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Kinetic Relations for a Lattice Model of Phase Transitions

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Abstract

The aim of this article is to analyse travelling waves for a lattice model of phase transitions, specifically the Fermi-Pasta-Ulam chain with piecewise quadratic interaction potential. Firstly, for fixed, sufficiently large subsonic wave speeds, we rigorously prove the existence of a family of travelling wave solutions. Secondly, it is shown that this family of solutions gives rise to a kinetic relation which depends on the jump in the oscillatory energy in the solution tails. Thirdly, our constructive approach provides a very good approximate travelling wave solution.

1. Introduction

This article is concerned with travelling waves and the associated kinetic relations for the Fermi-Pasta-Ulam chain with a piecewise quadratic interaction potential. The aims of this article are threefold. First, for fixed large, but subsonic wave speed, the existence of a family of travelling heteroclinic waves is established (here, heteroclinic is understood in the sense that the asymptotic states are in different wells of the interaction potential). We are not aware of such non-uniqueness results for related lattice models in the literature. Methodologically, the existence result is an extension of earlier work [15], where the existence of a symmetric travelling wave is shown. Here we show that this solution is embedded in a one-parameter family of solutions, parametrised by a family of functions in the kernel of the associated linearised operator. Secondly, the chosen parametrisation of solutions gives rise to a parametrisation of the so-called kinetic relation (relating the wave speed to the so-called configurational force). This significantly extends the previous result [15], where the symmetry of the travelling wave implied a trivial force-free kinetic relation. To avoid possible confusion, we emphasise that the family of kinetic relations found here is a parametrisation for

fixed wave speed. That is, the kinetic relation is not unique. Thirdly, we demonstrate the numerical potential of the framework employed here. Below we provide explicit approximate solutions, henceforth called *profiles*, which show a small deviation from the exact solution, see the plots in Section 5. Furthermore, we prove rigorously that the profiles differ from the exact solution by at most $\frac{0.5}{c^2}$ in the L^∞-norm, where c is the wave speed. This should be contrasted with the traditional representation of the solution as an infinite sum of Fourier-like components, where error bounds on the solution do not seem to exist in the literature.

The motivation for this article is the quest to identify kinetic relations. Kinetic relations specify a relationship between the configurational force and the velocity of a phase boundary [1,21]. The rationale for investigating kinetic relations for lattice models is lucidly described in [23,22]; here we remark that alternative proposals to resolve the ill-posedness of the macroscopic equations of elasticity with nonconvex energy density exist, including vanishing viscosity [13] or interfacial energy [20]. We instead aim to use kinetic relations *derived* from first principles. Two comments on the kinetic relation below (see Equation (47)) seem in place. First, we emphasise that the kinetic relation is in this setting *not* a unique relation between the configurational force and the wave velocity c. Rather, for fixed c, the kinetic relation is a multi-valued map with values describing the configurational force. Second, the kinetic relation has a simple and explicit form, unlike previous representations as a formal sum. Our analysis is, however, restricted to a relatively small range of large subsonic velocities (see Theorem 1 below for the precise formulation).

We show that the kinetic relation can be given a thermomechanical interpretation, rather than a purely mechanical one. This is in line with the thinking of O. Penrose in [12], who discusses the derivation of irreversible macroscopic equations from Newtonian mechanics. In Penrose's words, "The model must contain, in addition, some nonmechanical ingredient. What can this extra non-mechanical ingredient be?". Here we show that for the problem of a moving phase boundary, the purely mechanical microscopic (lattice) model gives rise to a thermomechanical kinetic relation. It is, however, not clear how to classify solutions, using a probabilistic characterisation of "good" or "bad" solutions, as in [12].

We study the Fermi-Pasta-Ulam chain (1) given below with bi-quadratic potential energy, where to our knowledge the first investigation is due to Balk, Cherkaev and Cherkaev [4,5]. In [4], the authors study associated initial-value problems and solve them numerically. They observe macroscopic irreversibility for the microscopic Hamiltonian system, and explain this phenomenon by an energy transfer to high frequency oscillations. We consider travelling waves, where time is no longer an independent variable and thus such a thermalisation is harder to define; yet the discussion in Section 4 gives an interpretation of our findings in the spirit of [4].

The precise setting is as follows. The Fermi-Pasta-Ulam chain is defined by the equation of motion

$$\ddot{u}_j(t) = V'(u_{j+1}(t) - u_j(t)) - V'(u_j(t) - u_{j-1}(t)) \tag{1}$$

for every $j \in \mathbb{Z}$; it describes the motion of a one-dimensional chain of atoms $\{q_j\}_{j \in \mathbb{Z}}$ on the real line by the deformation $u_j \colon \mathbb{R} \to \mathbb{R}$, where $j \in \mathbb{Z}$ numbers the atoms. Equation (1) describes the evolution governed by Newton's law, with neighbouring atoms being linked by springs.

The argument of the elastic potential is the discrete strain, which is given by the difference of the deformations $u_{j+1}(t) - u_j(t)$. We consider phase transitions and thus face the difficulty that $V \colon \mathbb{R} \to \mathbb{R}$ is nonconvex. As in several previous studies [4, 5, 23, 24, 15], we consider the simplest possible bistable elastic potential V, namely a piecewise quadratic function. Specifically, we define

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

In this article, we confine the analysis to the one-dimensional case and refer the reader to [17] for an analysis of bistable atomistic interactions on two-dimensional lattices. Molecular dynamics simulations make it possible to investigate a broader class of configurations than we can study in the travelling wave frame and more realistic interaction potentials; recent investigations of the kinetics of detwinning are due to Hildebrand and Abeyaratne [9], and the analysis of martensitic microstructure evolution by Kastner and Ackland [10].

