still completely integrable, is the famous Toda chain, see [Tod70, DKKZ74, Hén74] with potential

$$\Phi(r) = \exp(1 - r) - (1 - r). \tag{1.2}$$

For our purposes it is convenient to use the atomic distances $r_\alpha = x_{\alpha+1} - x_\alpha$ and velocities $v_\alpha = \dot{x}_\alpha$ as the basic variables, changing (1.1) to the system

$$\dot{r}_\alpha = v_{\alpha+1} - v_\alpha \,, \quad \dot{v}_\alpha = \Phi'(r_\alpha) - \Phi'(r_{\alpha-1}). \tag{1.3}$$

Rather than investigating solutions of (1.3) for finite N, we focus on the thermodynamic limit $\varepsilon = 1/N \to 0$ in the *hyperbolic* scaling of the *microscopic* coordinates t and α, which is defined by the *macroscopic* time $\overline{t} = \varepsilon t$ and particle index $\overline{\alpha} = \varepsilon\alpha$. It is natural to scale the atomic positions in the same way, i.e. $\overline{x} = \varepsilon x$, which leaves atomic distances and velocities scale invariant. For a survey on other reasonable scaling we refer to §2 and [GHM06a].

Our main goal is to derive a micro-macro transition for the atomic chain, i.e. we aim to replace the high dimensional ODE (1.1) by a few macroscopic PDEs. The derivation of such a continuum limit is simple as long as the atomic data vary on the macroscopic scale only, see (1.9) below. If, however, the atomic data oscillate on the microscopic scale, the problem is tremendously complicated, because then distances and velocities *do not* converge to macroscopic functions. Instead, at each point in the macroscopic space-time, the local (r, v)-distribution converges to a nontrivial Young-measures, see §5. We interpret the microscopic oscillations as a form of temperature in the chain, see §2, and refer to oscillation-free limits as *cold*.

The main problem in the case of temperature is to find an appropriate description for the structure and evolution of the oscillations. Even if we are interested in the macroscopic behavior of averaged quantities only, the microscopic oscillations determine the evolution of the *internal energy*, that is, the amount of energy which is stored in purely microscopic motion. In other words, any reasonable macroscopic limit for oscillatory solutions needs to describe thermodynamic effects, such as creation of temperature and transport of heat. Unfortunately, no rigorous theory is known that applies without further assumptions.

Numerical simulations as discussed in §5 and §6, as well as rigorous results for the Toda chain, cf. [HFM81, Kam91, VDO91, DKKZ96, DM98], suggest that for certain solutions of (1.1), the arising microscopic oscillations can be described by *modulated traveling waves*. Traveling waves are highly oscillatory exact solutions of (1.1). The most relevant kind for our purposes are *wave trains* which are periodic functions of a single phase variable, depending on four characteristic parameters. Modulated wave trains arise when these parameters vary on the macroscopic scale.

A characteristic property of wave trains is that the arising Young measures are supported on closed curves. As a consequence, they correspond to a very special kind of temperature which is not related to our usual notion of thermalization. However, they give rise to a thermodynamically consistent macroscopic theory involving temperature, entropy, and so on. Moreover, if cold initial data form macroscopic shocks, then Newton's equations self-organize into microscopic oscillations in form of modulated wave trains, and in this sense our notion of temperature turns out to be generic.

Some aspects of the problems addressed in this article have much in common with certain *zero dispersion limits*, which we will briefly discuss next to illustrate our point of view. This is not to be confused with so called zero diffusive-dispersive limits, where diffusive effects prevail, cf. e.g. [Sch82, KL02]. The most prominent example is Burger's equation

$$\partial_{\overline{t}} u + u\, \partial_{\overline{\alpha}} u = 0, \tag{1.4}$$

which, on a formal level, is the zero dispersion limit of the KdV equation

$$\partial_{\overline{t}} u + u\, \partial_{\overline{\alpha}} u + \varepsilon\, \partial_{\overline{\alpha}}^3 u = 0. \tag{1.5}$$

The main question is under which conditions the solutions of (1.5) converge as $\varepsilon \longrightarrow 0$ to (weak) solutions of (1.4). The rigorous theory for this problem was developed by Lax and Levermore in [LL83, Ven85] by relying on the complete integrability of (1.5).

It is well known that generic initial data u_{ini} yield a critical time $\overline{t}_{\mathrm{crit}}$ such that (1.4) has a unique smooth solution for $0 < \overline{t} < \overline{t}_{\mathrm{crit}}$, but for $\overline{t} > \overline{t}_{\mathrm{crit}}$ solutions exist in a weak sense only, having at least one discontinuity at some $\overline{\alpha}_{\mathrm{crit}}$, and satisfying $\partial_{\overline{t}} u + \frac{1}{2}\partial_{\overline{\alpha}}(u^2) = 0$ in the sense of distributions.

Imposing the same initial datum u_{ini} for KdV, the typical behavior for $\varepsilon \to 0$ is as follows, see for instance the surveys in [Lax86, Lax91, LLV93]. For $0 < \overline{t} < \overline{t}_{\mathrm{crit}}$ the solutions u_ε of (1.5) converge strongly to the unique smooth solution of (1.4). However, for $\overline{t} > \overline{t}_{\mathrm{crit}}$ the KdV-solutions become highly oscillatory in a neighborhood of $\overline{\alpha}_{\mathrm{crit}}$ with wavelength $1/\sqrt{\varepsilon}$, and converge to a weak limit $\langle u \rangle$ only. The main point is that $\langle u \rangle$ does *not* satisfy Burgers equation, i.e. $\partial_{\overline{t}} \langle u \rangle + \frac{1}{2}\partial_{\overline{\alpha}} \langle u \rangle^2 \neq 0$, because $\langle u \rangle^2 \neq \langle u^2 \rangle$.

A discrete zero dispersion limit was studied in [GL88], replacing (1.4) by

$$\dot{u}_\alpha + \tfrac{1}{2}\, u_\alpha\, (u_{\alpha+1} - u_{\alpha-1}) = 0. \tag{1.6}$$

This scheme is equivalent to a dispersive spatial discretization of (1.4), because the identification $u_\alpha(t) = u(\varepsilon t,\, \varepsilon\alpha)$ transforms (1.6) into $\partial_{\overline{t}} u + u\, \nabla^{\pm\varepsilon} u = 0$ with $\nabla^{\pm\varepsilon} u(\overline{t},\, \overline{\alpha}) = \big(u(\overline{t},\, \overline{\alpha} + \varepsilon) - u(\overline{t},\, \overline{\alpha} - \varepsilon)\big)/2\varepsilon$, The numerical study in [GL88] provides evidences for the same qualitative limiting behavior as for KdV. Further examples for numerical schemes with interesting zero dispersion limit can be found in [HL91] and [LL96].

Towards modulation theory, [GL88] found a simple description for *modulated binary oscillations*, which provides an *approximate* solution of (1.6) satisfying $u_\alpha \approx v_\alpha + (-1)^\alpha\, w_\alpha$, where v_α and w_α vary on the macroscopic scale only. The modulation equations for binary oscillations read

$$\partial_{\overline{t}} a + a\, \partial_{\overline{\alpha}} b = 0, \quad \partial_{\overline{t}} b + b\, \partial_{\overline{\alpha}} a = 0. \tag{1.7}$$

where $a = v + w$ and $b = v - w$. This system is strictly hyperbolic if and only if a and b have the same sign, and conservation laws for $\ln a$ and $\ln b$ imply that strictly positive initial data stay positive for all times.

Let $a = a(\overline{t}, \overline{\alpha})$ and $b = b(\overline{t}, \overline{\alpha})$ be a smooth solution of (1.7) defined until $\overline{t}_{\mathrm{crit}}$, and denote the corresponding modulated binary oscillations by

$$u_\alpha^{\mathrm{mod}}(t) = v(\varepsilon t,\, \varepsilon\alpha) + (-1)^\alpha\, w(\varepsilon t,\, \varepsilon\alpha). \tag{1.8}$$

It is proven in [GL88] that (1.8) indeed yields approximate solutions of the microscopic system for $t < \varepsilon^{-1}\overline{t}_{\mathrm{crit}}$ in the sense that $u_\alpha^{\mathrm{mod}}(t) - u_\alpha(t)$ converges to zero as $\varepsilon \to 0$ for $\overline{t} < \overline{t}_{\mathrm{crit}}$ if $u_\alpha(0) = u_\alpha^{\mathrm{mod}}(0)$. For larger times we expect that modulated binary oscillations are not longer close to an exact solution.

Returning to the atomic chain (1.1), we next derive the macroscopic evolution of *cold* data, i.e. we assume macroscopic fields $r(\overline{t}, \overline{\alpha})$ and $v(\overline{t}, \overline{\alpha})$ such that $r_\alpha(t) = r(\varepsilon t,\, \varepsilon\alpha)$, $v_\alpha(t) = v(\varepsilon t,\, \varepsilon\alpha)$. Substitution into (1.3) yields

$$\partial_{\overline{t}}\, r - \nabla^{+\varepsilon} v \;=\; 0, \quad \partial_{\overline{t}}\, v - \nabla^{-\varepsilon}\Phi'(r) \;=\; 0, \tag{1.9}$$

In the limit $\varepsilon \to 0$ we formally obtain the so called *p-system* consisting of the macroscopic conservation laws for mass and momentum given by

$$\partial_{\overline{t}}\, r - \partial_{\overline{\alpha}}\, v = 0, \quad \partial_{\overline{t}}\, v - \partial_{\overline{\alpha}}\, \Phi'(r) = 0. \tag{1.10}$$

It is well known that, for convex Φ, the p-system is hyperbolic and that for smooth solutions the energy is conserved according to

$$\partial_{\overline{t}} \left(\tfrac{1}{2} v^2 + \Phi(r)\right) - \partial_{\overline{\alpha}} \left(v\, \Phi'(r)\right) = 0. \tag{1.11}$$

In analogy to the previous discussion, the p-system describes the thermodynamic limit for cold atomic data as long as these data are smooth on the macroscopic scale. However, we will show next that, if the nonlinearity forms a shock, then the p-system is no longer a thermodynamically consistent model for the macroscopic evolution. For simplicity, we assume that the flux function Φ' is convex so that all eigenvalues of (1.10) are genuinely nonlinear. According to the Lax theory of hyperbolic system, cf. [Smo94, Daf00, LeF02], a shock wave propagates with a constant shock speed c so that r and v satisfy the Rankine-Hugoniot jump conditions across the shock given by

$$-c[\![r]\!] - [\![v]\!] = 0, \quad -c[\![v]\!] - [\![\Phi'(r)]\!] = 0, \tag{1.12}$$

where $[\![\cdot]\!]$ denotes the jump. However, (1.12) implies that the jump condition for the energy must be violated, i.e. for shocks with (1.12) we have

$$-c[\![\frac{1}{2} v^2 + \Phi(r)]\!] - [\![v\, \Phi'(r)]\!] \neq 0.$$

Consequently, the p-system predicts some production for the macroscopic energy (the Lax criterion selects only shocks with negative production).

In contrast, Newton's equations always conserve mass, momentum *and* energy. Therefore, the p-system cannot describe the thermodynamic limit beyond the shock at which the atomic data start to oscillate. Indeed, some amount of energy is dissipated into *internal energy* leading to a *dispersive shock fan*. It is one of the merits of modulation theory that it can describe the microscopic oscillations emerging from cold shocks as discussed in §6.

The article is organized as follows. In §2: we briefly sketch the thermodynamical framework. We survey some existence and approximation results of *wave trains* and *solitons* in §3, including multi-phase wave trains, thermodynamic properties and new a priori estimates. §4 gives a brief overview on Whitham's modulation theory applied to FPU chains, leading to a system of four conservation laws for wave train parameters. In §5 we briefly summarize some aspects of numerical justification by evaluating the aforementioned Young measures and testing assumptions of modulation theory. The shock problem for cold Riemann data is discussed in §6, and we characterize the behavior of all macroscopic fields at the shock front by assuming that is consists of a generic soliton.

2 Thermodynamic framework

Thermodynamics describes the evolution of deformation and heat on the macroscopic scale in a body, which may be isolated from the surroundings or is subjected to external supply of mechanical forces and heat. In the following we will illustrate the strategy of thermodynamics for a macroscopic body in one space dimension, that is microscopically constituted by an atomic chain. To this end thermodynamics considers, at any *Lagrangian space-time point* $(\bar{t}, \bar{\alpha})$ a certain number of *specific densities* $u_j(\bar{t}, \bar{\alpha})$, $j = 1...M$, and determines these fields by means of a system of PDEs for given initial and boundary data. The most important densities in 1D are the specific volume (mean distance) r, the macroscopic velocity v, and the specific total energy $E = \frac{1}{2}v^2 + U$, uniquely decomposed into kinetic energy and specific internal energy U.

The PDE system relies on M equations of balance that read in regular points

$$\partial_{\bar{t}} u_j + \partial_{\bar{\alpha}} F_j = P_j, \quad j \in \{1, 2, \ldots, M\}, \tag{2.1}$$

where f_j and P_j are called *fluxes* and *productions*, respectively. The fundamental balance equations are the conservation laws for mass, momentum and energy given by

$$\partial_{\bar{t}} r - \partial_{\bar{\alpha}} v = 0 \;, \quad \partial_{\bar{t}} v + \partial_{\bar{\alpha}} p = 0 \;, \quad \partial_{\bar{t}} E + \partial_{\bar{\alpha}} f = 0, \tag{2.2}$$

where p denotes the pressure and f is the energy flux, satisfying $f = pv+q$ with heat flux q. Further conservation laws are possible, but those are material and process dependent.

In order that (2.1) becomes a closed system for the variables, thermodynamics has to model constitutive equations that relate, in a material dependent manner, the fluxes and productions to the densities themselves and/or their time and space derivatives. The generality of the constitutive functions is restricted by universal principles like Galileian invariance and the *entropy principle*, and by material dependent symmetry principles. The entropy principle consists of several parts, see [MR98] for more details.

1. There exists an entropy pair (S, g), given by (material dependent) constitutive functions in terms of the densities u_j, so that the entropy density S is a concave function.

