Discrete dynamic models for phase transitions

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The problem under consideration is easy to formulate. Consider a one-dimensional chain of atoms $\{q_j\}_{j\in\mathcal{Z}}$ on a torus ($\mathcal{Z} := \mathbb{Z}/L\mathbb{Z}$ with $L \in \mathbb{N}$) or on the real line ($\mathcal{Z} := \mathbb{Z}$). For each atom, the deformation is given by $u_k\colon \mathbb{R} \to \mathbb{R}$. The equations of motion are governed by Newton's law, which, in suitable units, reads

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

for every $k \in \mathcal{Z}$ (on the torus, indices are counted modulo L). This is a spatially discretized, one-dimensional version of the well-studied equations of motions of an elastic material

$$u_{tt}(x) = \operatorname{Div}(\sigma(Du(x))). \tag{2}$$

Discretized equations as (1) are intrinsically interesting, as they correspond to forward-backward equations. This become apparent in the travelling wave formulation

$$u_j(t) = u(j - ct) \text{ for } j \in \mathcal{Z}, \tag{3}$$

since then Equation (1) transforms into

$$c^2\ddot{u}(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)). \tag{4}$$

This is the Euler-Lagrange function for the action functional

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

Many problems, such models of crystal lattices, photonic structures, and Josephson junctions, can be described by lattice differential equations, of which (4) is one instance. There are a number of mathematical problems associated with lattice differential equations in general. A number of interesting papers [1, 2, 3] give a good insight into this field.

Such spatially discrete models are of interest in mathematical material science. In that context, an additional challenge can occur, which is at the centre of the present investigation. Namely, to describe phase transitions in solids ("martensitic" phase transformations), the interaction potential V is assumed to be *non-convex*. For the naïve continuum limit (2) of Equation (1), this corresponds to an ill-posed elliptic-hyperbolic problem. The travelling wave ansatz (3) singles out solutions and allows us to gain insight into the motion of a phase boundary. The existence of travelling waves will have implications for the prediction of a *kinetic relation*, which relate the velocity of a phase boundary to a configurational force.

Here, the existence of travelling waves is analysed rigorously for a special case, namely nearest-neighbour interaction with a piecewise quadratic energy,

$$V(\epsilon) = \frac{1}{2}\min\{(\epsilon+1)^2, (\epsilon-1)^2\} \tag{5}$$

The aim is to investigate the existence of solutions to (4) with V given by (5). It is shown that on a torus of length L, the existence of solutions with the strain distribution

$$\epsilon > 0 \text{ on } (0, \tfrac{L}{2}) \text{ and } \epsilon < 0 \text{ on } (\tfrac{L}{2}, L) \tag{6}$$

depends on the wave speed c: for some velocities c, a solution exists, while for other velocities nonexistence of a solution with strain distribution (6) can be proved.

For the real line ($\mathcal{Z} := \mathbb{Z}$), the existence of heteroclinic waves with the strain distribution

$$\epsilon > 0 \text{ for } x > 0 \text{ and } \epsilon < 0 \text{ for } x < 0$$

can be proved rigorously for sufficiently large velocities below the wave speed 1. Previous results [4, 6] were formal in the sense that they relied on physical considerations, namely the so-called *causality principle for a steady-state solution* [5]. This approach addresses the issue of the non-integrability of the Fourier transform of potential solutions (with singularities stemming from zeros of the dispersion relation). It seems natural to request a rigorous mathematical framework for problems of this kind, and a sketch of how to address this issue was contributed for the particular problem under consideration.

References

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