For the strain, (2) implies that

$$\sigma(\varepsilon) := \varepsilon + 1 - 2H(\varepsilon) = \varepsilon + H(-\varepsilon) - H(\varepsilon) \tag{3}$$

equals $V'(\varepsilon)$ wherever V is differentiable, that is, for every $\varepsilon \neq 0$. Here, H is the symmetrised Heaviside function,

$$H(x) = \begin{cases} 0 & \text{for } x < 0 \\ \frac{1}{2} & \text{for } x = 0 \\ 1 & \text{for } x > 0 \end{cases}.$$

With the travelling wave ansatz $u_j(t) = u(j - ct)$ for $j \in \mathbb{Z}$, Equation (1) reduces to

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

In terms of the discrete strain $\varepsilon(x) := u(x) - u(x-1)$, the travelling wave equation is

$$c^2 \varepsilon''(x) = \Delta_1 V'(\varepsilon(x)), \tag{4}$$

where

$$\Delta_1 f(x) := f(x+1) - 2f(x) + f(x-1)$$

is the *discrete Laplacian*. Specialising the potential to the choice made in (2), Equation (4) becomes

$$c^2 \varepsilon''(x) = \Delta_1 \left[\varepsilon(x) + H\left(-\varepsilon(x)\right) - H\left(\varepsilon(x)\right) \right] = \Delta_1 \varepsilon(x) - 2\Delta_1 H\left(\varepsilon(x)\right). \quad (5)$$

For the sake of clarity, we order into linear and nonlinear part and rewrite (5) as

$$c^2 \varepsilon'' - \Delta_1 \varepsilon = -2\Delta_1 H(\varepsilon). \quad (6)$$

The aim of this article is to show the existence of a family of heteroclinic travelling wave solutions for this nonlinear advance-delay equation, and study the associated kinetic relations. We prove in Theorem 1 that a three-parameter family of solutions exists; this is also the dimension of the solution space one wold expect from a counting argument. Further, one can show, using arguments from distribution theory akin to those in [14], that every bounded solution with a single phase boundary at the origin is of the kind described in Theorem 1.

In [18], it is shown that travelling wave solutions for the Fermi-Pasta-Ulam chain with biquadratic potential appear naturally for solutions of initial-value problems. Their numerical experiments demonstrate that after a transient regime, travelling-wave like motion is observed. Further, it is also pointed out that travelling waves can have an energy supply from infinity, unlike the problem of a resting source studied by Sommerfeld [19].

2. Existence of a family of travelling waves

In a previous study [15], the authors proved the existence of a symmetric travelling wave solution to (6). One purpose of this note is to show that there is a family of travelling waves, parametrised by the average in the (averaged) asymptotic profiles. The travelling wave solution of [15] has zero average and is thus symmetric. In the framework employed here, the solution is represented as a sum of a (here explicitly given) profile and a corrector in $L^2(\mathbb{R})$. At the heart of the existence proof is the observation that suitable functions in the kernel of the linear operator

$$L := \left(c^2 \partial^2 - \Delta_1 \right) \quad (7)$$

can be superimposed on the symmetric solution profile. A suitable choice of these kernel functions can achieve the desired symmetry change.

We focus on single-transition waves, where exactly one interface is present that separates the atoms in one phase from those in the other. It is not restrictive to assume that the interface is positioned at the origin. We thus seek solutions ε to (6) which are defined on the real line and have the property that

$$\varepsilon > 0 \text{ for } x > 0 \text{ and } \varepsilon < 0 \text{ for } x < 0. \quad (8)$$

Then, and only then, it follows directly that

$$f(x) := \Delta_1 H(\varepsilon) = \begin{cases} 1 & \text{for } x \in (-1, 0) \\ -1 & \text{for } x \in (0, 1) \\ 0 & \text{else,} \end{cases} \tag{9}$$

that is, the nonlinear right-hand side turns into a function that only depends on the spatial variable, and one is left to solve

$$c^2 \varepsilon'' - \Delta_1 \varepsilon = -2f(x). \tag{10}$$

An analogous simplification has been employed for related lattice problems, e.g., the Frenkel-Kontorova problem, notably by Atkinson and Cabrera [3] (see also [6]). Kresse and Truskinovsky [11] give a clear account for the Frenkel-Kontorova problem and highlight that the single-transition interface condition (8) probably does not hold for low wave speeds c. As pointed out by Kresse and Truskinovsky, a rigorous argument needs to prove that the single-transition condition (8) holds, since only then is the solution found for (10) a solution of the original system (6).

We point out that the right-hand side $-2f$ of Equation (10), given in (9), is compactly supported on $[-1, 1]$, and hence its Fourier transform exists. We recall that for $g\colon \mathbb{R} \to \mathbb{R}$, the Fourier transform (if defined) is

$$F[g] := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) \exp(-i\kappa x) \, \mathrm{d}x;$$

the Fourier sine transform (if defined) is given by

$$F_{\mathrm{s}}[g](\kappa) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sin(\kappa x) g(x) \, \mathrm{d}x = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} \sin(\kappa x) g(x) \, \mathrm{d}x.$$

The relation

$$F[g] = -i F_{\mathrm{s}}[g]$$

holds for odd functions $g\colon \mathbb{R} \to \mathbb{R}$.