2. The constitutive laws closing (2.1) yield a further balance equation

$$\partial_{\bar{t}} S + \partial_{\bar{\alpha}} g = \Sigma \geq 0 \quad \text{with} \quad \Sigma = 0 \Longleftrightarrow P_j = 0, \tag{2.3}$$

   where Σ denotes the non-negative *entropy production*.

3. The definition of (absolute) temperature T_{macro} is given by

$$T_{\text{macro}} = \frac{\partial U}{\partial S}. \tag{2.4}$$

   Note that this phenomenological definition is a priori unrelated to any microscopic model.

4. The law of Clausius-Duhem holds, i.e. $T_{\text{macro}} g = q$.

This abstract framework is the basic paradigm of Rational Thermodynamics and assumed to hold in all cases. However, the constitutive laws depend on the chosen macroscopic scaling and are generally unknown. Nevertheless, the scaling predicts the way in which the fluxes (and productions) can and cannot depend on the densities. For instance, in the hyperbolic scaling, the macroscopic equations must be invariant (to leading order) under $(\bar{t}, \bar{\alpha}) \mapsto (\lambda\bar{t}, \lambda\bar{\alpha})$, whereas the parabolic scaling $(\bar{t}, \bar{\alpha}) = (\varepsilon^2 t, \varepsilon\alpha)$ implies macroscopic invariance under $(\bar{t}, \bar{\alpha}) \mapsto (\lambda^2\bar{t}, \lambda\bar{\alpha})$.

Therefore, in the hyperbolic scaling all constitutive relations for the fluxes must be local, i.e. F_j depends pointwise on the densities u_j, so that (2.2) is a first order system. We mention that hyperbolicity of (2.1) is guaranteed if the entropy S is a concave function, see [MR98]. Generally, for the hyperbolic scaling, all constitutive relations can be encoded in a Gibbs equation with a single thermodynamic potential. On the other hand, for parabolic scaling, we expect that the fluxes depend (mainly) on the spatial derivatives of the densities. In the simplest case the energy flux f is given by Fourier's law, i.e. $f = \partial_{\bar{\alpha}} U$, so that the energy balance leads to the heat equation.

In conclusion, we sketch the macroscopic thermodynamics for the atomic chain (1.1) as it results from modulated wave trains. It turns out that the macroscopic system

(2.1) consists of the three fundamental and a fourth equation, the *conservation of wave number* $\partial_{\bar{t}} k - \partial_{\bar{\alpha}} \omega = 0$, with wave number k and frequency ω. In addition, there is a fifth conservation law for the entropy S, i.e. $\Sigma = 0$ in (2.3), and all fluxes are given by the thermodynamic potential $U = U(r, k, S)$ through the Gibbs equation

$$\mathrm{d}E = \omega\,\mathrm{d}S - p\,\mathrm{d}r - g\,\mathrm{d}k + v\,\mathrm{d}v. \tag{2.5}$$

Note that the equation of state depends on the chain, i.e. on the potential Φ, whereas (2.5) is universal. From (2.4) and (2.5), we infer that the macroscopic temperature T_{macro} equals the wave train frequency ω. Interestingly, here there is a difference between T_{macro} and the kinetic temperature defined as the mean kinetic energy of the atoms, see §3. However, it turns out that the Clausius-Duhem law is satisfied, i.e. we find $q = \omega g$.

3 Traveling waves

Traveling waves are exact solutions of the infinite chain (1.1) for $N = \infty$ of the form $x_\alpha(t) = x(\alpha - ct)$ depending on a single phase variable ϕ and traveling with a constant speed c. In the context of the macroscopic limits that we consider, relevant traveling waves are solitons, which vanish as $\phi \to \pm\infty$, and wave trains, which are periodic in ϕ. Due to Galilean invariance, we can allow additional drift in space-time of the form

$$x_\alpha(t) = r\alpha + vt + y_\alpha(t),$$

where the profile $y_\alpha(t)$ solves the modified lattice equations

$$\ddot{y}_\alpha = \Phi'(r + y_{\alpha+1} - y_\alpha) - \Phi'(r + y_\alpha - y_{\alpha-1}) \tag{3.1}$$

and traveling waves $y_\alpha(t) = \mathbb{Y}(\alpha - ct)$ solve the second order advance-delay differential equation

$$c^2 \partial_{\phi\phi} \mathbb{Y}(\phi) = \Phi'(r + \mathbb{Y}(\phi + 1) - \mathbb{Y}(\phi)) - \Phi'(r + \mathbb{Y}(\phi) - \mathbb{Y}(\phi - 1)). \tag{3.2}$$

3.1 Wave trains

Normalizing the period of wave trains to 1 and using $c = \omega/k$ with wave number k and frequency ω, we obtain the form

$$x_\alpha(t) = r\alpha + vt + \mathbb{X}(k\alpha + \omega t), \tag{3.3}$$

where $\mathbb{X}(\varphi)$ is the 1-periodic *wave profile* function. There are unique choices for the average distance r and the average velocity v such that $\int_0^1 \mathbb{X}(\varphi)\mathrm{d}\varphi = 0$. Upon substitution into Newton's equations, we obtain the analogue of (3.2)

$$\omega^2 \partial_{\varphi\varphi} \mathbb{X} = \Phi'(r + \mathbb{X}(\varphi + k) - \mathbb{X}(\varphi)) - \Phi'(r + \mathbb{X}(\varphi) - \mathbb{X}(\varphi - k)), \tag{3.4}$$

with the three parameters r, k, ω. Another useful formulation is the fixed point equation, or nonlinear eigenvalue problem, for $\mathbb{V} = \partial_\varphi \mathbb{X}$

$$\omega^2 \mathbb{V} = \mathcal{F}(\mathbb{V}) := \hat{A}_k \partial\Phi \left(r + \hat{A}_k \mathbb{V} \right), \tag{3.5}$$

where the operator $\hat{A}_k$ and the Nemyckii operator $\partial\Phi$ are defined by

$$\begin{aligned}
(\hat{A}_k \mathbb{V})(\varphi) &:= A_k \mathbb{V}(\varphi) - k \int_0^1 \mathbb{V}(s) \mathrm{d}s \,, \quad A_k \mathbb{V}(\varphi) := \int_{\varphi - k/2}^{\varphi + k/2} \mathbb{V}(\tau) \mathrm{d}\tau \\
\partial\Phi(\mathbb{V})(\varphi) &:= \Phi'(\mathbb{V}(\varphi)).
\end{aligned}$$

Distances and velocities of the microscopic wave trains are then

$$r_\alpha(t) = r + A_k \mathbb{V}(k\alpha + \omega t + k/2) \,, \quad v_\alpha(t) = v + \omega \mathbb{V}(k\alpha + \omega t). \tag{3.6}$$

Existence and approximation of wave trains

We give an overview of the variational approach to wave train existence and approximation by numerical schemes that are based on maximizing

$$\mathcal{W}(\mathbb{V}) = \int_0^1 \Phi\Big(r + \hat{A}_k \mathbb{V} \Big) \, \mathrm{d}\varphi, \; \mathbb{V} \in H_\gamma := \left\{ \mathbb{V} \in L^2([0,1]) \,:\, \frac{1}{2} \|\mathbb{V}\|_{L^2}^2 \le \gamma \right\}.$$

Problem 3.1. *For given parameters r, k and $\gamma > 0$ we seek maximizers of $\mathcal{W}$ in H_γ, i.e. we solve $W(r, k, \gamma) = \max_{\mathbb{V} \in H_\gamma} \mathcal{W}(\mathbb{V})$.*

Theorem 3.2. *Problem 3.1 always has a solution. In particular, there exists a maximizer $\mathbb{V}$ with $\| \mathbb{V} \|_{L^2} = \sqrt{2\gamma}$ together with a positive Lagrangian multiplier $\omega_1^2 > 0$ such that $\mathbb{V}$ and ω^2 solve* (3.5).

Scheme 3.3. *Let any parameter set for problem 3.1 be given, and let $\mathbb{V}_0 \in H_\gamma$ be an arbitrary initial datum with $\hat{A}_k \mathbb{V}_0 \neq 0$. Then we define inductively two sequences $(\mathbb{V}_n)_{n \in \mathbb{N}} \subset H_\gamma$ and $(\omega_n)_{n \in \mathbb{N}}$ by the following iteration step*

$$\mathbb{V}_{n+1} = \frac{1}{f_n} \mathbb{W}_n \,, \quad \mathbb{W}_n = \mathcal{F} \mathbb{V}_n \,, \quad f_n = \frac{\| \mathbb{W}_n \|_{L^2}}{\sqrt{2\gamma}} \,, \quad \omega_{n+1} = \sqrt{f_n}.$$

In [Her04] it is proved that this scheme is compact, and numerical simulations indicate that 3.3 converges.

Remark 3.4. In fact, Theorem 3.3.2 in [Her04] proves that every closed cone of functions that is invariant under $\mathcal{F}$ contains at least one traveling wave. For the cone of even monotone functions used below, this was also shown in [FV99], Theorem 2.14.

By means of Scheme 3.3 we can compute wave trains with prescribed parameter $\gamma = \frac{1}{2}\,\|\mathbb{V}\|_{L^2}^2$. There are variants of 3.3 which allow to prescribe either the entropy S or the temperature T of a wave train (for the definition of S and T see §3.1 below). Hence, wave trains are parametrized (at least) by (k, r, γ), as well as trivially by v; the latter is relevant for the modulation equations discussed in §4. On may view the parameter ω of the wave train equation (3.4) depending on (r, k, γ) via a 'dispersion relation', here expressed as the Lagrange multiplier. We emphasize, that it is not known whether the set of wave trains is a smooth three-dimensional manifold of orbits; note that phase shifts $\mathbb{V}(\cdot + s)$ trivially give rise to an (at least) one-dimensional kernel of the linearization $\omega^2 - D\mathcal{F}(\mathbb{V})$ of (3.5) spanned by $\partial_\varphi \mathbb{V}$. Moreover, for given parameters there is a discrete multiplicity of solutions, because solutions for mk, $m \in \mathbb{N}$, are solutions for k as well, though these do not have minimal period 1. We conjecture that wave trains are unique in cones defined by monotonicity properties of $\mathbb{V}$ as discussed below.

Existence and approximation of multi-phase wave trains

We present new results concerning the existence of multi-phase waves, which will be published with full details elsewhere. As before, our variational approach is essentially restricted to convex interaction potentials Φ, but allows for arbitrary large amplitudes.

For simplicity we consider only two-phase wave trains having two wave numbers k_1 and k_2. However, all results can easily be generalized to other multi-phase wave trains. Moreover, to avoid technicalities we always suppose that Φ is defined on the whole real axis with bounded and continuous second derivative Φ''.

A *two-phase wave train* is an exact solution of Newton's equations satisfying

$$x_\alpha(t) = r\alpha + vt + \mathbb{X}(k_1\alpha + \omega_1 t,\, k_2\alpha + \omega_2 t). \tag{3.7}$$

Here r, v, k_1, k_2, ω_1 and ω_2 are given parameters, and the profile function $\mathbb{X}$ is assumed to have zero average and be 1-periodic with respect to each phase variable $\varphi_i = k_i\alpha + \omega_i t$. The ansatz (3.7) gives rise to the advance-delay differential equation

$$\big(\omega_1^2\,\partial_{\varphi_1}^2 + \omega_2^2\,\partial_{\varphi_2}^2\big)\mathbb{X} = \nabla^-\partial\Phi\big(r + \nabla^+\mathbb{X}\big) \tag{3.8}$$

where $\nabla^\pm$ are difference operators defined by

$$\big(\nabla^\pm\mathbb{X}\big)(\varphi_1,\, \varphi_2) := \pm\mathbb{X}(\varphi_1 \pm k_1,\, \varphi_2 \pm k_2) \mp \mathbb{X}(\varphi_1,\, \varphi_2)$$

Our aim is to identify an optimization problem with a single scalar constraint such that (3.8) is equivalent to the corresponding Euler-Lagrange equation with multiplier ω_1^2. Consequently, we regard the ratio $\beta = \omega_2/\omega_1$ as parameter of this problem.

Let $\mathcal{T}_2 \cong [0,\, 1] \times [0,\, 1]$ be the two dimensional torus with its canonic Lebesgue measure, and let all function spaces which follow be defined on $\mathcal{T}_2$. We consider the

Sobolev space

$$H_0^1 = \left\{ X \in H^1 : \int_{\mathcal{T}_2} X = 0 \right\}, \quad \| X \|_{H_0^1}^2 := \int_{\mathcal{T}_2} (\partial_{\varphi_1} \mathbb{X})^2 + \beta^2 (\partial_{\varphi_2} \mathbb{X})^2. \tag{3.9}$$

This norm is equivalent to the standard norm on H_0^1 as long as $\beta \neq 0$. Let E be the canonic embedding $E : H_0^1 \to L^2$, and E^* its adjoint operator $E^* : L^2 \to H^{-1} = (H_0^1)^*$. Note that E is compact, and that here we have identified L^2 with its dual L^{2^*}. By $\triangle$ we denote the Laplace operator corresponding to (3.9), i.e.

$$\triangle := \partial_{\varphi_1}^2 + \beta^2 \, \partial_{\varphi_2}^2.$$

Recall that $-\triangle : H_0^1 \to H^{-1}$ is an isometric isomorphism between Hilbert spaces, and that the difference operators $\nabla^\pm : L^2 \to L^2$ are continuous with $(\nabla^+)^* = -\nabla^-$. Moreover, our assumptions on Φ imply that the convex functional $\mathbb{X} \mapsto \int_{\mathcal{T}_2} \Phi(\mathbb{X})$ is well defined and continuous on L^2.

