Travelling waves in atomistic chains and kinetic relations

Johannes Zimmer
(joint work with Hartmut Schwetlick)

Martensitic materials pose good test problems for the analysis of the passage from atomistic to continuum. The reason is that on the microscopic level, they can be well approximated by a chain of atoms governed by Newton's equations; thus, the system is *microscopically Hamiltonian*. However, martensitic materials can undergo phase transitions, and moving phase boundaries can generate dissipation, so that the system is *macroscopically dissipative*. The simplest possible situation for which this phenomenon can be understood is that of a single phase boundary propagating in a one-dimensional chain of atoms $\{q_j\}_{j\in\mathbb{Z}}$ on the real line. Neighbouring atoms are linked by a spring with elastic potential V, and it is convenient to assume that only nearest neighbours interact. The longitudinal elongation of atom k is given by $u_k\colon \mathbb{R}\to\mathbb{R}$. The argument of the elastic potential V is the discrete strain, that is, the difference of the deformations, $u_{k+1}(t)-u_k(t)$. The springs are bistable, with the two stable states representing two stable phases. The equations of motion are assumed to be governed by Newton's law, so that in suitable units

$$\ddot{u}_k(t) = V'(u_{k+1}(t)-u_k(t)) - V'(u_k(t)-u_{k-1}(t)) \tag{1}$$

for every $k\in\mathbb{Z}$. A travelling wave *ansatz* is $u_k(t)=u(k-ct)$ for $k\in\mathbb{Z}$; with this formulation, Equation (1) becomes

$$c^2\ddot{u}(x) = V'(u(x+1)-u(x)) - V'(u(x)-u(x-1)). \tag{2}$$

We remark that the Hamiltonian is

$$\int_{\mathbb{R}} \left[\tfrac{1}{2}c^2\dot{u}(t)^2 + V(u(t+1)-u(t))\right]\,\mathrm{d}t.$$

Equation (2) is an instance of a so-called *lattice differential equation*. Models of crystal lattices, photonic structures, and Josephson junctions, furnish other examples of lattice differential equations. A number of interesting papers [2, 4, 5] demonstrates the variety of problems and methods encountered in this field.

It is convenient to reformulate the travelling-wave formulation (2) in terms of the discrete strain $\epsilon(x)=u(x)-u(x-1)$; it then simply reads

$$c^2\epsilon''(x) = \Delta_1 V'(\epsilon(x)), \tag{3}$$

where $\Delta_1 g(x) := g(x+1)-2g(x)+g(x-1)$ is the discrete Laplacian. Though one would like to treat smooth nonconvex potentials, rigorous results are presently only available for the special interaction potential

$$V(\epsilon) = \frac{1}{2}\min\{(\epsilon+1)^2,(\epsilon-1)^2\}. \tag{4}$$

This potential also appears in other works [9, 10]. For this choice of V, (3) becomes

$$c^2\epsilon''(x) = \Delta_1\epsilon(x) - 2\Delta_1 H(\epsilon(x)), \tag{5}$$

with H denoting the Heaviside function. The wave travels with speed c.

To formulate the result, we introduce the *dispersion relation* $D_c(\kappa) = 4\sin^2\left(\frac{\kappa}{2}\right) - c^2\kappa^2$. We choose a velocity regime so that the the dispersion relation vanishes for exactly one positive value, which we denote κ_0. This assumption restricts the analysis to fast subsonic, almost sonic wave speeds. We remark that for martensitic phase transitions, there is a distinction between fast (*umklapp*) and slow (*schiebung*) martensitic transformations. The former move with a velocity close to that of an elastic wave, the latter are observable under an optical microscope [3, 8].

It is then possible to show that there exists, for fixed wave speed c close to the sound speed $c_0 := 1$, a *family* of solutions of (5). Every family is heteroclinic in the sense that the strain is negative (positive) for negative (positive) arguments. This corresponds to solutions with the strain in one well for negative arguments and in the second well for positive arguments. The precise formulation is as follows.

Theorem 1. *Suppose the dispersion relation has one positive zero κ_0 with $\kappa_0^2 < \frac{1}{2}$. Then there exists a family of heteroclinic wave solutions, parametrised by a real number ξ with $|\xi| \leq 1$. The solutions are such that $\epsilon(x) > 0$ for $x > 0$ and $\epsilon(x) < 0$ for $x < 0$ for all admissible values of the parameter ξ.*

We briefly discuss the Rankine-Hugoniot condition, and introduce the notation $[\![f]\!]$ for $f(s(t)+,t) - f(s(t)-,t)$, where $s(t)$ is the position of the interface. We write $f(s-)$ respectively $f(s+)$ for the one-sided limit of f in s from the left respectively from the right.