One aim of this article is to show that the kernel of the linear operator (7) heavily influences essential qualitative properties of the solution, including the kinetic relation. To be specific, let us introduce the *dispersion relation*

$$D(\kappa) := -c^2 \kappa^2 + 4 \sin^2 \left(\frac{\kappa}{2} \right). \tag{11}$$

For the linear part $L\varepsilon = c^2 \varepsilon'' - \Delta_1 \varepsilon$ of Equation (5), it holds that

$$F[L\varepsilon] = F\left[c^2 \varepsilon'' - \Delta_1 \varepsilon\right] = D(\kappa) F[\varepsilon],$$

and analogously for the Fourier sine transform,

$$F_{\mathrm{s}}[L\varepsilon] = F_{\mathrm{s}}\left[c^2 \varepsilon'' - \Delta_1 \varepsilon\right] = D(\kappa) F_{\mathrm{s}}[\varepsilon].$$

We fix the wave speed c,

$$c := \pm \frac{\sin\left(\frac{\kappa_0}{2}\right)}{\frac{\kappa_0}{2}}; \tag{12}$$

this choice ensures that the dispersion relation $D(\kappa)$ has *only one* positive zero, namely κ_0. We point out that the latter property does not determine the sign of c. Hence, unlike in [15], we allow for both signs in the definition (12) of c.

The following theorem makes the same assumptions as the previous existence result [15, Theorem 3.1], but shows that there is a family of solutions, rather than one solution.

Theorem 1. *Suppose the dispersion relation* (11) *has one positive zero* κ_0 *with* $\kappa_0^2 < \frac{1}{2}$. *Then there exists a family of heteroclinic solutions to Equation* (6), *parametrised by two real numbers* ξ, η *with* $|\xi| \leq 1$ *and* $|\eta|$ *sufficiently small. The solutions satisfy the sign condition* (8) *for all admissible parameter values* ξ *and* η.

Theorem 1 is an immediate consequence of Lemma 1 to Lemma 3 below. To formulate these statements, we sketch the setting and focus on how the dispersion relation determines the ansatz, in particular the difference to the ansatz for the symmetric wave.

As before [15], we write the solution ε of (10) (equivalently, the solution of (6) with the sign condition (8)) as a linear combination of a *profile* and a *corrector*, that is,

$$\varepsilon := \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}. \tag{13}$$

The profile function collects all parts of the solution ε corresponding to the singularities of

$$\frac{F[-2f]}{D(\kappa)}; \tag{14}$$

since the solution ε is formally given by the inverse Fourier transform of (14), the corrector is then a function in $L^2(\mathbb{R})$ and satisfies an equation which can be solved by Fourier methods in $L^2(\mathbb{R})$.

The profile ε_{pr} is defined as follows. Let α and β be constants, with

$$\alpha := c^2 \frac{\kappa_0^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}} > 0 \tag{15}$$

and $\beta > 0$ chosen such that

$$\gamma^2 := \left(1 + \frac{\kappa_0^2}{\beta^2}\right)^{-1} := c^2 \alpha \frac{1 - c^2}{\kappa_0^2} = c^4 \frac{1 - c^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}. \tag{16}$$

Then, we define the *profile function* as

$$\varepsilon_{\text{pr}}(x) := \varepsilon_{\text{pr}}^{\text{osc}}(x) + \varepsilon_{\text{pr}}^{\text{nonosc}}(x) \tag{17}$$

with

$$\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}(x) := \frac{\alpha}{\kappa_0^2} \cdot 2 \sin^2\left(\tfrac{\kappa_0}{2}x\right)(\mathrm{sign}(x) + \xi) + \eta \sin\left(\kappa_0 x\right) \tag{18}$$

(with $\xi, \eta \in \mathbb{R}$ two free parameters); and

$$\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x) := \mathrm{sign}(x) \cdot \alpha \frac{1 - \exp\left(-\beta\,|x|\right)}{\beta^2} + \frac{-2}{c^2}\Delta_1\left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right](x) + \varepsilon_{\mathrm{2nd}}(x), \tag{19}$$

where

$$\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}(x) := \mathrm{sign}(x) \cdot \frac{1}{4}\,|x|^2 \tag{20}$$

is a contribution with a jump, and

$$\varepsilon_{\mathrm{2nd}}(x) := \frac{7}{60}\frac{129}{128}\frac{x \exp\left(-\frac{\sqrt{30}}{2}\,|x|\right)}{c^2}\left(\sqrt{30} + 15\,|x| - \frac{115}{86}\sqrt{30}\,|x|^2\right) \tag{21}$$

is a second order correction in $L^2(\mathbb{R})$.

This is a rearrangement of the terms of the profile given in [15], with a new contribution in form of an asymmetric oscillatory term in (18), namely

$$\varepsilon_{\mathrm{asym}} := \frac{\alpha}{\kappa_0^2} \cdot 2 \sin^2\left(\tfrac{\kappa_0}{2}x\right)\xi. \tag{22}$$

We point out the essential properties of this term. First, it is the only term that breaks the point symmetry of the solution. Second, it is in the kernel of the linear operator L of (7), since $2\sin\left(\frac{\kappa_0}{2}\right)^2 = 1 - \cos\left(\kappa_0 x\right)$, and the affine functions along with $\sin\left(\kappa_0 x\right)$ and $\cos\left(\kappa_0 x\right)$ are in the kernel of L.

Lemma 1. *There is a function $\varepsilon_{\mathrm{cor}} \in L^2(\mathbb{R})$ such that $\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ solves Equation (10) for all values of $\xi, \eta \in \mathbb{R}$.*

Proof. The asymmetric oscillatory term of (22) is chosen to be in the kernel of the operator $L := \left(c^2\partial^2 - \Delta_1\right)$ from (7). It thus follows readily that the profile function $\varepsilon_{\mathrm{pr}}$ satisfies an equation

$$\left(c^2\partial^2 - \Delta_1\right)\varepsilon_{\mathrm{pr}}(x) = -2f(x) + \Phi(x), \tag{23}$$

where $\Phi \in L^2(\mathbb{R})$ is a continuous localised function already obtained in [15].