The spaces and operators from above allow to regard the wave train equation as an equation in H^{-1}. In particular, (3.8) is equivalent to

$$-\omega_1^2 \triangle X = E^* \big(\nabla^+\big)^* \, \partial\Phi\big(r + \nabla^+ E \, \mathbb{X}\big), \tag{3.10}$$

where the Nemyckii operator $\partial\Phi : L^2 \to L^2$ with $\mathbb{X} \mapsto \Phi'(\mathbb{X})$ is the Gateaux differential of the functional (3.11). For fixed $\gamma > 0$ we define the closed convex set $H_\gamma \in L^2$ and the convex Gateaux differentiable functional $\mathcal{W}$ as follows

$$H_\gamma = \left\{ X \in H_0^1 \; : \; \tfrac{1}{2} \| X \|_{H_0^1}^2 \leq \gamma \right\}, \quad \mathcal{W}(\mathbb{X}) := \int_{\mathcal{T}_2} \Phi\big(\nabla^+ E \, \mathbb{X}\big). \tag{3.11}$$

Now (3.10) yields the following constrained optimization problem.

Problem 3.5. *For given parameters r, k_1, k_2, $\gamma > 0$ and $\beta \neq 0$ we seek maximizers of $\mathcal{W}$ in H_γ, i.e. we solve*

$$W(r, \, k_1, \, k_2, \, \beta, \, \gamma) = \max_{\mathbb{X} \in H_\gamma} \mathcal{W}(\mathbb{X}).$$

Theorem 3.6. *Problem 3.5 always has a solution. In particular, there exists a maximizer $\mathbb{X}$ with $\| \mathbb{X} \|_{H_0^1} = \sqrt{2\gamma}$ together with a positive Lagrangian multiplier $\omega_1^2 > 0$ such that $\mathbb{X}$ and ω_1^2 solve* (3.10).

Remark 3.7. By construction, (3.10) is an identity in H^{-1}. However, $\mathbb{X} \in H^1$ implies that the right hand side of (3.10) is again an element of H^1, and the theory of elliptic regularity provides $\mathbb{X} \in H^3$. Moreover, we can prove further regularity by exploiting Sobolev's embedding theorems.

In analogy to the single-phase wave trains, we can solve the optimization problem 3.5 iteratively using an adapted abstract approximation scheme.

Geometry and phase velocity of wave trains

Since the modulation equations for the macroscopic limit of the chain depend on wave trains, it is essential to understand properties of wave trains and their parameter variation. Motivated by numerical simulations, we investigate geometric properties of wave trains in the phase space of distances and velocities. With the shock problem in mind, see §6, we are also interested in the transition to solitons as the wave number tends to zero.

From (3.5) we infer that if $(\mathbb{V}, \omega, k, r)$ is a solution to (3.5), then $(-\mathbb{V}, \omega, 1-k, r)$ is also a solution, and vice versa: $\mathbb{V}(\varphi; k) = -\mathbb{V}(\varphi + 1/2; 1-k)$. In case of a binary oscillation, $k = 1/2$, the symmetry implies that (3.4) reduces to the planar Hamiltonian ODE

$$\omega^2 \partial_{\varphi\varphi} \mathbb{X} = \Phi'(r - 2\mathbb{X}) - \Phi'(r + 2\mathbb{X}). \tag{3.12}$$

More generally, for rational $k = n/m$ equation (3.4) can be written as an m-dimensional second order Hamiltonian ODE with components $\mathbb{X}_j = \mathbb{X}(\cdot + jn/m)$, $j = 0, \dots m-1$. This system is equivariant under the $\mathbb{Z}_m$ action $\mathbb{X}_j \to \mathbb{X}_{j+1}$, where indices are taken modulo m, and $\mathbb{Z}_m$ lies in the isotropy subgroup of wave trains.

The microscopic phase space of distances and velocities is in fact the phase space of the ODE (3.12) for $k = 1/2$. Therefore, the orbits

$$Q := \{(r + A_k\mathbb{V}(\varphi + k/2), v + \omega\mathbb{V}(\varphi)) \,|\, 0 \le \varphi < 1\} \tag{3.13}$$

are convex, non self-intersecting curves and nested for different ω with fixed (r, k).

We can prove some of these properties for general wave number k, see also Figure 5.4, and define the positive cones

$$\begin{aligned} \mathcal{M}_\pm \;:=\; & \{\mathbb{V}(1+\varphi) = \mathbb{V}(\varphi),\, \int_0^1 \mathbb{V}(s)\mathrm{d}s = 0,\, \mathbb{V}(\varphi) = \mathbb{V}(-\varphi), \\ & \mathrm{sgn}(\mathbb{V}(\varphi_1) - \mathbb{V}(\varphi_2)) = \pm 1,\, 0 < \varphi_1 < \varphi_2 < 1/2\}, \end{aligned}$$

so that $\mathbb{W} \in \mathcal{M}_\pm$ has unique global extrema at $\varphi = 0$ and $\varphi = 1/2$, and $\mathbb{W}(\varphi_1) = \mathbb{W}(\varphi_2)$ is equivalent to $\varphi_1 \in \{\varphi_2, -\varphi_2, 1-\varphi_2\}$. By symmetry $\mathbb{W} \in \mathcal{M}_\pm$, implies $\mathbb{W}(\cdot + 1/2) \in \mathcal{M}_\mp$. The basis of the following results is the observation $\mathcal{F} : \overline{\mathcal{M}_\pm} \to \mathcal{M}_\pm$, which was noted in [FV99]. Throughout this article, we are only interested in wave trains in $\mathcal{M}_+ \cup \mathcal{M}_-$, and conjecture that wave trains are unique within these cones.

Let $Q_\Phi = \{\Phi''(r + A_k\mathbb{V}(\varphi)) \mid 0 < \varphi \le 1\}$. We will estimate the phase velocity $c_{\mathrm{ph}} := \omega/k$ of wave trains and the size of Q in terms of

$$M := \max Q_\Phi(\mathbb{V}) \,, \quad m := \min Q_\Phi(\mathbb{V}).$$

Remark 3.8. Note that $\sqrt{m}$, $\sqrt{M}$ are the characteristic velocities of the p-system. Applying Theorem 3.10 below for monotone Φ'', these values are attained at $\varphi = 0, 1/2$, respectively.

Next, we report our main, new results concerning the general geometry and phase velocity of wave trains; full proofs will appear elsewhere.

Theorem 3.9. *Assume $\Phi'' > 0$. Then (3.5) has solutions $(\omega, \mathbb{V}) \in \mathbb{R}_0 \times \mathcal{M}_+$ for any $(\gamma, r, k) \in \mathbb{R}^2 \times (0, 1/2)$ such that $k \to 0 \Leftrightarrow \omega \to 0$.*

More precisely, the phase velocity of these wave trains satisfies

$$b(k)\sqrt{m} \;\leq\; \frac{|\omega|}{k} \;\leq\; \sqrt{M}, \tag{3.14}$$

where $b(k) \in (0, 1/2)$, $b(k) = 1/2$ for $k \leq 2\varphi_*$ with $\mathbb{V}(\varphi_*) = 0$ the unique root of $\mathbb{V}$. For $2\varphi_* < k < 1/2$, we can take

$$b(k) = \frac{1}{4} - \frac{\int_{-k/4}^{k/4} |\mathbb{V}(\varphi)|^2 + |\mathbb{V}(\varphi + 1/2)|^2 \mathrm{d}\varphi}{4||\mathbb{V}||_2^2}.$$

Theorem 3.9 states that the lower phase velocity bound of wave trains is estimated by a correction of the p-system characteristic. Indeed, small amplitude wave trains have $m \sim \Phi''(r)$, so that the harmonic phase velocities $\sqrt{m}\sin(\pi k)/\pi k$ apply, which, being *smaller* than $\sqrt{m}$, necessitate a correction such as $b(k)$.

Theorem 3.10. *Assume $\Phi'' > 0$ and consider solutions $\mathbb{V} \in \mathcal{M}_+$ to (3.5) for given (r, k, γ). Then the curve Q is smooth, closed, convex and non self-intersecting. Its unique extrema in r-direction lie at $\varphi = -k/2, (1-k)/2$ and in v-direction at $\varphi = 0, 1/2$, and it is bounded by $|\omega| \leq k\sqrt{M}$ and*

$$\frac{1}{2}k|\mathbb{V}(\varphi)| \;\leq\; |A_k\mathbb{V}(\varphi)| \;\leq\; \sqrt{k}||\mathbb{V}||_2. \tag{3.15}$$

If Φ'' is monotone, and ω independent of (r, k), then ω is a strictly monotone function of γ and the curves Q are nested near the extrema in r- and v-directions for fixed (r, k). The sign of monotonicity is that of ω.

While the unique points on Q with vertical and horizontal slope lie at $\varphi = (1 - k)/2, 1/2$ and $\varphi = 0, -k/2$, the limiting profile for $k \to 0$ is not necessarily parametrized by φ. Indeed, for a limiting soliton, we expect that only one of these pairs converges to the point (r, v) of the soliton's background state as $k \to 0$.

The harmonic dispersion relation (3.18) renders ω a function of k, so that the last part of Theorem 3.10 does not apply. Indeed, in this case $\mathbb{V}$ is independent of k and ω, see (3.17).

Remark 3.11. The estimates on the size of Q imply that a nontrivial solitary limit as $k \to 0$ requires unbounded norm parameter γ, growing at least like $1/k$. Since Theorem 3.9 also implies $\omega \to 0$ as $k \to 0$, we expect that the monotonicity of γ in ω holds in general for small ω.

Nestedness of Q near the extrema in r and v directions for fixed (r, k) is a biproduct of our approach. However, it seems difficult to prove the numerical observation that the entire phase plots are nested.

Thermodynamics of wave trains

Wave trains represent exact solutions of Newton's equations which are highly oscillating on the microscopic scale. However, on the macroscopic scale we cannot resolve the microscopic oscillations but must pass to a thermodynamic description involving energy, pressure, temperature and the like. It turns out that for each wave train all these thermodynamic quantities are constant on the macroscopic scale. As a consequence, we can interpret each exact wave train solution of Newton's equation as a "thermodynamic state" of the chain. This idea turns out to be fruitful in modulation theory discussed in §4, where we allow for macroscopic modulations of the thermodynamic states.

Most thermodynamic quantities are defined as mean values of the oscillating atomic data in a wave train solution:

$$\begin{aligned} W &= \int_0^1 \Phi(r + A_k \mathbb{V}(\varphi))\,\mathrm{d}\varphi && \text{specific internal potential energy density,} \\ p &= -\int_0^1 \Phi'(r + A_k \mathbb{V}(\varphi))\,\mathrm{d}\varphi && \text{pressure = negative specific force density,} \\ K &= \frac{\omega^2}{2}\int_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi && \text{specific internal kinetic energy density,} \end{aligned}$$

and further

$$\begin{aligned} T &= 2K && \text{kinetic temperature,} \\ F &= K - W && \text{specific internal action density,} \\ U &= K + W && \text{specific internal energy density,} \\ E &= \frac{1}{2}v^2 + U && \text{specific total energy density.} \end{aligned}$$

Note that $K = \omega^2\gamma$, where γ is norm parameter used above. All these quantities are constants for exact wave trains. However, in modulation theory they become fields in $\overline{t}$ and $\overline{\alpha}$ whose macroscopic evolution is described by the modulation equations. In particular, although all quantities are defined by integrals over the phase variable φ, in modulation theory they represent *specific densities*.

There are other important thermodynamic quantities which are not directly related to mean values of the atomic data. It turns out that

$$S := \omega \int_0^1 \mathbb{V}(\varphi)^2\ \mathrm{d}\varphi\ , \quad g := -\int_0^1 \mathbb{V}(\varphi)\,\Phi'(r + A_k \mathbb{V}(\varphi))\,\mathrm{d}\varphi \tag{3.16}$$

can be interpreted as the macroscopic *entropy density* and *entropy flux*, respectively. It is proven in [Her04, DHM06] that any smooth family of wave trains provides an equation of state together with a corresponding Gibbs equation.

independent variables	*thermodynamic potential*	*Gibbs equation*
$(r,\ k,\ \gamma)$	$W = W(r,\ k,\ \gamma)$	$\mathrm{d}W = \omega^2\,\mathrm{d}\gamma\ -\ p\,\mathrm{d}r\ -\ g\,\mathrm{d}k$
$(r,\ k,\ \omega)$	$F = F(r,\ k,\ \omega)$	$\mathrm{d}F = S\,\mathrm{d}\omega\ +\ p\,\mathrm{d}r\ +\ g\,\mathrm{d}k$
$(r,\ k,\ S)$	$U = U(r,\ k,\ S)$	$\mathrm{d}U = \omega\,\mathrm{d}S\ -\ p\,\mathrm{d}r\ -\ g\,\mathrm{d}k$

The different variants of equations of state and Gibbs equations are all equivalent as long as the respective changes of coordinates are well defined.

The Gibbs equation becomes very important in modulation theory, where it provides the closure for the modulation equations. In particular, if the equation of state is known, then all other constitutive relations are determined by the Gibbs equation.

Examples for wave trains

For a few specific potential, explicit expressions are known for both the profile functions and the equation of state. The following examples are taken from [Her04, DHM06].

