Riemann Problems in FPU Chains

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We impose Riemann initial data to FPU chains and study the solutions on the hyperbolic macroscopic scale.

The setting. FPU chains, named after the famous Fermi-Pasta-Ulam experiments, consist of N identical particles that are coupled in a nonlinear nearest neighbor potential $\Phi : \mathbb{R} \to \mathbb{R}$ by Newton's law of motion

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

Here $x_\alpha(t)$ is the atomic position which depends on the *microscopic* time t and the particle index α. Rather than regarding (1) as high-dimensional system of ODEs we aim to establish a *thermodynamic limit* by means of the *hyperbolic scaling*. To this end we introduce a small *scaling parameter* $\varepsilon = 1/N$ and define the *macroscopic* time $\overline{t} = \varepsilon t$ and particle index (=material space) $\overline{\alpha} = \varepsilon\alpha$. The macroscopic, or *thermodynamic*, limit is then related to the limit $\varepsilon \to 0$.

The simplest macroscopic model for FPU chains results by assuming *cold motion*, i.e., we suppose that the atomic distances $r_\alpha(t) = x_{\alpha+1} - x_\alpha$ and velocities $v_\alpha = \dot{x}_\alpha$ vary on the macroscopic scale only. This gives rise the two-scale ansatz $r_\alpha(t) = R(\varepsilon t, \varepsilon\alpha)$ and $v_\alpha(t) = V(\varepsilon t, \varepsilon\alpha)$ where R and V are macroscopic functions. Substitution into (1) and formal expansions with respect to ε yield at leading order

$$\partial_{\overline{t}} R - \partial_{\overline{\alpha}} V = 0, \quad \partial_{\overline{t}} V - \partial_{\overline{\alpha}} \Phi'(R) = 0, \quad \partial_{\overline{t}} \left(\tfrac{1}{2}V^2 + \Phi(R)\right) - \partial_{\overline{\alpha}} \left(V\Phi'(R)\right) = 0, \tag{2}$$

The first two equations form the *p-system* (which is strictly hyperbolic for convex Φ) and correspond to the macroscopic *conservation laws* for *mass* and *momentum*. Moreover, for *smooth* solution these equations imply the third identity, that is *conservation of energy*.

Dispersive shocks. The p-system provides a reasonable thermodynamic description for FPU chains as long as the functions R and V are smooth, see [DHR06, DH07] for a discussion, but typically there exists a critical time $\overline{t}_{\mathrm{crit}}$ at which a macroscopic shock is formed. In this case the PDEs (2) must be accompanied by the Rankine Hugeniot conditions

$$c[\![R]\!] + [\![V]\!] = 0, \quad c[\![V]\!] + [\![\Phi'(R)]\!] = 0, \quad c[\![\tfrac{1}{2}V^2 + \Phi(R)]\!] + [\![V\Phi'(R)]\!] = 0, \tag{3}$$

with *shock speed* c, which formulate the conservation laws across the shock. However, typically a shock *cannot* satisfy *all* three

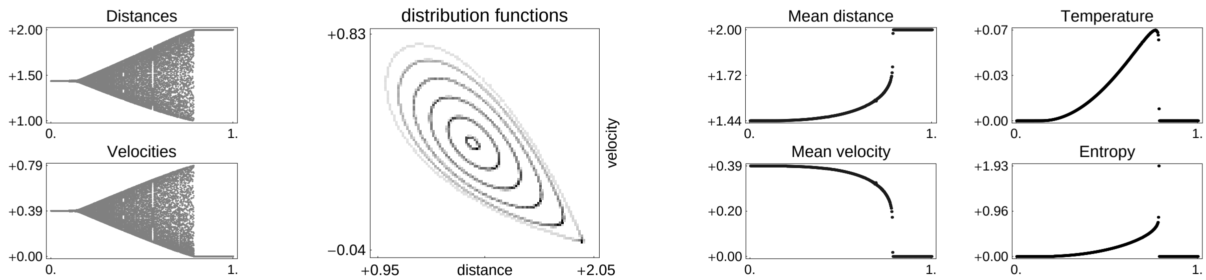

Fig. 1 Example of a dispersive shock. *Microscopic (Left)*: Snapshots of atomic distances and velocities. *Mesoscopic (Middle)*: Superposition of several local distribution functions within the dispersive shock. *Macroscopic (Right)*: Snapshots of thermodynamic fields.

jump conditions simultaneously (Lax shocks for the p-system have negative energy production). In contrast to the p-system FPU chains conserve mass momentum *and* energy for all times, and therefore the atoms beyond a cold shock start to oscillate. These oscillations can be interpreted as *temperature* and propagate on the macroscopic scale. This phenomenon gives rise to so-called dispersive shocks, and can be observed in many zero dispersion limits, see [Lax91, El05] for an overview. The creation of temperature in FPU chains is investigated in [DH07, HR07] by imposing cold Riemann initial data for (1). The arising dispersive shocks, see Figure 1, can be viewed as rarefaction waves for Whitham's modulation equation, compare [FV99, DHM06] and references therein, and obey remarkable dynamical and geometric properties.