This implies that $\varepsilon_{\mathrm{cor}}$ is found as the $L^2(\mathbb{R})$-solution of

$$\left(c^2\partial^2 - \Delta_1\right)\varepsilon_{\mathrm{cor}}(x) = \Phi(x) \tag{24}$$

already described in [15]. Hence, by Equations (23) and (24) we deduce that $\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ solves Equation (10). $\square$

Lemma 2. *The profile contribution $\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}$ satisfies*

$$x \cdot \varepsilon_{\mathrm{pr}}^{\mathrm{osc}}(x) \geq 0$$

for all $x \in \mathbb{R}$ as long as $|\xi| \leq 1$ and $|\eta|$ is sufficiently small.

Proof. Observe from (18) that $\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}$ satisfies the claim if η is small enough and there holds

$$x \left(\mathrm{sign}(x) + \xi \right) \geq 0$$

for all $x \in \mathbb{R}$. It is easy to see that this implies the upper bound $|\xi| \leq 1$. □

Lemma 3. *The profile contribution $\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}$ satisfies*

$$c^2 \varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x) > 0.5 \ for \qquad |x| > 0.385, \tag{25}$$

$$\frac{c^2 \varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x)}{x} > 1.2 \ for \ 0 < |x| \leq 0.385. \tag{26}$$

In particular, it obeys the single transition condition (8).

Proof. Let us recall for $x > 0$ the definition (17) of the profile function

$$\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x) := \alpha \frac{1 - \exp\left(-\beta|x|\right)}{\beta^2} + \frac{-2}{c^2} \Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right](x) + \varepsilon_{\mathrm{2nd}}(x).$$

Thus, with

$$t = t\left(\kappa_0\right) := \frac{\alpha c^2}{\beta^2} = \frac{\frac{\kappa_0^2}{1-c^2}}{\kappa_0^2 + \beta^2},$$

we can write

$$c^2 \varepsilon_{\mathrm{pr}}(x) = t \left(1 - \exp\left(-\beta\,|x|\right)\right) - 2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right](x) + c^2 \varepsilon_{\mathrm{2nd}}(x). \tag{27}$$

For $\kappa_0^2 \leq \frac{1}{2}$, we can estimate

$$1.57 \leq t \leq \mathring{t} := \lim_{\kappa_0 \to 0} t = 1.6. \tag{28}$$

Furthermore, the monotonicity of β in κ_0 implies as in [15, (46)]

$$\left| \exp\left(-\beta x\right) - \exp\left(-\mathring{\beta}x\right) \right| < 0.01, \tag{29}$$

with $\frac{1}{\mathring{\beta}^2} := \frac{2}{15}$. As in [15], we define

$$W(x) := \mathring{t} \left(1 - \exp\left(-\mathring{\beta}x\right)\right) - 2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right] + c^2 \varepsilon_{\mathrm{2nd}}, \tag{30}$$

which is a function that only depends on x and not on κ_0. To prove the lemma, we will utilise the following properties of $W(x)$,

$$W(x) > 0.58 \quad \text{for} \qquad x > 0.385, \tag{31}$$

$$W(x) > 1.5 \cdot x \text{ for } 0 < x \leq 0.385. \tag{32}$$

(i) $x > 0.385$. We define

$$W_1 := t \exp\left(-\beta x\right) - \mathring{t} \exp\left(-\mathring{\beta} x\right)$$

and obtain from (27)

$$
\begin{aligned}
c^2 \varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}} &\geq t\left(1 - \exp\left(-\beta x\right)\right) - 2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right] + c^2 \varepsilon_{\mathrm{2nd}} \\
&= \left(t - 2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right] + c^2 \varepsilon_{\mathrm{2nd}} - \mathring{t} \exp\left(-\mathring{\beta} x\right)\right) - W_1 \\
&= t - \mathring{t} + W - W_1.
\end{aligned}
$$

It follows from (28) that

$$\left|t - \mathring{t}\right| \leq 0.03. \tag{33}$$

Hence, we estimate as in [15] with (33), (29) and (28) in the second step that

$$
\begin{aligned}
|W_1| &\leq \left|t - \mathring{t}\right| \frac{\exp\left(-\beta x\right) + \exp\left(-\mathring{\beta} x\right)}{2} + \left|\exp\left(-\beta x\right) - \exp\left(-\mathring{\beta} x\right)\right| \frac{t + \mathring{t}}{2} \\
&< 0.03 \cdot 1 + 0.01 \mathring{t} \leq 0.046 =: E_1.
\end{aligned}
$$

Thus, (31) ensures for all $x > 0.385$ that

$$\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x) > 0.58 - (0.03 + E_1) > 0.5, \tag{34}$$

as claimed.