The harmonic chain with interaction potential $\Phi(r) = c_0 + c_1\,r + \frac{c_2}{2}\,r^2$. Here the linearity of Φ' implies that (3.5) may be solved by means of Fourier transform. Some simple calculations yield the following family of traveling waves, parameterized by $(r,\ k,\ \gamma)$,

$$\mathbb{V}(\varphi)\ =\ 2\sqrt{\gamma}\,\sin(2\pi\varphi), \qquad A_k\mathbb{V}(\varphi + k/2)\ =\ (\sin(\pi\,k)/\pi)\,\mathbb{V}(\varphi). \tag{3.17}$$

Here $\mathbb{V}$ is independent of (r, k) and $A_k\mathbb{V}$ independent of r. Degeneracy of the harmonic chain is also reflected by the *harmonic dispersion relation*

$$\omega(k) = \sqrt{c_2}\sin(\pi k)/\pi, \tag{3.18}$$

which provides the frequency ω as function of k, and does not depend on r or γ. Consequently, for the harmonic chain we cannot choose r, k and ω as set of independent variables. From (3.17) we infer that the equation of state reads

$$W(r,\ k,\ \gamma) = c_0 + c_1\,r + \frac{1}{2}\,c_2\,r^2 + \omega(k)^2\gamma,$$

which implies $g(r,\ k,\ \gamma) = -c_2\,\sin(2\pi k)\gamma$ and $S(r,\ k,\ \gamma) = 2\omega(k)\gamma$. Moreover, we can replace γ by S, and obtain

$$U(r,\ k,\ S) = c_0 + c_1 r + \frac{1}{2}c_2 r^2 + \omega(k)S. \tag{3.19}$$

The hard sphere model with interaction radius r_0. Here all atomic interaction are modeled as elastic collision between hard spheres with radius r_0. This gives rise to an interaction potential Φ with

$$\Phi(r) = +\infty \quad \text{for} \quad r < r_0, \quad \Phi(r) = 0 \quad \text{for} \quad r \geq r_0.$$

Although this potential is not smooth the notion of traveling waves may be generalized to this case, and again we are able to derive explicit expressions for wave trains. Some basic arguments lead to the following family of traveling waves, parameterized by $(r,\, k,\, \omega)$,

$$\mathbb{V}(r,\, k,\, \varphi) = \begin{cases} -(r - r_0)/k & \text{if} \quad 0 \le \varphi < k, \\ +(r - r_0)/(1 - k) & \text{if} \quad k \le \varphi < 1. \end{cases}$$

Note that here the frequency $\omega > 0$ is a free parameter and may be chosen independently of r and k. The corresponding equation of state reads

$$U(r,\, k,\, S) = \tfrac{1}{2}\,(r - r_0)^{-2}\, S^2\, k\,(1 - k). \tag{3.20}$$

We mention that the hard sphere model describes the high energy limit for certain potentials, see [Tod81] for the Toda potential, and [FM02], as well as §3.2, for Lennard-Jones potentials.

The third example is the *small amplitude limit*, where the amplitude δ of $\mathbb{V}$ is defined as the first fourier coefficient, i.e. for odd $\mathbb{V}$ we find $\delta = \int_0^1 \mathbb{V}(\varphi)\,\cos(2\pi\varphi)\,\mathrm{d}\varphi$. To identify the leading order terms we expand the nonlinear interaction potential Φ around the mean distance r up to fourth order. To leading order the frequency ω must satisfy the harmonic dispersion relation which now reads $\Omega_0(r,\, k) = \sqrt{\Phi''(r)}\,\sin(k\,\pi)/\pi$. According to [DHM06], the amplitude δ and the action F can be expressed in powers of $\omega - \Omega_0(r,\, k)$ as follows

$$\begin{aligned} \delta^2 &= \frac{\omega^2 - \Omega_0(r,\, k)^2}{2\,\Omega_0(r,\, k)^2}\, G(r,\, k), \\ F(r,\, k,\, \omega) &= -\Phi(r) + G(r,\, k)(\omega - \Omega_0(r,\, k))^2 + \mathcal{O}\big((\omega - \Omega_0(r,\, k))^3\big), \end{aligned} \tag{3.21}$$

where $G(r,\, k)$ is given by

$$G(r,\, k) = \frac{\Phi''(r)^2}{2\,\pi^2\,\Phi''(r)\,\Phi^{(4)}(r)\,\big(1 - \cos(2\pi k)\big) + \big(\Phi'''(r)\big)^2\big(1 + \cos(2\pi k)\big)}.$$

3.2 Solitary waves

Homoclinic orbits in ODEs are typically accompanied by large wave length periodic orbits in the sense that there exists a parameter curve of periodic orbits converging to the homoclinic orbit as the period tends to infinity [VF92]. For the lattices we consider, the situation is similar: wave trains exist for arbitrarily larger wave number and limit to solitons as the wave number tends to zero. This was proven for certain monotone waves and potentials under growth assumptions in [PP00] by a mountain pass approach.

We thank Karsten Matthies (University of Bath) for providing notes on which the remaining part of this section is based. We report some of his joint work with Gero

Friesecke, mainly concerning solitons in (1.1) in the form (3.1) for a large class of possibly non-convex potentials Φ.

A prototype of physically realistic interaction is given by the standard Lennard-Jones potentials

$$\Phi(r) = a\Big(r^{-m} - r_*^{-m}\Big)^2 \text{ for } r > 0, \quad a > 0,\ m \in \mathbb{N}.$$

where Φ is minimized when neighbouring particles are placed at some specific equilibrium distance $r = r_* > 0$, and tends to infinity as the neighbour distance tends to zero.

Since the particle positions x_α corresponding to displacements y_α are $x_\alpha = r_*\alpha + y_\alpha$, this means that $\Phi(r)$ must have a minimum at $r = r_*$ and that $\Phi(r) \to \infty$ as $r \to 0$. More precisely we assume:

(H1) (Minimum at r_*) $\Phi \in C^3(0,\infty)$, $\Phi(r_*) = \Phi'(r_*) = 0$, $\Phi''(r_*) > 0$
(H2) (Growth) $\Phi(r) \geq c_0 r^{-1}$ for some $c_0 > 0$ and all r close to 0 and $\Phi(r) = \infty$ for $r \leq 0$.
(H3) (Hardening) $\Phi'''(r) < 0$ in $(0, r_*]$, $\Phi(r_* + r) < \Phi(r_* - r)$ in $(0, r_*)$.

Here we seek solitons whose profile $\mathbb{Y}(\phi)$ solves (3.2) with $r = r_*$. The construction in [FW94] for the existence of solitons is based on the variational problem

$$\begin{aligned}&\text{Minimize } \gamma_*(\mathbb{Y}) := \frac{1}{2}\int_{\mathbb{R}} \partial_\phi \mathbb{Y}(\phi)^2 d\phi \text{ among } \mathbb{Y} \in W^{1,2}_{\text{loc}}(\mathbb{R}) \text{ satisfying}\\ &\partial_\varphi \mathbb{Y} \in L^2(\mathbb{R}),\ \mathcal{W}_*(\mathbb{Y}) := \int_{\mathbb{R}} \Phi(r + \mathbb{Y}(\phi+1) - \mathbb{Y}(\phi))\mathrm{d}\phi. \qquad (3.22)\end{aligned}$$

Remark 3.12. It is instructive to compare this ansatz with the one used for wave trains in §3.1, where the real line is replaced by the unit interval and $\mathcal{W}$ maximized for fixed norm parameter γ. This lead to a relatively simple convex maximization problem for convex potentials. In contrast, (3.22) is a kind of dual problem, where $\mathcal{W}_*$ is fixed and the norm parameter γ_* minimized; a more challenging formulation that allows for non-convex potentials.

The goal is to determine the Γ-limit of the variational problem and the limiting profile in the high-energy regime. Since this regime is highly discrete and involves strong forces, neither classical continuum approximations nor weak coupling approximations are possible.

The limiting profile for $\mathcal{W}_*(\mathbb{Y}) \to \infty$ was derived in [FM02]. Here we recover this as a corollary of the following Γ-convergence result. We let

$$H^* := \{\mathbb{Y} \in W^{1,2}_{\text{loc}}(\mathbb{R}) | \mathbb{Y}(0) = 0, \partial_\phi \mathbb{Y} \in L^2(\mathbb{R})\},$$

and for every displacement profile $\mathbb{Y}$ we denote the relative displacement profile by $r(\phi) = \mathbb{Y}(\phi+1) - \mathbb{Y}(\phi)$. As in (3.22) we consider the functional γ_* on

$$\begin{aligned} H^*_K &= \{\mathbb{Y} \in H^* \,|\, \mathcal{W}_*(\mathbb{Y}) = K\}\\ H^*_\infty &= \{\mathbb{Y} \in H^* \,|\, r(\phi) \geq -r_*; \forall \phi \in \mathbb{R}\\ &\qquad \exists \text{ compact nonempty set } S_{\mathbb{Y}} \subset \mathbb{R} \text{ with } r_{|S_{\mathbb{Y}}} = -r_*\}.\end{aligned}$$

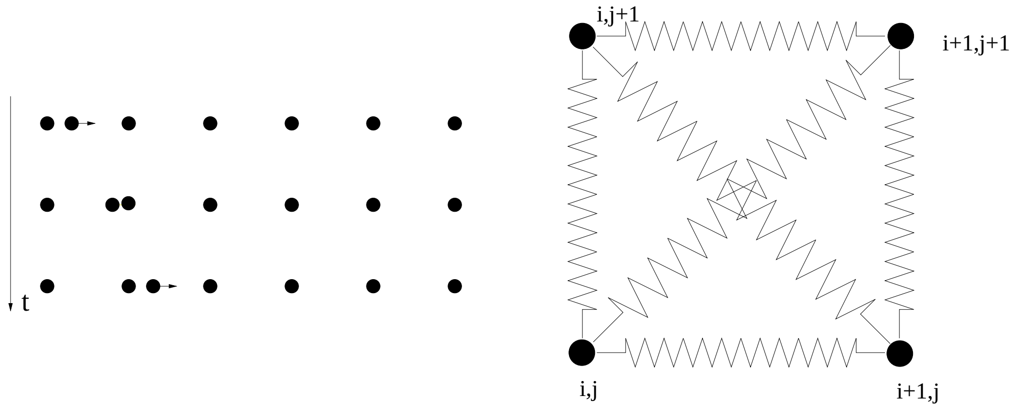

Figure 3.1: Left: Hard-sphere soliton. Right: cell of springs in 2D lattice.

Theorem 3.13. (Γ-convergence) *Assume that the interaction potential satisfies (H1), (H2). Then the problem 'Minimize $\gamma_*(\mathbb{Y})$ for $\mathbb{Y} \in H_K^*$' Γ-converges to the problem 'Minimize $\gamma_*(\mathbb{Y})$ for $\mathbb{Y} \in H_\infty^*$' in the sense that*

1. (lim-inf-inequality) *If $\mathbb{Y}^{(K)} \rightharpoonup \mathbb{Y}$ in H^* with $\mathbb{Y}^{(K)} \in H_K^*$, $\mathbb{Y}^{(K)}$ translation normalized (i.e. $r^{(K)}(0) = \min_{\phi\in\mathbb{R}} r^{(K)}(\phi)$), then $\mathbb{Y} \in H_\infty^*$ and $\gamma_*(\mathbb{Y}) \leq \liminf_{K\to\infty} \gamma_*(\mathbb{Y}^{(K)})$,*

2. (Existence of recovery sequence) *For all $\mathbb{Y} \in H_\infty^*$ there exists a sequence $\mathbb{Y}^{(K)} \in H_K^*$ with $\mathbb{Y}^{(K)} \rightharpoonup \mathbb{Y}$ in H^* and $\gamma_*(\mathbb{Y}^{(K)}) \to \gamma_*(\mathbb{Y})$.*

A consequence is the following piecewise linear asymptotic displacement profile, corresponding to piecewise constant velocity profile.

Corollary 3.14. (*Asymptotic shape of minimizers) Every translation normalized sequence $\mathbb{Y}^{(K)}$ of minimizers of γ_* on H_K^* converges in H weakly to the up to translation unique minimizer $\mathbb{Y}_\infty$ of the limit problem, where*

$$\mathbb{Y}_\infty(\phi) = \begin{cases} 0, & \phi \leq 0 \\ -r_*\phi, & \phi \in [0,1] \\ -r_*, & \phi \geq 1. \end{cases}$$

In a mechanical interpretation, this is a compression wave localized on a single atomic spacing. The limiting dynamics are hard-sphere dynamics like in a Boltzmann gas, see Figure 3.1. In particular the work shows that dispersionless transport of energy is not restricted to the long-wave regime.

We mention that Friesecke and Matthies analyse a two dimensional counterpart of (3.1) in [FM03], see Figure 3.1. The existence of longitudinal solitary waves along one of the lattice directions was shown for typical potentials under some mild nondegeneracy assumptions. These traveling waves are unique, i.e. there are no other localized traveling wave in the same direction, e.g. there do not exist transversal traveling waves. It is surprising that purely harmonic springs are included here, because solitary waves do not occur in harmonic chains.

4 Modulation Theory

4.1 Macroscopic evolution of data with temperature

In this section we use the theory of Young measures, see for instance [Tay96, War99, Daf00], and derive some restrictions for any thermodynamic limit of the chain.

Let $\Omega = \{(\overline{t},\, \overline{\alpha}) : 0 \le \overline{t} \le \overline{t}_{\rm fin},\, \overline{\alpha} \in [0,\, 1]\}$, and let $(N_i)_i$ be a sequence with $N_i \to \infty$. Moreover, for any i let $Q^{(i)}_\alpha(t) = (r^{(i)}_\alpha(t)\, v^{(i)}_\alpha(t))$, $0 \le t \le N_i \overline{t}_{\rm fin}$ and $\alpha = 1,\, ...,\, N_i$, be a solution of Newton's equation, and suppose that the total energy of the initial data is proportional to N_i, i.e.

$$\sum_{\alpha=1}^{N_i} \left(\frac{1}{2} \big(v^{(i)}_\alpha(0)\big)^2 + \Phi\big(r^{(i)}_\alpha(0)\big) \right) = \mathcal{O}(N_i). \tag{4.1}$$

Under some suitable assumptions on the potential (say boundedness of Φ'' for simplicity) the functions $Q^{(i)}_\alpha(t)$ are compact with respect to the convergence of Young measures in the following sense. There is at least a subsequence, still denoted by $(N_i)_i$, and a family of probability measures $(\overline{t},\, \overline{\alpha}) \mapsto \mu(\overline{t},\, \overline{\alpha},\, dQ)$ such that for any continuous observable $\psi = \psi(Q) = \psi(r,\, v)$ the following convergence is satisfied

$$\int_\Omega \psi\big(Q^{(i)}\big(N_i\, \overline{t},\, N_i\, \overline{\alpha}\big)\big)\, \xi\big(\overline{t},\, \overline{\alpha}\big)\; \mathrm{d}\overline{t}\, \mathrm{d}\overline{\alpha} \;\xrightarrow{i\to\infty}\; \int_\Omega \langle\psi\rangle\big(\overline{t},\, \overline{\alpha}\big)\, \xi\big(\overline{t},\, \overline{\alpha}\big)\; \mathrm{d}\overline{t}\, \mathrm{d}\overline{\alpha}. \tag{4.2}$$

Here ξ is an smooth test function, and $\langle\psi\rangle\big(\overline{t},\, \overline{\alpha}\big)$ is given by

$$\langle\psi\rangle\big(\overline{t},\, \overline{\alpha}\big) = \int_{\mathbb{R}^2} \psi(Q)\, \mu\big(\overline{t},\, \overline{\alpha},\, dQ\big). \tag{4.3}$$

For fixed $\big(\overline{t},\, \overline{\alpha}\big) \in \Omega$, the probability measure $\mu\big(\overline{t},\, \overline{\alpha},\, dQ\big)$ describes the microscopic oscillations in the vicinity of $\big(\overline{t},\, \overline{\alpha}\big)$, and for any observable Ψ the number $\langle\Psi\rangle\big(\overline{t},\, \overline{\alpha}\big)$ gives the *local mean value* of Ψ.

