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Travelling waves for a Frenkel–Kontorova chain

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Abstract

In this article, the Frenkel–Kontorova model for dislocation dynamics is considered, where the on-site potential consists of quadratic wells joined by small arcs, which can be spinodal (concave) as commonly assumed in physics. The existence of heteroclinic waves—making a transition from one well of the on-site potential to another—is proved by means of a Schauder fixed point argument. The setting developed here is general enough to treat such a Frenkel–Kontorova chain with smooth (C^2) on-site potential. It is shown that the method can also establish the existence of two-transition waves for a piecewise quadratic on-site potential.

MSC: 37K60; 34C37; 58F03; 70H05

1. Introduction

In 1938, Frenkel and Kontorova proposed a fundamental model of dislocation dynamics [8]. The model is given by Newton's equation of motion for a chain of atoms,

$$mu_k'' = \beta(u_{k+1} - 2u_k + u_{k-1}) - 2\pi \frac{\tilde{\alpha}}{\gamma} g' \left(\frac{2\pi}{\gamma} u_k \right) \tag{1}$$

with some constants $\tilde{\alpha}$, β, γ, describing the displacement u_k of atom $k \in \mathbb{Z}$ in a one-dimensional chain. The nonlinearity is the derivative of an on-site potential describing the interaction with atoms above and below the chain of atoms considered. The periodicity of the nonlinearity thus

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reflects the periodic nature of a crystalline lattice. The Frenkel–Kontorova chain is a fundamental model of dislocation dynamics, describing how an imperfection (dislocation) travels through a crystalline lattice; see for example the survey [3]. The simplest motion that may exist is that of a travelling wave, $u_j(t) = u(j - ct)$ with wave speed c. This *ansatz* transforms (1), after rescaling, into

$$c^2 u'' - \Delta_D u + g'(u) = 0 \tag{2}$$

on $\mathbb{R}$, where Δ_D is the discrete Laplacian,

$$\Delta_D u(x) := u(x+1) - 2u(x) + u(x-1).$$

In the original paper [8], the on-site potential g is sinusoidal. A dislocation corresponds to a heteroclinic wave in the sense that the states near $-\infty$ are in one well of g and the states near $+\infty$ are in another well, which we here take to be a neighbouring one; see Fig. 1 for a plot of an approximate solution, where the dislocation is in travelling wave coordinates positioned at the origin; the oscillations in the left half plane take place in one well of the on-site potential, and the solutions in the positive half plane take place in the neighbouring well. It thus suffices to consider potentials g with two wells only, say

$$g(u) = \frac{1}{2}\alpha u^2 - \alpha\psi(u), \tag{3}$$

which leads to the reformulation of (2) as

$$c^2 u'' - \Delta_D u + \alpha u - \alpha\psi'(u) = 0 \tag{4}$$

(in the setting considered here, it is easy to show that a solution to (4) with a two-well on-site potential is also a solution to the same equation with a suitable periodic continuation of the on-site potential).

The study of equation (4) has a long history in mechanics. Initial work by Frank and van der Merwe [7] resorted to the analysis of the continuum approximation of (1), the sine-Gordon equation, is analysed. This simplifies the analysis significantly, but already Schrödinger [18] pointed out the difference between PDE limits and underlying lattice equations. Indeed, the analysis of (1) has proved to be very hard. To the best of our knowledge, all existing analytic results, spanning more than 50 years, rely on the assumption that g is piecewise quadratic; then the force g' in (1) is piecewise linear and Fourier methods can be applied. We refer the reader to papers by Atkinson and Cabrera [2], Earmme [5] and extensive work by Truskinovsky and collaborators, covering the so-called Fermi–Pasta–Ulam–Tsingou chain with piecewise quadratic interaction [22] and the Frenkel–Kontorova model [14]. Kresse and Truskinovsky have studied the case of an on-site potential with different moduli (second derivatives at the minima) [15]. We also mention important contributions by Slepyan, for example [21,20]. Flytzanis, Crowley and Celli [6] apply Fourier techniques to a problem where the potential consists of three parabolas, the middle one being concave.

A difficulty with a piecewise quadratic on-site potential is that it is not smooth, but has a cusp. One would expect the physical potential to be smooth, but the use of Fourier methods automatically leads to singularities in the force. Does the presence or absence of this singularity affect the existence of waves? The answer is neither obvious from physical view, since the singularity can