(ii) $0 < x \leq 0.385$: For this range of x, we base our argument on estimating the derivative of $\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}$. We observe

$$
\begin{aligned}
c^2 \left(\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}\right)' &\geq \beta t \exp\left(-\beta x\right) + \left(-2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right] + c^2 \varepsilon_{\mathrm{2nd}}\right)' \\
&\geq \mathring{\beta}\mathring{t} \exp\left(-\mathring{\beta} x\right) + \left(-2\Delta_1 \left[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}\right] + c^2 \varepsilon_{\mathrm{2nd}}\right)' - W_2 \\
&= W' - W_2,
\end{aligned} \tag{35}
$$

where W is defined in (30), and

$$W_2 := \mathring{\beta}\mathring{t} \exp\left(-\mathring{\beta} x\right) - \beta t \exp\left(-\beta x\right).$$

Next, we want to show that W_2 is small. Since [15, (43)] and (28) imply

$$\mathring{\beta}\mathring{t} \geq \beta t \geq \mathring{\beta}\sqrt{\tfrac{20}{21}} \cdot 1.57 > 0.95 \cdot \mathring{t}\mathring{\beta},$$

we deduce $\left|\mathring{\beta}\mathring{t} - \beta t\right| < 0.05 \mathring{t}\mathring{\beta}$, and can estimate

$$|W_2| \leq \left|\exp\left(-\beta x\right) - \exp\left(-\mathring{\beta}x\right)\right| \frac{\mathring{\beta}\mathring{t} + \beta t}{2}$$

$$+ \left|\mathring{\beta}\mathring{t} - \beta t\right| \left(\frac{\exp\left(-\beta x\right) + \exp\left(-\mathring{\beta}x\right)}{2}\right)$$

$$\leq 0.01 \cdot \mathring{t}\mathring{\beta} + \left|\mathring{\beta}\mathring{t} - \beta t\right| \cdot 1 < 0.06\mathring{t}\mathring{\beta} < 0.3 =: E_2.$$

Thus, we deduce from (35)

$$c^2 \varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}(x) \geq \int_0^x c^2 \left(\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}\right)' \, \mathrm{d}\xi \geq W(x) - E_2 x = 1.2 \cdot x,$$

which is the claim for all $0 < x \leq 0.385$ by (32).

Since $\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}}$ is an odd function, the claimed statement for $x < 0$ follows by symmetry.   □

Proof of Theorem 1. Lemma 1 provides a solution

$$\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}} = \varepsilon_{\mathrm{pr}}^{\mathrm{osc}} + \varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}} - \varepsilon_{\mathrm{cor}}$$

of the non-autonomous linear equation (10). As described above, ε is a solution of (6) if it satisfies the single transition condition (8). We verify the latter in two steps. Firstly, we combine Lemma 3 with Corollary 3.9 in in [15], namely

$$|\varepsilon_{\mathrm{cor}}(x)| < \frac{0.48}{c^2} \text{ and } |\varepsilon'_{\mathrm{cor}}(x)| < \frac{1.1}{c^2},$$

to deduce that the non-oscillatory part $\varepsilon_{\mathrm{pr}}^{\mathrm{nonosc}} - \varepsilon_{\mathrm{cor}}$ satisfies the sign condition by. Secondly, by Lemma 2, the oscillatory contribution $\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}$ satisfies the single transition condition (8) for $|\xi| \leq 1$. By additivity, ε then satisfies the single transition condition (8) as well and is thus a solution to (6) as claimed.   □

3. The Rankine-Hugoniot condition

We now show that the family of waves of Theorem 1 satisfy the Rankine-Hugoniot condition. As for the symmetric case [15], the argument is simple due to the chosen framework. Namely, with $\varepsilon(x) = \varepsilon_{\mathrm{pr}}(x) - \varepsilon_{\mathrm{cor}}(x)$ with $\varepsilon_{\mathrm{cor}} \in L^2(\mathbb{R})$ as in Section 2, follows that macroscopic quantities such as the Rankine-Hugoniot condition can be directly read off from the profile function $\varepsilon_{\mathrm{pr}}$. This profile is explicitly known, see Equations (17), (18) and (19).

Let us write $s(t)$ for the position of the interface, and introduce the notation $[\![f]\!]$ for $f(s(t)+, t) - f(s(t)-, t)$ (here, $x_0\pm$ is the shorthand notation for the limits from the left and the right at x_0). In the setting of continuum

mechanics, for an interface moving with velocity c, either the strain u_x or the velocity $\dot{u}$ may be discontinuous at the interface. However, the moving interface must satisfy the *Rankine-Hugoniot* conditions [1, Equations (2.6) and (2.7)]

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

which we combine by writing for $\varepsilon = u_x$

$$\rho c^2 \, [\![\varepsilon]\!] = [\![\sigma(\varepsilon)]\!]. \tag{36}$$

Here, one has $\rho \equiv 1$ and, thanks to (3), $[\![\sigma(\varepsilon)]\!] = [\![\varepsilon]\!] - 2$, so (36) is equivalent to

$$[\![\varepsilon]\!] = \frac{2}{1 - c^2}. \tag{37}$$

For the family of solutions of Section 2, although the strain is continuous, it oscillates at $\pm\infty$. Thus, the jump in ε in (37) needs to be understood in the sense

$$[\![\varepsilon]\!] = \bar{\varepsilon}_+ - \bar{\varepsilon}_-, \tag{38}$$

where $\bar{\varepsilon}_\pm$ are the limits of the *averaged strains*

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

and

$$\bar{\varepsilon}_- := \lim_{x \to -\infty} \lim_{s \to \infty} \frac{1}{s} \int_{x-s}^x \varepsilon(\xi) \, \mathrm{d}\xi.$$

As mentioned at the beginning of this section, only $\varepsilon_{\mathrm{pr}}$ contributes to the asymptotic strains $\bar{\varepsilon}_\pm$. An elementary calculation shows that (16) implies

$$\bar{\varepsilon}_+ = \alpha \left(\frac{1+\xi}{\kappa_0^2} + \frac{1}{\beta^2} \right) + \frac{-2}{c^2} \frac{1}{2} = \frac{\alpha}{\kappa_0^2} \gamma^{-2} - \frac{1}{c^2} + \frac{\alpha\xi}{\kappa_0^2} = \frac{1}{1-c^2} + \frac{\alpha\xi}{\kappa_0^2}. \tag{39}$$

Analogously

$$\bar{\varepsilon}_- = -\alpha \left(\frac{1-\xi}{\kappa_0^2} + \frac{1}{\beta^2} \right) - \frac{-2}{c^2} \frac{1}{2} = -\frac{1}{1-c^2} + \frac{\alpha\xi}{\kappa_0^2}. \tag{40}$$

Thus, as in the symmetric case,

$$[\![\varepsilon]\!] = \bar{\varepsilon}_+ - \bar{\varepsilon}_- = 2\frac{1}{1-c^2}, \tag{41}$$

and, via (38), we have verified the Rankine-Hugoniot condition (37).