Here we consider the *common* probability distribution of distance and velocity instead of their separate statistics so that any measure $\mu\big(\overline{t},\, \overline{\alpha},\, dQ\big)$ can be interpreted as a weight function defined on the *microscopic state space* which is spanned by distance and velocity.

In §1 we have seen that Newton's equations are equivalent to the two *microscopic conservation laws* (1.3), from which one can derive the microscopic conservation of energy $\dot{e}_\alpha(t) = -f_\alpha(t) + f_{\alpha+1}(t)$ with $e_\alpha(t) = \frac{1}{2} v^2_{\alpha+1}(t) + \Phi(r_\alpha(t))$ and $f_\alpha(t) = -v_\alpha(t)\, \Phi'(r_\alpha(t))$. As a direct consequence, *every* Young measure limit must satisfy the following *macroscopic* conservation laws of mass, momentum and energy

$$\begin{aligned} \partial_{\overline{t}} \langle r\rangle - \partial_{\overline{\alpha}} \langle v\rangle &= 0, \\ \partial_{\overline{t}} \langle v\rangle - \partial_{\overline{\alpha}} \langle \Phi'(r)\rangle &= 0, \\ \partial_{\overline{t}} \big\langle \tfrac{1}{2} v^2 + \Phi(r)\big\rangle - \partial_{\overline{\alpha}} \langle v\, \Phi'(r)\rangle &= 0. \end{aligned} \tag{4.4}$$

This system of PDEs gives some restrictions for any young measure limit of the atomic chain. However, in general we can not express the fluxes in terms of the densities, and hence the system (4.4) is not closed, i.e. it does not determine the macroscopic evolution completely. We mention that (4.4) shows that any Young measure limit is a *measure-valued* solution of the p-system in the sense of DiPerna, see [Hör97, Daf00]. In addition, it is a measure-valued solution of the energy equation (1.11).

Within modulation theory we will start with some assumptions concerning the structure of the microscopic oscillations in the chain. Afterwards we will identify further macroscopic evolution laws extending (4.4), and constitutive relations that close the extended system.

4.2 Whitham modulation equations for wave trains

Here we describe Whitham's modulation theory for the atomic chain with hyperbolic scaling. For further examples concerning modulation theories of discrete system we refer to [HLM94, SW00, FP99, DK00, GM04, GM06], and to [GHM06a, GHM06b] for an overview.

A *modulated traveling wave* is an approximate solution of Newton's equation (1.1) satisfying

$$x_\alpha(t) = \frac{1}{\varepsilon}X(\varepsilon t,\, \varepsilon\alpha) + \tilde{\mathbb{X}}\Big(\varepsilon t,\, \varepsilon\alpha,\, \frac{1}{\varepsilon}\Theta(\varepsilon t,\, \varepsilon\alpha)\Big), \tag{4.5}$$

where X and Θ are macroscopic functions. The generic traveling wave parameters $(r,\, v,\, k,\, \omega)$ now are macroscopic fields depending on $(\overline{t},\, \overline{\alpha})$, and read

$$\omega = \partial_{\overline{t}}\Theta, \quad k = \partial_{\overline{\alpha}}\Theta, \quad v = \partial_{\overline{t}}X \quad r = \partial_{\overline{\alpha}}X. \tag{4.6}$$

The microscopic oscillations are described by

$$\tilde{\mathbb{X}}(\overline{t},\, \overline{\alpha},\, \varphi) = \mathbb{X}\big(r(\overline{t},\, \overline{\alpha}),\, v(\overline{t},\, \overline{\alpha}),\, k(\overline{t},\, \overline{\alpha}),\, \omega(\overline{t},\, \overline{\alpha}),\, a(\overline{t},\, \overline{\alpha}),\, \varphi\big), \tag{4.7}$$

where $\mathbb{X}(r,\, v,\, k,\, \omega,\, a,\, \varphi)$ is a smooth family of 1-periodic wave trains depending on the parameters $\vec{u} = (r,\, v,\, k,\, \omega,\, a)$ as well as on the phase φ. We use an additional parameter a, which might be the entropy S or the parameter γ. However, in any case we impose an abstract dispersion relation

$$\omega = \Omega(r,\, k,\, a). \tag{4.8}$$

The modulation equations are PDEs which describe the macroscopic evolution of the modulated parameter $(r,\, v,\, k,\, \omega,\, a)$, and ensure that (4.5) indeed provides approximate solutions. For their formal derivation we use Whitham's variational approach, see [Whi74, FV99, DHM06], and [GHM06a, GHM06b] for a more general setting.

In a first step we insert the ansatz (4.5) into the expression for the total action in the atomic chain, and expand all arising terms in powers of ε. This gives rise to the *reduced action integral*

$$\text{total action} = \mathbb{L}(X,\, \Theta,\, a) = \int\limits_0^{\overline{t}_{\mathrm{fin}}} \int\limits_0^1 L\big(\vec{u}(\overline{t},\, \overline{\alpha})\big)\, \mathrm{d}\overline{\alpha}\, \mathrm{d}\overline{t}, \tag{4.9}$$

with $L(\vec{u}) = \mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u},\, \cdot))$ and

$$\mathcal{L}(\vec{u},\, \mathbb{X}) = \int_0^1 \left(\frac{1}{2}(v + \omega\, \partial_\varphi \mathbb{X})^2 - \Phi(r + \nabla_k \mathbb{X})\right) \mathrm{d}\varphi,$$

where $(\nabla_k \mathbb{X})(\varphi) = \mathbb{X}(\varphi + k)$. In a second step we apply the principle of least action to (4.9). The variation with respect to a gives $\partial_a L = 0$, which recovers the dispersion relation (4.8), and the variations with respect to X and Θ yield

$$\partial_{\overline{t}} \partial_v L + \partial_{\overline{\alpha}} \partial_r L = 0 \quad \text{and} \quad \partial_{\overline{t}} \partial_\omega L + \partial_{\overline{\alpha}} \partial_k L = 0, \tag{4.10}$$

respectively. Moreover, the definitions (4.6) imply two further evolution equations, namely $\partial_{\overline{t}} r - \partial_{\overline{\alpha}} v = 0$ and $\partial_{\overline{t}} k - \partial_{\overline{\alpha}} \omega = 0$.

In the last step we reformulate all macroscopic identities by using the thermodynamic definitions from §3, and as a consequence we find that the modulation equations take the form

$$\partial_{\overline{t}} \Big(r,\, v,\, k,\, S\Big) + \partial_{\overline{\alpha}} \Big(-v,\, +p,\, -\omega,\, +g\Big) = 0. \tag{4.11}$$

These equations represent the macroscopic conservation laws for mass, momentum, wave number and entropy. Moreover, they imply the conservation of energy via

$$\partial_{\overline{t}} E + \partial_{\overline{\alpha}} \,\big(pv + g\omega\big) = 0. \tag{4.12}$$

and thus we can regard the system (4.11) as an extension of (4.4). Recall that the closure for (4.11) and (4.12) is provided by the equation of state $E = \frac{1}{2}v^2 + U(r,\, k,\, S)$ and the Gibbs equation (2.5). However, for almost all interaction potential Φ we lack explicit expressions for the equations of state, and therefore we cannot characterize the properties of (4.11).

Finally, we display the modulation equations for the harmonic chain

$$\partial_{\overline{t}} \Big(r,\, v,\, k,\, S\Big) - \partial_{\overline{\alpha}} \Big(v,\, c_2\, r,\, \omega(k),\, \omega'(k)\, S\Big) = 0, \tag{4.13}$$

which follow from (4.11) by means of the equation of state (3.19), and the harmonic dispersion relation (3.18).

4.3 The justification problem

So far, there is no known rigorous derivation of the modulation equations for the nonlinear case. For this reason we formulate a conjecture, following similar results for partial differential equations [KSM92, Sch98, Mie02]. We assume that the potential Φ is sufficiently smooth, and that a smooth family of traveling waves $\mathbb{X}(\vec{u},\,\varphi)$ with independent parameters $\vec{u} = (r,\, v,\, k,\, \omega)$ is given. Moreover, we assume that the following set $\mathcal{M}$ is open

$$\mathcal{M} = \left\{ \vec{u} = (r,\, v,\, k,\, \omega) \;\middle|\; \begin{array}{l} \text{the system (4.11) is strictly hyperbolic in } \vec{u}, \\ \text{the traveling wave } \mathbb{X}(\vec{u},\,\cdot) \text{ is linearly stable} \end{array} \right\}.$$

For a given solution $\vec{\overline{u}} = \vec{\overline{u}}(\overline{t},\,\overline{\alpha})$ of (4.11) we define

$$M^{\varepsilon}_{\alpha}(t) = \begin{pmatrix} \widetilde{r}(\varepsilon t,\,\varepsilon\alpha) + (\hat{A}_k\mathbb{V})\Big(\vec{\overline{u}}(\varepsilon t,\,\varepsilon\alpha),\, \tfrac{1}{\varepsilon}\widetilde{\Theta}(\varepsilon t,\,\varepsilon\alpha) + \tfrac{1}{2}\widetilde{k}(\varepsilon t,\,\varepsilon\alpha)\Big) \\ \widetilde{v}(\varepsilon t,\,\varepsilon\alpha) + \widetilde{\omega}(\varepsilon t,\,\varepsilon\alpha)\,\mathbb{V}\Big(\vec{\overline{u}}(\varepsilon t,\,\varepsilon\alpha),\, \tfrac{1}{\varepsilon}\widetilde{\Theta}(\varepsilon t,\,\varepsilon\alpha)\Big) \end{pmatrix},$$

where $\mathbb{V}$ abbreviates $\partial_{\varphi}\mathbb{X}$, and the modulated phase $\widetilde{\Theta}$ is given by (4.6). We believe that the following conjecture is in the heart of the matter.

Conjecture 4.1. *Let $\vec{\overline{u}}$ be a sufficiently smooth solution of Whitham's equation defined for $\overline{t} \in [0,\, \overline{t}_{\mathrm{fin}}]$, and suppose that $\vec{\overline{u}}$ takes values in $\mathcal{M}$. Then there exists a suitable Banach space Υ_{ε}, and some exponent $\kappa > 0$ such that*

$$\|Q^{\varepsilon}(t) - M^{\varepsilon}(t)\|_{\Upsilon_{\varepsilon}} = \mathcal{O}(\varepsilon^{\kappa}), \quad \|Q^{\varepsilon}(0)\|_{\Upsilon_{\varepsilon}} = \mathcal{O}(1) \tag{4.14}$$

for all ε, and all t with $0 \le \varepsilon t \le \overline{t}_{\mathrm{fin}}$.

At the moment we are far from being able to prove this conjecture in this general form. However, it does hold rigorously for the harmonic chain and the hard sphere model.

The proof for the harmonic chain essentially relies on the linearity of Newton's equations, which allows to control the residuum, see [DHM06]. In addition, there is further rigorous derivation of (4.11) in the context of Wigner measures. For the details we refer to [Mie06], and for similar results to [Mac02, Mac04]. The rigorous justification for the hard sphere model is based on the observation that both the microscopic dynamics and the macroscopic equations become much simpler in the Eulerian representation of thermodynamics, cf. [Her04]

On a formal level we expect a close relation between stability of wave trains and hyperbolicity of modulation equations; if Whitham's equations (4.11) are not hyperbolic, then the corresponding initial value problem is ill-posed, which indicates that traveling waves are unstable due to a Benjamin-Feir instability, see e.g. [Whi74, BM95]. However, for arbitrary interaction potential Φ, neither stability criterions nor hyperbolicity conditions are available up to now. Having linearly degenerate eigenvalues, the harmonic chain and hard sphere model are not prototypical and do not provide further insight. Only the small amplitude limit gives some criteria for the hyperbolicity of (4.11). Starting with the equation of state (3.21) we can compute the characteristic speeds for (4.11), see [DHM06], and end up with the following criterion. The system (4.11) has four real eigenvalues, and is thus hyperbolic, if

$$\begin{aligned}\hat{N}(r,\,k) =& \Big(\Phi'''(r)\Big)^2 \Big(7 - 8\cos(2\pi k) + \cos(4\pi k)\Big) + \\ & \Phi''(r)\,\Phi^{(4)}(r)\Big(4\cos(2\pi k) - 3 - \cos(4\pi k)\Big)\end{aligned}$$

is positive, but has two imaginary eigenvalues for $\hat{N}(r,\,k) < 0$. For $k = 1/2$ the corresponding formula was already given in [Fla96].

5 Numerical justification of modulation theory

Although there is no rigorous justification for the modulation equations (4.11), numerical simulations strongly indicate that they provide the right thermodynamic description for a wide class of initial value problems for the atomic chain. We refer to [DH06] which gives a detailed thermodynamic interpretation of several numerical experiments. The main results can be summarized as follows.

(*i*) If all macroscopic fields are smooth, then the arising oscillations in the atomic data can be described in terms of modulated traveling waves, and the macroscopic dynamics is governed by the modulation system (4.11).

(*ii*) Modulated traveling waves describe the microscopic oscillations emerging when cold data form shocks.

(*iii*) If the shocks emerge from data with temperature, then usually the microscopic oscillations exhibit a more complicated structure, and (single-phase) modulation theory fails in this case.

Concerning the last item, results for the Toda chain suggest a hierarchy of modulation models, enumerated by the number of phases, where shocks on a lower level require the model of the next level, see e.g. the review [LLV93] and the references therein.

Note that these numerical observation are valid only if the interaction potential Φ is convex, the macroscopic scale results from the hyperbolic scaling, and the microscopic initial data are given by modulated traveling waves.