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Towards FPU-Riemann solvers. An important building block for a macroscopic theory for FPU chains are *atomistic Riemann solvers* that predict the thermodynamic limit for cold Riemann initial data. In the simplest case Φ''' has no zeros so that all shocks for the p-system have a non-vanishing energy production. Under this assumption we can describe the atomistic Riemann solver in terms of *wave sets* as follows. For given left state $u_{\rm L} = (r_{\rm L},\, v_{\rm L})$ the corresponding wave set $\mathcal{W}^{\rm FPU}[u_{\rm L}]$ consists of four smooth curves in $(r,\, v)$–space that emanate from u_L, see the left picture in Figure 2. The curves $\mathcal{R}_{\pm}[u_{\rm L}]$ come from the Lax theory for hyperbolic systems and contain all possible right states $u_{\rm R}$ that can be connected from $u_{\rm L}$ by a single rarefaction wave (where $+$ and $-$ correspond to 1– and 2–waves, respectively). However, instead of Lax-shock curves we find two *dispersive shock curves* $\mathcal{D}_{\pm}[u_{\rm L}]$. These four curves decompose the $(r,\, v)$–space into four regions, and encode the solutions to all Riemann problems, see Figure 2.

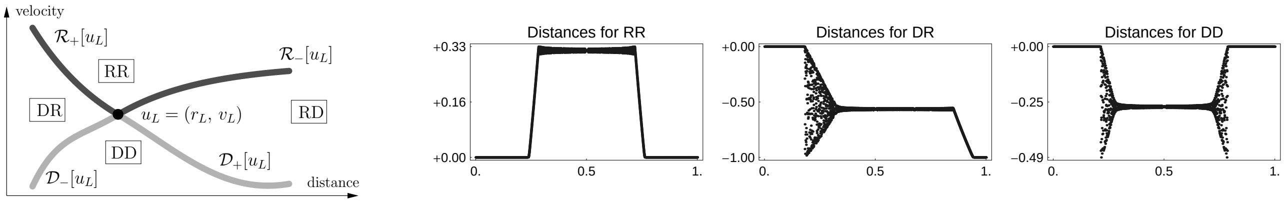

Fig. 2 *Left*: Sketch of the atomistic Riemann solver for strictly concave Φ'. The wave sets $\mathcal{W}^{\rm FPU}[u_{\rm L}]$ consist of rarefaction (R) curves and dispersive shock (D) curves, and decompose the plane into 4 regions DD, RD, RR, and RD. *Right*: Prototypical Examples for Riemann solutions corresponding to RR, DR and DD.

Conservative shocks in FPU chains. We show in [HR07] that for potentials with non-convex flux, i.e., roots in Φ''', there exist curves of Riemann initial data where *all* jump conditions in (3) are satisfied, and the corresponding *conservative* shocks are *undercompressive*. Numerical results and heuristic arguments show that *supersonic* conservative shocks occur in the macroscopic limit of the FPU chain, whereas the chain is not capable to produce *subsonic* conservative shocks. Moreover, adapting LeFloch's *conservative Riemann solver* for the p-system, see [LeF02], we can predict *modified wave sets* that build up a FPU-Riemann solver with supersonic undercompressive conservative shocks, see Figure 3.

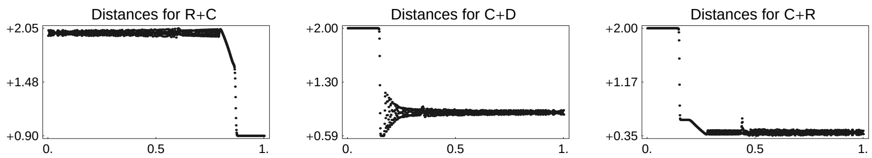

Fig. 3 For *supersonic* conservative shocks the modified wave sets involve the following composite waves. *Left*: Rarefaction wave with attached conservative shock. *Middle*: Conservative shock followed by a dispersive shock. *Right*: Conservative shock followed by a rarefaction wave.

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