4. The kinetic relation

A central observation of this note is that the kinetic relation is for fixed velocity (with $\kappa_0 \leq \frac{1}{2}$ and the wave speed c as in (12)) not uniquely determined, but essentially parametrised by a family of functions in the kernel of the linear operator L from Equation (7), in the following sense: if the profile $\varepsilon_{\mathrm{pr}}$ contains no functions in $\ker(L)$ other than the zero function, then the kinetic relation is trivial, namely the zero function. This is the case for a symmetric profile [15]. In the asymmetric case, the profile $\varepsilon_{\mathrm{pr}}$ contains nonzero functions from $\ker(L)$, and it is those kernel functions that render the kinetic relation non-trivial.

Before discussing this in detail, let us recall the definition of a kinetic relation, after introducing the notation $\{\sigma\} := \frac{1}{2}\left(\sigma(s(t)+,t) + \sigma(s(t)-,t)\right)$ for the average stress across the discontinuity. A moving interface can dissipate energy, and the amount of dissipation is measured by the *configurational force* (or *driving force*). Namely, if the strain on both sides of the interface is constant, say ε_l for the strain on the left and ε_r for the strain on the right, then, the *configurational force* acting on an interface is

$$f := [\![V(\varepsilon)]\!] - \{V'(\varepsilon)\}[\![\varepsilon]\!] \tag{42}$$

(see, for example, [1, Equation (2.11)]). Since the configurational force depends on the speed c of the interface, we write $f = f(c)$. Furthermore,

$$R(c) := cf(c) \tag{43}$$

is the (macroscopic) *rate of the energy dissipation* or *energy flux* [1, Equation (2.10)]. The entropy inequality requires that $fc \geq 0$.

Here, the waves can oscillate, possibly widely, on both sides of the interface. We thus have to interpret Equation (42) in an averaged sense,

$$f = [\![V(\langle\varepsilon\rangle)]\!] - \{V'(\langle\varepsilon\rangle)\}[\![\langle\varepsilon\rangle]\!], \tag{44}$$

where we define for a asymptotically periodic function $\phi(x)$ values at infinity by

$$\langle\phi\rangle_{\pm} := \lim_{x\to\pm\infty}\lim_{s\to\pm\infty}\frac{1}{s}\int_x^{x+s}\phi(\xi)\,\mathrm{d}\xi.$$

By definition, we recover $\langle\varepsilon\rangle_{\pm} = \bar{\varepsilon}_{\pm}$, where $\bar{\varepsilon}_{\pm} = \pm\frac{1}{1-c^2} + \frac{\alpha}{\kappa_0^2}\xi$ by (39) and (40). Let us represent the strain as follows

$$\varepsilon(x) = \bar{\varepsilon}_{\pm} + \frac{\alpha}{\kappa_0^2}\left(\operatorname{sign}x + \xi\right)\cos\kappa_0 x + \eta\sin\kappa_0 x + \varepsilon_0(x),$$

where $\varepsilon_0(x) \to 0$ as $|x| \to \infty$. Thus, we obtain

$$V\left(\langle\varepsilon\rangle_{\pm}\right) = V\left(\bar{\varepsilon}_{\pm}\right) = \frac{1}{2}\left((\bar{\varepsilon}_{\pm} \mp 1)^2\right)$$

and

$$[\![V(\langle\varepsilon\rangle)]\!] = \frac{1}{2}\left(\bar{\varepsilon}_+^2 - \bar{\varepsilon}_-^2\right) - (\bar{\varepsilon}_+ + \bar{\varepsilon}_-).$$

Further, we find

$$\{V'(\langle\varepsilon\rangle)\} = \{\langle\varepsilon\rangle\} = \frac{\bar{\varepsilon}_+ + \bar{\varepsilon}_-}{2}$$

and

$$[\![\langle\varepsilon\rangle]\!] = \bar{\varepsilon}_+ - \bar{\varepsilon}_-,$$

which yields for f in (44)

$$f = -(\bar{\varepsilon}_+ + \bar{\varepsilon}_-) = -2\frac{\alpha}{\kappa_0^2}\xi. \tag{45}$$

Now we observe that

$$\langle V(\varepsilon)\rangle_{\pm} = \frac{1}{2}\left((\bar{\varepsilon}_{\pm} \mp 1)^2 + \frac{1}{2}\left(\frac{\alpha}{\kappa_0^2}\left(\pm 1 + \xi\right)\right)^2 + \frac{1}{2}\eta^2\right).$$

Hence, it holds that

$$\langle V(\varepsilon)\rangle_{\pm} - V\left(\langle\varepsilon\rangle_{\pm}\right) = \frac{1}{4}\left(\frac{\alpha}{\kappa_0^2}\left(\pm 1 + \xi\right)\right)^2 + \frac{1}{4}\eta^2,$$

and we deduce

$$[\![\langle V(\varepsilon)\rangle - V\left(\langle\varepsilon\rangle\right)]\!] = \left(\frac{\alpha}{\kappa_0^2}\right)^2\xi. \tag{46}$$