In this section we give an brief survey on the numerical justification from [DH06], and present a typical example with periodic boundary conditions and smooth macroscopic fields. Moreover, in §6 we study the numerical solution of a Riemann problem with cold initial data, and give an improved discussion of its macroscopic limit.

In order to study the macroscopic behavior of the atomic chain for large N we must evaluate the thermodynamic properties of the numerical data which are the macroscopic fields of the local mean values, and the local distribution functions of the atomic data. The computation of both mean values and distribution functions relies on *mesoscopic space-time windows*. In what follows let $\mathcal{F} = I_{\mathrm{T}}^{\mathcal{F}} \times I_{\mathrm{P}}^{\mathcal{F}}$ be such a window where I_{T} and I_{P} are sets of time steps and particle indices, respectively. The window F is mesoscopic if and only if it is very small on the macroscopic scale, but contains a lot of particles as well as time steps, i.e. $\sharp I_{\mathrm{T}}, \sharp I_{\mathrm{P}} \sim N^{\kappa}$ for some exponent κ with $0 < \kappa < 1$. In particular, any F describes the microscopic vicinity of a certain macroscopic point $Z_{\mathcal{F}} = (\overline{t}_{\mathcal{F}}, \overline{\alpha}_{\mathcal{F}})$.

For any atomic observable ψ we can easily compute the mean value $\langle\psi\rangle_{\mathcal{F}}$ of ψ with respect to each window $\mathcal{F}$ by a simple averaging formula. Note that there is a close relation to the notion of Young measures. In particular, if the atomic data converge for $N \to \infty$ in the sense of Young measures, then $\langle\psi\rangle_{\mathcal{F}}$ is a good approximation for $\langle\psi\rangle(\overline{t}_{\mathcal{F}}, \overline{\alpha}_{\mathcal{F}})$ from (4.3). Moreover, by means of $\mathcal{F}$ we can compute the complete measure $\mu\big(\overline{t}_{\mathcal{F}}, \overline{\alpha}_{\mathcal{F}}, dQ\big)$, see [DH06] for the details.

The micro-macro transition of modulation theory relies on the hypothesis that all atomic oscillations can be described by modulated wave trains. If this is right, then the microscopic distributions functions within any space-time window $\mathcal{F}$ must be equivalent to an exact wave train. Of course, the parameters of this wave train may depend on $\mathcal{F}$. In order to justify this hypothesis for given $\mathcal{F}$, we have to identify four wave train parameters, namely the specific length $r_{\mathcal{F}}$, the mean velocity $v_{\mathcal{F}}$, the wave number $k_{\mathcal{F}}$ and a fourth parameter which might be the parameter $\gamma_{\mathcal{F}}$, the frequency $\omega_{\mathcal{F}}$, the entropy $S_{\mathcal{F}}$, or the temperature $T_{\mathcal{F}}$.

The values of $r_{\mathcal{F}}$, $v_{\mathcal{F}}$ and $T_{\mathcal{F}}$ are given by mean values of microscopic observables. This reads $r_{\mathcal{F}} = \langle r\rangle_{\mathcal{F}}$, $v_{\mathcal{F}} = \langle v\rangle_{\mathcal{F}}$, and $T_{\mathcal{F}} = \langle v^2\rangle_{\mathcal{F}} - \langle v\rangle_{\mathcal{F}}^2$. Determining $k_{\mathcal{F}}$ and $\omega_{\mathcal{F}}$ is not so obvious, because they have no immediate physical interpretation on the microscopic scale. To overcome this problem we introduce *auxiliary observables* Ψ_k and Ψ_ω, see [DH06] for their definitions, and set

$$k_{\mathcal{F}} := \langle\Psi_k\rangle_{\mathcal{F}}, \qquad \omega_{\mathcal{F}} := \langle\Psi_\omega\rangle_{\mathcal{F}}.$$

In the next step we start a numerical scheme similar to (3.3), which allows to prescribe the values $r_{\mathcal{F}}$, $v_{\mathcal{F}}$, $k_{\mathcal{F}}$ and $T_{\mathcal{F}}$, see [DH05] for details, and compute an exact wave train with these parameters. For any $\mathcal{F}$, the scheme yields a profile function $\mathbb{V}_{\mathcal{F}}$ as well as a frequency $\omega_{\mathcal{F}}^{\mathrm{TW}}$ which does not result from the auxiliary observable Ψ_ω but satisfies a dispersion relation.

Finally, we compare the microscopic distribution functions from the numerical data with their *macroscopic predictions* which can be expressed in terms of $\mathbb{V}_{\mathcal{F}}$. In particular, according to modulation theory, the support of the microscopic distribution functions must equal the curve

$$\varphi \mapsto Q^{\mathrm{TW}}(\varphi) = \Big(r_{\mathcal{F}} + \hat{A}_k \mathbb{V}_{\mathcal{F}}(\varphi + k_{\mathcal{F}}/2),\, v_{\mathcal{F}} + \omega_{\mathcal{F}}\, \mathbb{V}_{\mathcal{F}}(\varphi)\Big). \tag{5.1}$$

This rather strong prediction can be check for given numerical data.

Smoothly modulated initial data

We study the evolution of data with temperature by imposing initial data in form of smoothly modulated binary oscillations, i.e. we set

$$r_\alpha(0) = \begin{cases} r^{\,\mathrm{odd}}(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is odd}, \\ r^{\,\mathrm{even}}(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is even}, \end{cases} \qquad v_\alpha(0) \quad = \begin{cases} v^{\,\mathrm{odd}}(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is odd}, \\ v^{\,\mathrm{even}}(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is even}, \end{cases}$$

where $r^{\,\mathrm{odd}}$, $r^{\,\mathrm{even}}$, $v^{\,\mathrm{odd}}$ and $v^{\,\mathrm{even}}$ may be read off from Figure 5.1. We solved Newton's equation for the Toda chain with $N = 4000$ up to the macroscopic time $\overline{t}_{\mathrm{fin}} = 0.4$ by means of the Verlet scheme, see [SYS97, HLW02].

Figure 5.1 contains snapshots of the atomic data for several macroscopic times, where the black colored curves represent the local mean values, and Figure 5.2 shows the profiles for some macroscopic fields at time $\overline{t} = 0.4$. We observe that the atomic data are highly oscillating on the microscopic scale so that any appropriate mathematical descriptions of the limit $N \to \infty$ must rely on measures. The computation of wave number and frequency is illustrated in Figure 5.3, showing the oscillating values of the auxiliary observables Ψ_k and Ψ_Ω as well as their macroscopic mean values.

In Figure 5.4 we compare the microscopic distribution functions with their macroscopic predictions from modulation theory for six mesoscopic space-time windows at $\overline{t} = 0.4$. For each of these windows we represent the distribution function of microscopic data by a density plot with high (Gray) and low (White) probability for finding a particle. Note that the support of every distribution functions is contained in closed curves, and that the distribution functions vary on the macroscopic scale.

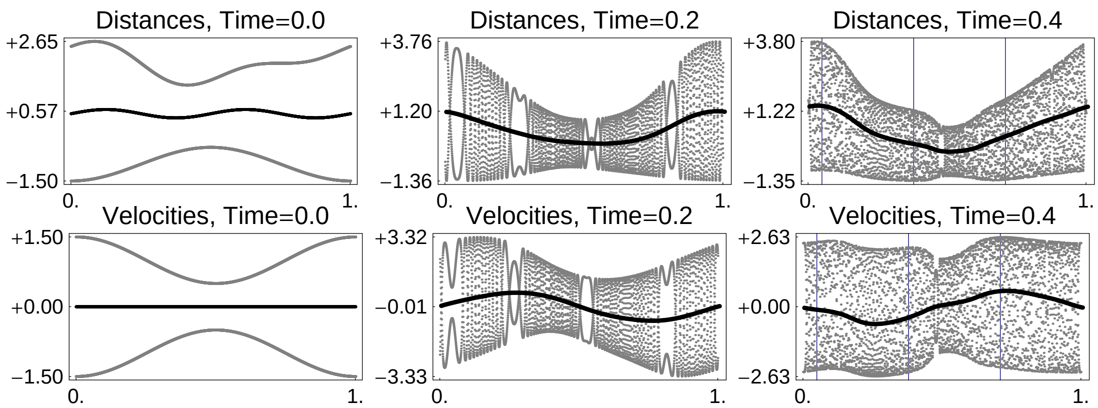

Figure 5.1: Snapshots of the atomic distances and velocities at several macroscopic times. The vertical lines at $\overline{t} = 0.4$ mark the space-time windows for Figure 5.4.

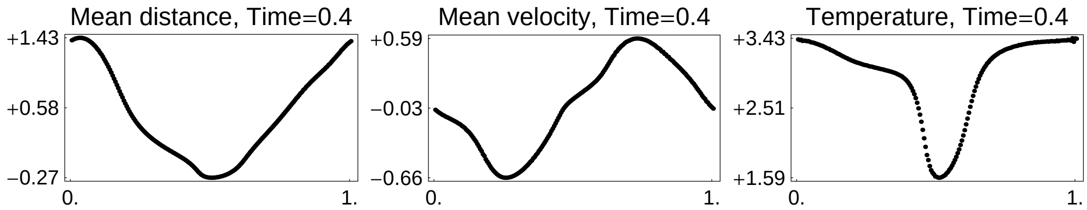

Figure 5.2: Selected macroscopic fields as functions of $\overline{\alpha}$ for $\overline{t} = 0.4$.

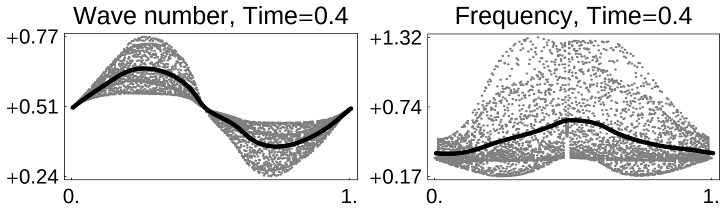

Figure 5.3: Wave number and frequency: oscillating auxiliary variables and macroscopic mean values.

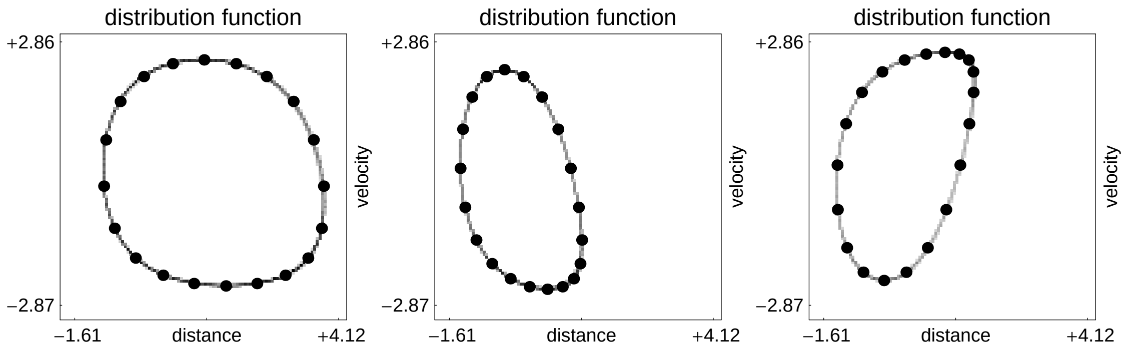

Figure 5.4: Distribution functions of the atomic data in three selected space-time windows at $\overline{t} = 0.4$; for the $\overline{\alpha}$-coordinates see Figure 5.1. Each picture contains a density plot of the atomic data (White and Gray) together with an illustration of the macroscopic prediction (Black).

The black dots in Figure 5.4 represent the macroscopic predictions: we project 20 points $Q_i = Q^{\mathrm{TW}}(i/20)$ of the curve (5.1), into the density plots. Figure 5.4 reveals that the curve (3.13) coincides with the support of the microscopic distribution functions, and that the distance between Q_{i+1} and Q_i is related to the gray level of the microscopic distribution functions. In conclusion, we can describe the microscopic oscillations within any window $\mathcal{F}$ by a periodic wave train. Moreover, we can conclude that the macroscopic evolution of the thermodynamic fields is indeed governed by the modulation equations (4.11), see the discussion in [DH06].

6 The shock problem

Since we expect a hyperbolic system describing the macroscopic limit, it is natural to investigate Riemann problems and interpret the results in terms of hyperbolic theory. A goal of this is to indicate selection principles for Riemann solvers that account for the macroscopic limit of atomic chains.

We would naively expect to find rarefaction fans, shocks and possibly contact discontinuities, that are selected by characteristic curves and entropy conditions and whose velocities are determined by characteristic velocities and Rankine-Hugoniot conditions.

It turns out that this picture is invalid when microscopic oscillations occur, leading to modulated wave trains as mentioned in §4. Instead, we find a situation very similar to the zero dispersion limit of the KdV equation mentioned in §1, where *dispersive shock fans* replace Lax-shock, and where velocities are not given by characteristic velocities of the limiting Burger's equation, corresponding to the p-system in our case. Faced with a large number of publications on this matter, we restrict references here to [LLV93, LP05, El05] and the bibliographies therein.

We focus on cold initial data, i.e. constant displacements and velocities with a single jump at some $\bar{\alpha}_*$, i.e.

$$(r,v)(\bar{\alpha},0) = (r_-,v_-)\,,\ \bar{\alpha} \le \bar{\alpha}_*\,,\ \text{and}\ (r,v)(\bar{\alpha},0) = (r_+,v_+)\,,\ \bar{\alpha} > \bar{\alpha}_*.$$

The macroscopic limit of the harmonic potential for such Riemann problems is cold and described by (4.13). It is therefore described by the corresponding p-system, which is a linear 1D wave equation, whose dynamics can be understood directly from the d'Alembert solution form, so there are only contact discontinuities.

For general nonlinear potentials, there is numerical evidence that dispersive shocks appear for initial data leading to Lax-shocks of the p-system, while rarefaction data leads to cold macroscopic limits described by the p-system. In Figure 6.1 we plot a typical situation for illustration, and sketch a dispersive shock fan in Figure 6.3. We are particularly interested in the transition of the Whitham modulation at its front.