The *Rankine-Hugoniot conditions* for strain u_x and velocity $\dot{u}$ read

$$[\![\sigma(u_x)]\!] = -\rho c\,[\![\dot{u}]\!]\,,$$
$$c\,[\![u_x]\!] = -\,[\![\dot{u}]\!]\,.$$

We combine these conditions and write for $\epsilon = u_x$

$$\rho c^2\,[\![\epsilon]\!] = [\![\sigma(\epsilon)]\!]\,. \tag{6}$$

Here, the solution can be shown to oscillate on both sides of the interface. It is, however, meaningful to consider the *averaged strains*, e.g.,

$$\bar{\epsilon}_+ := \lim_{x\to\infty}\lim_{s\to\infty}\frac{1}{s}\int_x^{x+s}\epsilon(\xi)\mathrm{d}\xi.$$

A direct calculation shows that the Rankine-Hugoniot condition holds,

$$\bar{\epsilon}_+ - \bar{\epsilon}_- = 2\frac{1}{1-c^2}. \tag{7}$$

To motivate kinetic relations, let us consider a heat-conducting thermoelastic body. We denote the heat flux by q, the specific entropy by s, the absolute temperature by T, and the material velocity (mass flux) by c. For a moving surface of discontinuity with normal n, the surface entropy production is $R := c\,[\![s]\!] + \left[\!\left[\frac{q\cdot n}{T}\right]\!\right]$. The second law of thermodynamics imposes the inequality $R \geq 0$. One can see that this restricts possible jumps for supersonic waves (shocks) as well as the constitutive structure of entropy production R for subsonic waves (kinks) [7]. For subsonic waves, this yields an additional condition $R = R(c)$.

A moving interface is exposed to the so-called *configurational force* f. Since the entropy production R is related to the configurational force, it is reasonable to define a *kinetic relation* as a functional relationship between f and wave speed c. We refer the reader to [6, 1] for more information on kinetic relations. The configurational force is given by

$$f := \int_{\bar{\epsilon}_-}^{\bar{\epsilon}_+} \sigma(\epsilon)\mathrm{d}\epsilon - \{\sigma\}\,[\![\epsilon]\!]\,. \tag{8}$$

Here, $\bar{\epsilon}_\pm$ is taken to be the limit of the averaged strain, $[\![\epsilon]\!] := \epsilon(s(t)+,t) - \epsilon(s(t)-,t)$ and $\{\sigma\} := \frac{1}{2}(\sigma(s(t)+,t) + \sigma(s(t)-,t))$. For the problem under consideration, one computes directly

$$f = -\frac{2c^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}} \cdot \xi. \tag{9}$$

We remark that contrary to the common assumption, f is not a function of c alone, but depends on a two-parameter family, with the wave speed being one parameter, and the other parameter ξ as in Theorem 1. This form of the kinetic relation is only valid for subsonic wave speeds with $\kappa_0^2 \leq \frac{1}{2}$ as in Theorem 1. Evidently, the kinetic relation is trivial, $f = 0$, for the symmetric wave, $\xi = 0$.

We close by pointing out that one would want to impose the validity of the entropy inequality $fc \geq 0$ for the solutions of Theorem 1. For $c > 0$, this inequality is violated for any solution with $\xi > 0$, while it holds for $\xi \leq 0$. Conversely, solutions with $\xi \geq 0$ satisfy the entropy inequality for $c < 0$; the symmetric solution, with trivial kinetic relation, satisfies the entropy inequality for positive and negative wave speeds.

References

[1] R. Abeyaratne, J. L. Knowles, *Kinetic relations and the propagation of phase boundaries in solids*, Arch. Rational Mech. Anal. **114** (1991), 119–154.

[2] S.-N. Chow, J. Mallet-Paret, W. Shen, *Traveling waves in lattice dynamical systems*, J. Differential Equations **149** (1998), 248–291.

[3] Föster, Scheil *Untersuchung des zeitlichen Ablaufes von Umklappvorgängen in Metallen*, Z. Metallkd. **32** (1940), 165–201.

[4] G. Friesecke, R. L. Pego, *Solitary waves on FPU lattices. I. Qualitative properties, renormalization and continuum limit*, Nonlinearity **12** (1999), 1601–1627.

[5] G. Iooss, K. Kirchgässner, *Traveling waves in in a chain of coupled nonlinear oscillators*, J. Comm. Math. Phys. **211** (2000), 439–464.

[6] L. Truskinovskiĭ, *Dynamics of nonequilibrium phase boundaries in a heat conducting nonlinearly lastic medium*, Prikl. Mat. Mekh. **51** (1987), 1009–1019.

[7] L. Truskinovsky, *Inertial effects in the dynamics of martensitic phase boundaries*, in Shape-Memory Materials and Phenomena — Fundamental Aspects and Applications (Liu, C. T. and Wuttig, M. and Otsuka, K. and Kunsmann, H., eds.) **48** (1992), 103–108.

[8] L. Truskinovsky, *Transition to detonation in dynamic phase changes*, Arch. Rat. Mech. Anal. **125** (1994), 375–397.

[9] L. Truskinovsky, A. Vainchtein, *Kinetics of martensitic phase transitions: Lattice model*, SIAM J. Appl. Math. **66** (2005), 1205–1221.

[10] L. Truskinovsky, A. Vainchtein, *Quasicontinuum models of dynamic phase transitions*, Contin. Mech. Thermodyn. **18** (2006), 1–21.