Hence we can rewrite the kinetic relation (42), using (45) and (46), as

$$f = -2\frac{\kappa_0^2}{\alpha} \cdot \left(\frac{\alpha}{\kappa_0^2}\right)^2 \xi = -2\frac{\kappa_0^2}{\alpha}[\![\langle V(\varepsilon)\rangle - V\left(\langle\varepsilon\rangle\right)]\!], \tag{47}$$

where $\frac{\kappa_0^2}{\alpha} = \frac{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}{c^2}$ is an even and positive function of c (as κ_0 is implicitly defined by (12)). Thus the kinetic relation is proportional to the jump in the oscillatory energy. The latter is the difference between the average of the energy and the energy of the averaged strain, $\langle V(\varepsilon)\rangle - V\left(\langle\varepsilon\rangle\right)$. The kinetic relation is thus nonzero except for the point-symmetric solution, where the jump vanishes and hence $\xi = 0$.

An interpretation of (47) is: the microscopic energy can be split in two parts, namely one where the local average of the energy equals the energy of the local average of the strain, and the remainder. Here, the solutions we find are asymptotically characterised by oscillations superimposed to an asymptotically constant strain state. For the latter, averaging and evaluating a (nonlinear) energy V commute, while this is not the case for oscillatory tails. So the split of the energy E can be written as a split into oscillatory and nonoscillatory contributions, $E = E_{\text{non}} + E_{\text{osc}}$. Then the expression for the kinetic relation shows that precisely the energy E_{osc} stored in the microscopic oscillations determines the macroscopic kinetic relation and thus

the macroscopic dissipation. A description of this observation would be that the energy stored in microscopic oscillations does converge in the continuum limit to the energy of the corresponding averaged (macroscopic) configuration; yet E_{osc} is not lost but enters the kinetic relation.

Since we consider travelling waves, there is no proper time variable involved. It does not make sense to speak of temperature in the sense of the famous experiment by Fermi, Pasta and Ulam [7], namely equipartition of energy over time among the Fourier modes; the rigid travelling wave frame does not permit such an equipartition for localised phase boundaries. Yet, E_{osc} is an energetic contribution that can be shown to give rise to the usual thermomechanical fields, such as heat flux Q (which we call here *radiation flux*). The precise derivation of these quantities can be found elsewhere [8]; however, they are not relevant for the discussion of the kinetic relation. A noteworthy observation, however, is that the kinetic relation depends on the oscillatory energy E_{osc}, and can thus be interpreted as a thermomechanical quantity.

One interpretation of this observation above is that there is no need for a selection criteria to pick the "correct" solution from the given family of kinetic relations. A molecular dynamics simulation would be carried out at some given temperature. As discussed above, it is the travelling wave frame does not allow the inclusion of temperature directly. However, instead of considering a full-fledged thermo-elastic macroscopic model as discussed in [2, 25], we suggest a reasonable approximation. To mimic temperature effects, we choose the intrinsic oscillatory energy E_{osc} such that it has the same value as the thermal energy. Thus the real temperature determines E_{osc} which in turn determines the kinetic relation. This procedure requires solutions which oscillate in front of the interface, to encode the required thermalisation.

We compare this interpretation to the established approach based on the causality principle [16]. The latter extends Sommerfeld's selection for the forced wave equation to moving inhomogeneities. A solution is found with Fourier methods, using a special integration path which can be interpreted as a vanishing viscosity approach. This principle has been employed for the phase transition lattice problem discussed here by Truskinovsky and Vainchtein [23] (similar arguments, here based on the Laplace transform, appear in [5]). The causality principle selects a solution which is asymptotically constant ahead of the interface. In the interpretation given above, this is a phase boundary entering a zero temperature region of the specimen. We remark that this solution is included in the solution family of Theorem 1.

As $\frac{\kappa_0^2}{\alpha}$ is even in c, the entropy inequality $fc \geq 0$ reads

$$- [\![\langle V(\varepsilon)\rangle - V(\langle\varepsilon\rangle)]\!]\, c \geq 0,$$

which can be written in terms of ξ as

$$-\xi \cdot c \geq 0.$$

We note that, as introduced in Theorem 1, the values of ξ are restricted to $|\xi| \le 1$. Observe that the entropy inequality holds if we use our choice in the sign of c to counter the sign of ξ. That is, $c > 0$ for $\xi \le 0$ and $c < 0$ for $\xi \ge 0$. In particular, this implies that in the limit cases $\xi \in \{-1, 1\}$, the travelling wave has to invade the region of asymptotically constant strain (see Figure 1).
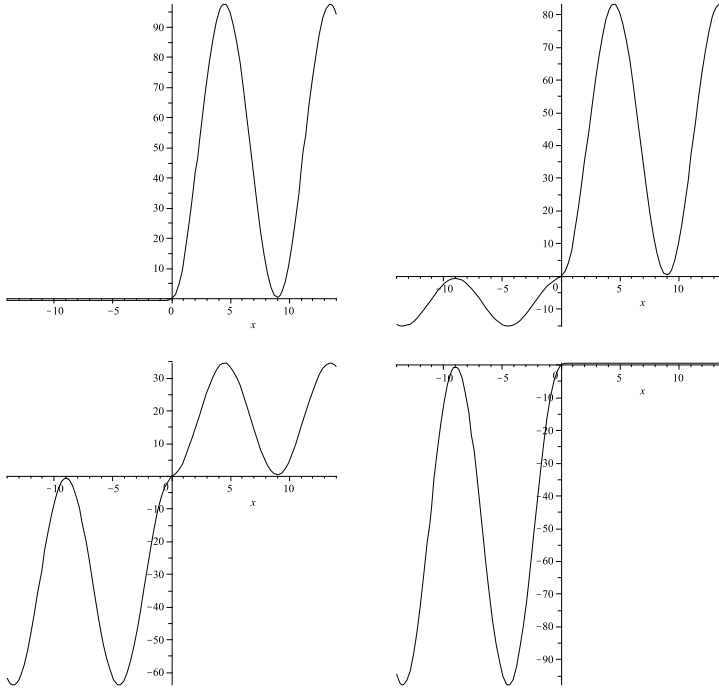