Remark 6.1. For convex flux, i.e. $\Phi''' > 0$, the p-system can be solved uniquely in terms of at most two rarefaction or shock waves [Smo94]. For non-convex flux the situation is more complicated, and the entropy conditions for the p-system no longer agree, because eigenvalues are no longer genuinely nonlinear [KS97, LeF02]. A specific choice of a convex-concave potential for (1.1), numerically yields a macroscopically cold, strong shock, connecting states with equal characteristic velocities, and traveling with a different Rankine-Hugoniot velocity. In particular, it is not a contact discontinuity or Lax shock, but a (fast) undercompressive shock. Details on this phenomenon will be published elsewhere.

The macroscopic dynamics in space-time for Riemann data appear to be self-similar, hence reducible to a macroscopic velocity variable $c = \alpha/t = \bar{\alpha}/\bar{t}$. More formally, we

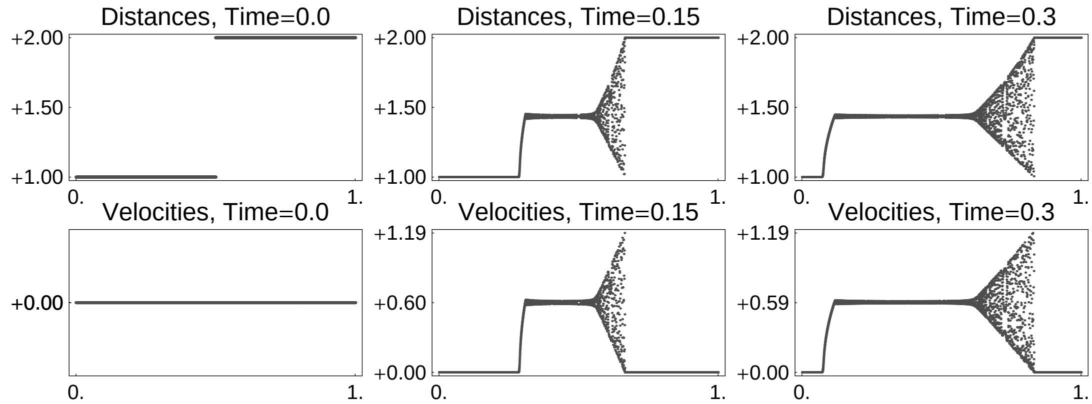

Figure 6.1: Riemann problem with $N = 4000$ and $\Phi(r) = (r-1)^2/2 - \cos(2(r-1))/4$ with one rarefaction wave and one dispersive shock: snapshots of atomic distances and velocities for $\bar{t} = 0.0$, $\bar{t} = 0.15$, and $\bar{t} = 0.3$.

assume that the Young measure $\mu(c)$ arising in the macroscopic limit for (initially cold) Riemann problems at each c is either a point measure or supported on a closed curve, corresponding to a wave train, so that from the modulation ansatz (4.5) we obtain $\tilde{\mathbb{X}}(c, \varphi)$ and analogously, from §4.3, an expression $M^\varepsilon(c, \varphi)$ for the vector of modulated distances and velocities. We use the phase variable φ to parametrize the support of $\mu(c)$. In case $\mu(c)$ is a point measure, we obtain a strong limit where $\tilde{\mathbb{X}}(c, \varphi) \equiv 0$.

A dispersive shock spans a range of speeds from the shock back velocity, c_b, to the shock front velocity, c_f. To ease notation, we assume $0 < c_\mathrm{b} < c_\mathrm{f}$, and that the constant states to the left and right of the dispersive shock are (r_-, v_-) and (r_+, v_+) as sketched in Figure 6.3.

It is instructive to view the modulation of wave trains in a dispersive shock as the selection of a curve in the set of wave trains $\tilde{\mathbb{X}}(c, \varphi)$ parametrized by $c_\mathrm{b} < c < c_\mathrm{f}$ in terms of the wave train parameters $(r(c), k(c), \omega(c))$. This curve bridges the energy jump between the constant states (r_-, v_-) and (r_+, v_+), and the wave trains become singular at c_b and c_f. Based on numerical evidence [HFM81] and results for the Toda chain [VDO91, Kam91], we assume that $M^\varepsilon(c_\mathrm{b}) \equiv (r_-, v_-)$ has zero amplitude, and the shock front $M^\varepsilon(c_\mathrm{f})$ corresponds to a *soliton* with background state (r_+, v_+), where $k(c_\mathrm{f}) = \omega(c_\mathrm{f}) = 0$. Note that this is a singular limit of (3.4) and that Theorem 3.10 implies infinite kinetic energy $\gamma(c_\mathrm{f})$. We plot wave trains and fields within a dispersive shock in Figure 6.2.

More precisely, the shock front is assumed to be a homoclinic orbit

$$\mathcal{H}(s) := \lim_{c \to c_\mathrm{f}} M^\varepsilon(c_\mathrm{f})$$

in the phase scaling $\varphi = \omega s$ with asymptotic state $\lim_{s \to \pm\infty} \mathcal{H}(s) = (r_+, v_+)$. We expect the convergence to the asymptotic state is exponential in s, thus L_p-norms of $[\mathcal{H}(s) - (r_+, v_+)]$ are finite. In terms of the wave train profile $\mathbb{X}$ and $\mathbb{V} = \partial_\varphi \mathbb{X}$ we

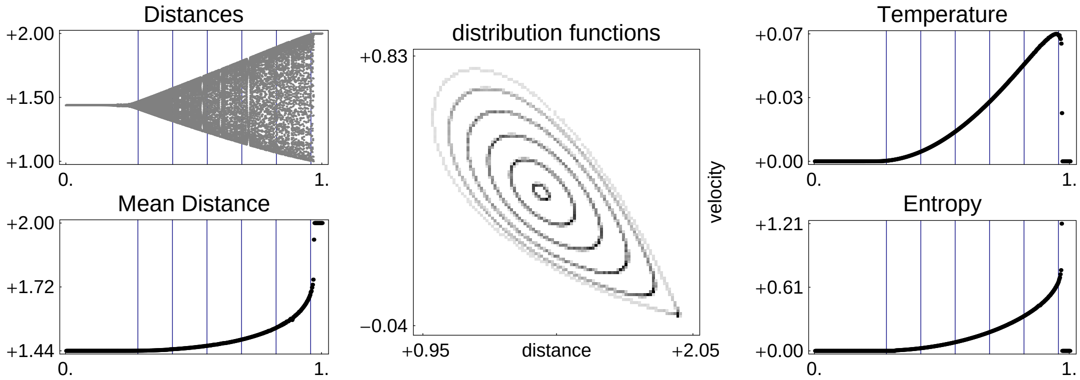

Figure 6.2: Example for dispersive shocks. Left: snapshots of atomic distances and their local mean values. Center: superposition of several distribution functions within the shock; positions of the space-time windows are marked by vertical lines. Right: snapshots of temperature and entropy.

can write the second component $\mathcal{H}_2$ of $\mathcal{H}$ as

$$\mathbb{H}(s) := \mathcal{H}_2(s) - v_+ = \lim_{c \to c_\mathrm{f}} \omega(c)\mathbb{V}(c, \omega(c)s) = \lim_{c \to c_\mathrm{f}} \frac{\mathrm{d}}{\mathrm{d}s}\mathbb{X}(c, \omega(c)s).$$

Both the vanishing amplitude at c_b and sinusoidal oscillations, and the homoclinic orbit at c_f are natural codimension-1 singularity along a curve of wave trains viewed as periodic orbits.

Assuming a soliton at the shock front means in particular that the modulation system does not have a strong shock, which is challenging to confirm numerically as discussed below. Instead, we conjecture that at the shock front the entropy S jumps and (r, v, k, ω) are continuous with unbounded derivative. Heuristically, the excess energy at the jump in the initial data cannot be dissipated by the conservative system, but is transported dispersively via oscillations with two new degrees of freedom, frequency and wave number.

Properties at and near the soliton

We predict the scaling of temperature and related quantities assuming the scaling in generic or conservative homoclinic bifurcations of ODEs [VF92], where the unfolding parameter, here c, is exponentially small in the period, here $1/\omega$. We thus expect $c_\mathrm{f} - c \sim \mathrm{e}^{-\kappa/\omega}$, for some $\kappa > 0$, and so

$$\omega(c) \sim k(c) \sim 1/\log(c_\mathrm{f} - c),$$

because Theorem 3.9 implies the same scaling in k. Indeed, this scaling could be confirmed for the case of Toda potential using the explicit solutions in [DKV95], and also appears in the formal derivations in [El05].

Temperature, entropy, entropy flux. The definition $T = \omega^2 \int_0^1 \mathbb{V}(\varphi)^2 \mathrm{d}\varphi$ of the temperature of a wave train yields

$$T(c)=\int_0^1 \left[\omega(c)\mathbb{V}(c,\varphi)\right]^2 \mathrm{d}\varphi=\omega(c)\int_0^{1/\omega(c)} \left[\omega(c)\mathbb{V}(c,\omega(c)s)\right]^2 \mathrm{d}s$$

and thus (assuming smoothness) the limiting temperature of the soliton

$$\lim_{c\to c_\mathrm{f}} T(c)=\lim_{c\to c_\mathrm{f}}\omega(c)\int_0^{1/\omega(c)} \left[\omega(c)\mathbb{V}(c,\omega(c)s)\right]^2 \mathrm{d}s=\int_0^\infty \mathbb{H}(s)^2\mathrm{d}s \lim_{c\to c_\mathrm{f}}\omega(c)=0,$$

because the L^2 norm of $\mathbb{H}$ is finite. Then the scalings of temperature T, entropy S and entropy flux g, see (3.16), are given by

$$T(c)\sim\left(\log(c_\mathrm{f}-c)\right)^{-1},\quad g(c)\sim S(c)=T(c)/\omega\sim 1,$$

where we used $cS'=g'$. We thus predict that the temperature is continuous for all c and decays to zero like $1/\log$. Entropy and entropy flux vanish in cold regions, but continuously approach a finite, non-zero value and jump to zero beyond the shock front.

Since the temperature also decays towards the shock back, we expect a unimodal curve $T(c)$ with a unique maximum, as is the case in e.g. a planar ODE where the interior of a homoclinic orbit is filled with periodic orbits and an elliptic equilibrium.

However, these scalings and limiting values are difficult to confirm numerically, because the $1/\log$ decay is hard to resolve, and the shock front could not be simulated in isolation from the rest of the modulation region due to boundary effects.

Norm parameter γ. On account of Theorem 3.10, the norm parameter γ grows at least like $1/k$, so that $\gamma(c)\geq -C\log(c_\mathrm{f}-c)$, for a constant $C>0$. This agrees with the prediction from the above entropy scaling, because

$$\gamma(c)=\frac{S}{2\omega}=\frac{T}{2\omega^2}\sim\frac{1}{\omega}\sim\log(c_\mathrm{f}-c).$$

Mean distance and velocity. Assuming that c unfolds the homoclinicity as a generic (or Hamiltonian) ODE, the flow time through a fixed small region near (r_+,v_+) grows logarithmically in c and thus for the average values we obtain the scaling

$$r(c)=r_+-r_1/\log(c_\mathrm{f}-c)+h.o.t.\quad v(c)=v_+-v_1/\log(c_\mathrm{f}-c)+h.o.t.,$$

with some constants r_1, v_2, since the limiting values are those of the corresponding Riemann data.

Note that the first equation in (4.4) implies $-cr'=v'$ in the sense of distributions, where $'=\mathrm{d}/\mathrm{d}c$. Therefore, $-c_\mathrm{f}r_1=v_1$, and so

$$c_\mathrm{f}=-v_1/r_1 \tag{6.1}$$

replaces the Rankine-Hugoniot jump condition.

Propagation speeds. The modulation equations yield five equations for the propagation speed of the shock front; four in term of leading order expansions such as $-cr' = v' \to -c = \mathrm{d}v/\mathrm{d}r$ above, and one jump condition $c[\![S]\!] = [\![g]\!]$. Indeed, in numerical simulations of dispersive shocks all these velocities are close to that obtained from the slope of the shock front in space-time.

The conservation of wave number implies $-ck' = \omega'$ and thus throughout the dispersive shock we have $-c = c_{\mathrm{g}} := \mathrm{d}\omega/\mathrm{d}k$, which is the group velocity and not the phase velocity $c_{\mathrm{ph}} := -\omega/k$ of wave trains. Note that here, $-c$ is the expected propagation velocity due to the choide of sign for ω in (3.3) and (4.7).

In particular, the shock front should move with the limiting group velocity, while the soliton speed naturally is the limiting phase velocity. However, in the solitary limit, phase and group velocity typically coincide, because for $L = 1/k$ we have the identity

$$c_{\mathrm{g}} = c_{\mathrm{ph}} - L\tfrac{\mathrm{d}c_{\mathrm{ph}}}{\mathrm{d}L},$$

where $\frac{\mathrm{d}c_{\mathrm{ph}}}{\mathrm{d}L}$ is exponentially small for generic and conservative homoclinic bifurcations in ODE [VF92]; the identity follows from $\frac{\mathrm{d}c_{\mathrm{ph}}}{\mathrm{d}k} = \frac{c_{\mathrm{g}}-c_{\mathrm{ph}}}{k}$.

Recall that the phase velocities of wave trains were estimated in (3.14) and rigorously imply that the soliton velocity is bounded (essentially) by p-system characteristics velocities c_-, c_- of the left and right states r_-, r_+. However, in numerical simulations, the shock front velocity c_{f} never exhausted these bounds, but was strictly between c_- and c_+.