Fig. 1. Numerical approximations to the solution ε for $\kappa_0 = 0.7$ and $\xi = 1$ (top left panel) $\xi = 0.7$ (top right panel), $\xi = -0.3$ (bottom left panel), and $\xi = -1$ (bottom right panel).

5. Qualitative properties of the profile

We refer to Figure 1 to illustrate how the asymmetry of the solution ε depends on the parameter ξ. The plots are numerical approximations of $\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ in the sense that we inverted the explicit representation of $\varepsilon_{\mathrm{cor}}$ in Fourier space numerically. Note in particular that for the bottom right plot ($\xi = -1$), the solution oscillates for negative values of x, whereas it converges rapidly to a constant for positive values of x as $x \to \infty$ (see also Figure 2, bottom right panel). For negative values of x, the gap of 0.5 that appeared in (25) of Lemma 3 is shown in the bottom left panel of Figure 2.
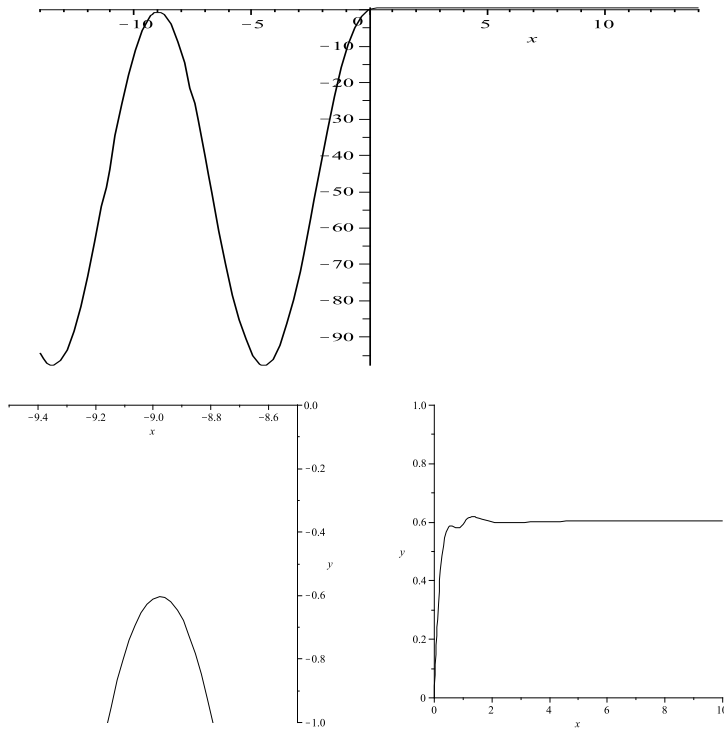
Fig. 2. A numerical approximation to the solution ε for $\kappa_0 = 0.7$ and $\xi = -1$. Top: Graph on $[-20, 20]$. Bottom left panel: Zoom to the first local maximum for negative values of x. Bottom right panel: Graph for $x \geq 0$.

We wish to emphasise that the profile $\varepsilon_{\mathrm{pr}}$ is a good approximation of the solution $\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ for all admissible values of ξ. Since the corrector is independent of ξ (see the proof of Lemma 1), we see from Figure 3 that the corrector is an order of magnitude smaller than the features of the profile function uniformly in ξ.

6. Discussion

We close with a brief outline of open questions. The result presented in this article are only proven for a small range of velocities just below the speed of sound. This restriction is of technical nature; only for this regime the existence of regimes can be proved rigorously. Numerical approximations suggest, however, that the same result holds true for a much larger range of subsonic velocities. However, the picture will change at even lower velocities, though, notably when the dispersion relation has more than one positive real root; there is no rigorous existence theory available at present. There is, however, one nonexistence result stating that in a range of very low
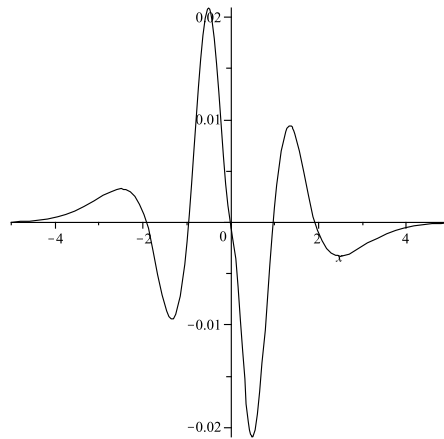
Fig. 3. A numerical approximation of the corrector $\varepsilon_{\mathrm{cor}}$ for $\kappa_0 = 0.7$.

velocities, no travelling waves with a single interface exist for the problem (1) studied here [14].

Another open problem is that of persistence of the findings under perturbations of the potential. Again no systematic and rigorous investigations exist; yet numerical experiments suggest [15] that solutions continue to exist if the cusp of the potential is smoothed; thus one would expect the results presented here to be preserved under this perturbation. An essential assumption, however, is that the wells are harmonic at the asymptotic strain states, and anharmonic lattices may lead to very different behaviour.

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