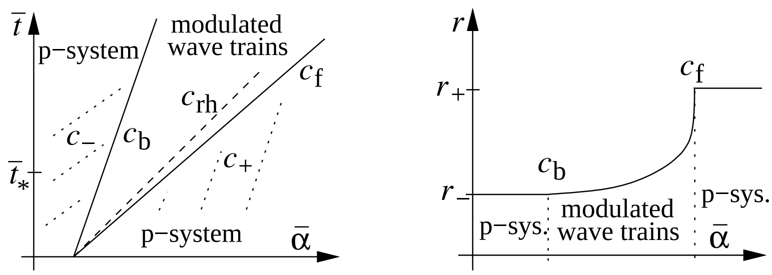

Figure 6.3: Left: Sketch of a dispersive shock for the macroscopic limit of a shock problem in (1.1). Dashed line is the p-system Lax shock with speed c_{rh}, dotted the p-system characteristic velocities $c_\pm$ of left and right states $(r_\pm, v_\pm)$. Right: sketch of the r-modulation at some time $\bar{t}_* > 0$ with $1/\log$ scaling at c_{f}.

On the other hand, the shock velocity of the p-system is given by the Rankine-Hugoniot condition $c_{\mathrm{rh}} = \sqrt{(\Phi'(r_-) - \Phi'(r_+))/(r_- - r_+)}$, and in all cases (for Φ' monotone) we numerically found the velocity ordering sketched in Figure 6.3, that is,

$$c_{\mathrm{b}} < c_+ < c_{\mathrm{rh}} < c_{\mathrm{f}} < c_-,$$

where $c_{\mathrm{rh}} - c_{\mathrm{f}} \sim 5\%$. Characteristics point into the dispersive shock fan, and indeed, we seem to find dispersive shocks only if $c_- < c_{\mathrm{rh}} < c_+$, see also Remark 6.1.

Finally, we mention that the velocity c_{b} of the shock back, where wave trains have small amplitude, numerically agrees with the prediction from harmonic modulation equations, i.e. $c_{\mathrm{b}} = \sqrt{\Phi''}(r_-)\sin(\pi k(c_{\mathrm{b}}))/\pi k_{\mathrm{b}}$.

Remarks and open problems

The occurrence of dispersive shocks has only been proven rigorously for some completely integrable cases, in particular the Toda chain [VDO91, Kam91]. Unfortunately, the literature on this issue is not easily accessible to non-specialists, and we found it inconclusive concerning the rigorous justification of a hyperbolic system of Whitham modulation equations. In fact, neither the observation that the shock front is a soliton, nor the scaling at the shock front, nor the velocity of the shock back seem to be worked out.

Similarly, to our knowledge, the selection mechanism for the soliton has not been formulated in terms of initial values for the Riemann problem (though the shock front velocity for the Toda shock problem can be computed explicitly [VDO91]). An observation towards a selection principle could be that in numerical experiments for vanishing initial velocities, the dispersive shock exhausts precisely the range between the initial jump in the r-component. We also observe that the dispersive shock in (c, r, v)-space is a graph over the plane $(0, r, v)$. In other words, the modulation parameter curve $(r, v, k, \omega)(c)$ appears to be selected in such a way that wave train orbits Q are (nested) level sets of an unknown function.

We hope that a study of the explicit solutions for the case of Toda potential, and results for zero dispersion limits mentioned in §1, provide more insight into the general situation, in particular the prediction of dispersive shocks and the shock front velocity.

Acknowlegdments

This work has been supported by the DFG Priority Program 1095 "Analysis, Modeling and Simulation of Multiscale Problems". We gratefully acknowledge notes by Karsten Matthies on which §3.2 is based, and fruitful discussions with Alexander Mielke and Thomas Kriecherbauer.

References

[BM95] T.J. Bridges and A. Mielke. A proof of the Benjamin-Feir instability. *Archive Rational Mech. Analysis*, 133:145–198, 1995.

[Daf00] C.M. Dafermos. *Hyperbolic Conservation Laws in Continuum Physics*, volume 325 of *Grundlehren d. mathem. Wissenschaften*. Springer, Berlin, 2000.

[DH05] W. Dreyer and M. Herrmann. On the approximation of periodic traveling waves for the atomic chain. WIAS preprint 1030, 2005.

[DH06] W. Dreyer and M. Herrmann. Numerical experiments on modulation theory for the nonlinear atomic chain. WIAS preprint 1031, revised version, 2006.

[DHM06] W. Dreyer, M. Herrmann, and A. Mielke. Micro-macro transition for the atomic chain via Whitham's modulation equation. *Nonlinearity*, 19(2):471–500, 2006.

[DK00] W. Dreyer and M. Kunik. Cold, thermal and oscillator closure of the atomic chain. *J. Phys. A: Math. Gen.*, 33:2097–2129, 2000.

[DKKZ74] P. Deift, S. Kamvissis, T. Kriecherbauer, and X. Zhou. The Toda lattice ii. existence of integrals. *Phys. Rev. B*, 9(4):1924–1925, 1974.

[DKKZ96] P. Deift, S. Kamvissis, T. Kriecherbauer, and X. Zhou. The Toda rarefaction problem. *Comm. Pure Appl. Math*, 49(1):35–83, 1996.

[DKV95] P. Deift, T. Kriecherbauer, and S. Venakides. Forced lattice vibrations, Part I. *Comm. Pure Appl. Math.*, 48:1187–1250, 1995.

[DM98] P. Deift and T. T-R McLaughlin. *A continuum limit of the Toda lattice*, volume 131/624 of *Mem. Americ. Math. Soc.* Americican Mathematical Society, 1998.

[El05] G.A. El. Resolution of a shock in hyperbolic systems modified by weak dispersion. *Chaos*, 15, 2005.

[Fla96] S. Flach. Tangent bifurcation of band edge plane waves, dynamical symmetry breaking and vibrational localization. *Physica D*, 91:223–243, 1996.

[FM02] G. Friesecke and K. Matthies. Atomic-scale localization of high-energy solitary waves on lattices. *Physica D*, 171:211–220, 2002.

[FM03] G. Friesecke and K. Matthies. Geometric solitary waves in a 2d mass spring lattice. *Discrete Contin. Dyn. Syst. Ser. B*, 3:105–114, 2003.

[FP99] G. Friesecke and R. L. Pego. Solitary waves on FPU lattices. I. Qualitative properties, renormalization and continuum limit. *Comm. Math. Phys.*, 12(6):1601–1627, 1999.

[FPU55] E. Fermi, J. Pasta, and S. Ulam. Studis on nonlinear problems. *Los Alamos Scientific Laboraty Report*, LA–1940, 1955.

[FV99] A.-M. Filip and S. Venakides. Existence and modulation of traveling waves in particle chains. *Comm. Pure Appl. Math.*, 51(6):693–735, 1999.

[FW94] G. Friesecke and J. A. D. Wattis. Existence theorem for solitary waves on lattices. *Comm. Math. Phys.*, 161(2):391–418, 1994.

[GHM06a] J. Giannoulis, M. Herrmann, and A. Mielke. Continuum descriptions for the dynamics in discrete lattices: derivation and justification. In A. Mielke, editor, *Analysis, Modeling and Simulation of Multiscale Problems*. Springer, 2006. To appear.

[GHM06b] J. Giannoulis, M. Herrmann, and A. Mielke. Redcution of hamiltonians and lagrangians in the passage from discrete to continuum models. In preparation, 2006.

[GL88] J. Goodman and P. Lax. On dispersive difference schemes. *Comm. Pure. Appl. Math.*, 41:591–613, 1988.

[GM04] J. Giannoulis and A. Mielke. The nonlinear Schrödinger equation as a macroscopic limit for an oscillator chain with cubic nonlinearities. *Nonlinearity*, 17:551–565, 2004.

[GM06] J. Giannoulis and A. Mielke. Dispersive evolution of pulses in oscillator chains with general interaction potentials. *Discr. Cont. Dynam. Systems Ser. B*, 6:493–523, 2006.

[Hén74] M. Hénon. Integrals of the Toda lattice. *Phys. Rev. B*, 9(4):1921–1923, 1974.

[Her04] M. Herrmann. *Ein Mikro-Makro-Übergang für die nichtlineare atomare Kette mit Temperatur.* Phd thesis, Humboldt-Universität zu Berlin, 2004.

[HFM81] B.L. Holian, H. Flaschka, and D.W. McLaughlin. Shock waves in the toda lattice: Analysis. *Phys. Rev. A*, 24(5):2595–2623, 1981.

[HL91] T. Y. Hou and P. Lax. Dispersive approximations in fluid dynamics. *Comm. Pure Appl. Math.*, 44:1–40, 1991.

[HLM94] M.H. Hays, C. D. Levermore, and P.D. Miller. Macroscopic lattice dynamics. *Physica D*, 79(1):1–15, 1994.

[HLW02] E. Hairer, Ch. Lubich, and G. Wanner. *Geometric Numerical Integration*, volume 31 of *Springer Series in Comp. Mathem.* Springer, Berlin, 2002.

[Hör97] L. Hörmander. *Lectures on Nonlinear Hyperbolic Differential Equations*, volume 26 of *Mathématiques & Applications*. Springer, Paris, 1997.

[Kam91] S. Kamvissis. *On the long time behavior of the double infinite Toda chain under shock initial data.* PhD thesis, New York University, 1991.

[KL02] C. Kondo and P.G. LeFloch. Zero diffusion-dispersion limits for hyperbolic conservation laws. *SIAM Math. Anal.*, 22:1320–1329, 2002.

[KS97] P. Krejči and I. Straškraba. A uniqueness criterion for the Riemann problem. *Hiros. Math. J.*, 27:307–346, 1997.

[KSM92] P. Kirrmann, G. Schneider, and A. Mielke. The validity of modulation equations for extended systems with cubic nonlinearities. *Proc. Roy. Soc. Edinburgh Sect. A*, 122:85–91, 1992.

[Lax86] P.D. Lax. On dispersive difference schemes. *Physica D*, 18:250–254, 11986.

[Lax91] P.D. Lax. The zero dispersion limit, a deterministic analogue of turbulence. *Comm. Pure Appl. Math.*, 44:1047–1056, 1991.

[LeF02] P. G. LeFloch. *Hyperbolic Conservation Laws.* Lectures in Mathematics: ETH Zürich. Birkhäser, Basel, 2002.

[LL83] P.D. Lax and C.D. Levermore. The small dispersion limit of the Korteweg-de Vries equation, I, II, III. *Comm. Pure Appl. Math.*, 36:no.3, 253–290; no.5, 571–593; no.6, 809–830, 1983.

[LL96] C.D. Levermore and J.G. Liu. Large oscillations arising in a dispersive numerical scheme. *Physica D*, 99:191–216, 1996.

[LLV93] P. D. Lax, C. D. Levermore, and S. Venakides. The generation and propagation of oscillations in dispersive initial value problems and their limiting behavior. In A.S. Fokas and V.E. Zakharov, editors, *Important developments in soliton theory*, pages 205–241. Springer, Berlin, 1993.

[LP05] P. Lorenzoni and S. Paleari. Metastability and dispersive shock waves in fermi-pasta-ulam system. oai:arXiv.org:nlin/0511026, 2005.

[Mac02] F. Maciá. *Propagación y control de vibraciones en medios discretos y continous.* PhD thesis, Universidad Complutense de Madrid, 2002.

[Mac04] F. Maciá. Wigner measures in the discrete setting: high-frequency analysis of sampling and reconstruction operators. *SIMA*, 36(2):347–383, 2004.

[Mie02] A. Mielke. The Ginzburg–Landau equation in its role as a modulation equation. In B. Fiedler, editor, *Handbook of Dynamical Systems II*, pages 759–834. Elsevier Science B.V., 2002.

[Mie06] A. Mielke. Macroscopic behavior of microscopic oscillations in harmonic lattices using wigner-husimi measures. to appear in Arch. Rat. Mech. Analysis, 2006.

[MR98] I. Müller and T. Ruggeri. *Rational Extended Thermodynamics*, volume 37 of *Springer Tracts in Natural Philosophy.* Springer, 2. edition, 1998.

[PP00] A. A. Pankov and K. Pflüger. Traveling waves in lattice dynamical systems. *Math. Meth. Appl. Sci.*, 23:1223–1235, 2000.

[Sch82] M.E. Schonbek. Convergence of solutions to nonlinear dispersive equations. *Comm. Part. Diff. Equa.*, 7:959–1000, 1982.

[Sch98] G. Schneider. Justification of modulation equations for hyperbolic systems via normal forms. *NoDEA Nonlinear Differential Equations Appl.*, 5(1):69–82, 1998.

[Smo94] J. Smoller. *Shock Waves and Reaction-Diffusion Equations*, volume 258 of *Grundlehren d. mathem. Wissenschaften*. Springer, 2. edition, 1994.

[SW00] G. Schneider and C. E. Wayne. Counter-propagating waves on fluid surfaces and the continuum limit for the Fermi-Pasta-Ulam model. In K. Gröger, B. Fiedler, and J. Sprekels, editors, *International Conference on Differential Equations*, pages 390–403. World Scientific, 2000.

[SYS97] R. D. Skeel, G. Yang, and T. Schlick. A family of symplectic integrators: Stability, accuracy, and molecular dynamics Applications. *SIAM J. Sci. Comput.*, 18:203–222, 1997.

[Tay96] M. E. Taylor. *Partial Differential Equations III: Nonlinear Theory*, volume 117 of *Applied Mathematical Sciences*. Springer, New York, 1996.

[Tod70] M. Toda. Waves in nonlinear lattices. *Prog. Theor. Phys.*, 45:174–200, 1970.

[Tod81] M. Toda. *Theory of nonlinear lattices*, volume 20 of *Springer Series in Solid-State Sci.* Springer, Berlin, 1981.

[VDO91] S. Venakides, P. Deift, and R. Oba. The Toda shock problem. *Comm. Pure Appl. Math.*, 44:1171–1242, 1991.

[Ven85] S. Venakides. The generation of modulated wavetrains in the solution of the Korteweg-de Vries equation. *Comm. Pure Appl. Math.*, 38:883–909, 1985.

[VF92] A. Vanderbauwhede and B. Fiedler. Homoclinic period blow-up in reversible and conservative systems. *Z. Angew. Math. Phys.*, 43:292–318, 1992.

[War99] G. Warnecke. *Analytische Methoden in der Theorie der Erhaltungsgleichungen*, volume 138 of *Teubner Texte z. Mathem.* B.G. Teubner, 1999.

[Whi74] G. B. Whitham. *Linear and Nonlinear Waves*, volume 1237 of *Pure And Applied Mathematics*. Wiley Interscience, New York, 1974.