NONEXISTENCE OF SLOW HETEROCLINIC TRAVELLING WAVES FOR A BISTABLE HAMILTONIAN LATTICE MODEL

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Abstract. The nonexistence of heteroclinic travelling waves in an atomistic model for martensitic phase transitions is the focus of this study. The elastic energy is assumed to be piecewise quadratic, with two wells representing two stable phases. We demonstrate that there is no travelling wave joining bounded strains in the different wells of this potential for a range of wave speeds significantly lower than the speed of sound. We achieve this using a profile-corrector method previously used to show existence of travelling waves for the same model at higher subsonic velocities.

1. Introduction

Is it possible for an elastic solid to exhibit a slow-moving phase boundary? We address this question using a Fermi-Pasta-Ulam (FPU) chain to model the material, which is a one-dimensional bi-infinite chain of identical point unit masses, representing atoms, joined to their nearest neighbours with springs. When modelling phase transitions, the springs typically have a nonconvex stored energy potential with different wells representing the different stable phases. Here we study materials

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Abbreviated Title: Nonexistence of Slow Lattice Waves with two distinct stable phases. This model with piecewise quadratic interactions was studied analytically and numerically by Balk *et al.* [2, 3].

The formulation is as follows. Let $u_j(t) \in \mathbb{R}$ be the displacement of the jth atom with respect to the uniform reference configuration at time $t \in \mathbb{R}$. The discrete strain is defined as $\varepsilon_j := u_j - u_{j-1}$. Denoting the potential function as $V\colon \mathbb{R} \to \mathbb{R}$ and assuming that the evolution of the dynamics is governed by Newton's second law one finds that the equation of motion is

$$u_j''(t) = V'(u_{j+1}(t) - u_j(t)) - V'(u_j(t) - u_{j-1}(t)), \qquad j \in \mathbb{Z}. \tag{1}$$

We say that a travelling wave solution represents a *phase transition* in the material if it has strains in both wells of the potential. Furthermore, a travelling wave representing a phase transition is *heteroclinic* if it asymptotically belongs to different wells. Such phase transitional travelling waves were first studied using Fourier analysis for a FPU chain with piecewise quadratic interaction potential by Truskinovsky and Vainchtein [12]. Schwetlick and Zimmer propose [8] an alternative framework to address the existence of subsonic phase transition waves very close to the speed of sound. Here we show that this framework, although used to prove existence, can be adapted to prove a seemingly contrary proposition, the nonexistence of single transition waves for a slow wave speed regime.

The question of what happens at subsonic wave speeds significantly lower than the speed of sound has, to the best of our knowledge, not been addressed in an analytical framework before. It has been conjectured by Peyrard and Kruskal [7] that travelling waves with low constant wave speeds do not exist for the related Frenkel-Kontorova model on finite domains. Here we show this conjecture is indeed true for the bi-infinite FPU chain as there is no travelling wave joining bounded strains in the different wells of the bilinear potential for wave speeds significantly lower than the speed of sound. Consequently this means that at low subsonic wave speeds there are no phase transitional solutions to the lattice differential equation (1) that makes a single transition between the potential wells. Remarkably, the methods are rather similar to those used to show the opposite result, namely the the existence of travelling waves for very fast subsonic waves [8]. Our result indicates that motion at the low wave speeds considered here may be less coherent than close to the speed of sound; it may be possible that there are travelling wave solutions with multiple interfaces, or solutions that are not of travelling wave type. In conjunction with [8], the result presented here describes a dichotomy: coherent single-interface travelling waves exist for high subsonic velocities but not for low speeds. Such a dichotomy between fast and slow martensitic transformations has been observed experimentally by Förster and Scheil [4] in the 1940's.

2. Mathematical Description

We consider a one-dimensional chain of atoms $\{q_n\}_{n\in\mathbb{Z}} \subset \mathbb{R}$ whose deformations are given as $u_j : \mathbb{R} \to \mathbb{R}$. We have made the assumption that the dynamics can be described by Newton's second law and that the equations of motion are given by (1). The system (1) is Hamiltonian and has the corresponding functional

$$\mathscr{H}[u] := \sum_{j\in\mathbb{Z}} \int_0^1 \left[\tfrac{1}{2}u_j'(t)^2 + V(u_{j+1}(t) - u_j(t))\right] \,\mathrm{d}t.$$

The motion of the phase boundary can be modelled as a travelling wave with strains in both wells of the potential. A solution of (1) is a *travelling wave* if it has the form

$$u_j(t) = u(j - ct), \qquad j \in \mathbb{Z}. \tag{2}$$

With the ansatz (2) the equations of motion (1) reduce to

$$c^2 u''(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)). \tag{3}$$

For the analysis of phase transitions in lattice models it is beneficial to reformulate equation (3) in terms of the *discrete strain*. We define the discrete strain as $\varepsilon(x) := u(x) - u(x-1)$ and specify the potential as a function of ε. In this study we consider the potential previously analysed in [2, 3, 12, 8],

$$V(\varepsilon) := \frac{1}{2} \min\left\{(\varepsilon+1)^2, (\varepsilon-1)^2\right\}. \tag{4}$$

So there are two wells joined at 0 by a cusp and the speed of sound is unity. Having wells at ±1 is immaterial however it is possible to rescale and translate the potential, as demonstrated by Schwetlick and Zimmer in [10], so that the wells are located at 0 and a small positive strain. Furthermore, we define the discrete Laplacian to be

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

Equation (3) can be now reformulated as the *discrete strain equation*

$$c^2 \varepsilon''(x) = \Delta_1 V'(\varepsilon(x)). \tag{5}$$

Given the explicit form of the potential (4) it is easy to check that (5) becomes

$$c^2 \varepsilon''(x) = \Delta_1 \varepsilon(x) - 2\Delta_1 H(\varepsilon(x)), \tag{6}$$

where H is the Heaviside function. Defining the linear operator $L_c := c^2\partial^2 - \Delta_1$ we rewrite (6) as the following nonlinear advance-delay differential equation

$$L_c \varepsilon(x) = -2\Delta_1 H(\varepsilon(x)). \tag{7}$$

We say that a travelling wave satisfies the *sign condition* or has a *single transition* if it satisfies the property

$$x \cdot \varepsilon(x) > 0 \text{ for every } x \neq 0. \tag{SC}$$

Condition (SC) is central to this paper as it implies that there is exactly one phase boundary, located at the origin in the moving frame coordinates.

The aim of this paper is to demonstrate that there exists a range of values for c, whose absolute values are much less than unity, such that there are no single-transition heteroclinic travelling wave solutions to (7).

3. Fourier Analysis and the Dispersion Relation

The Fourier transform of a function $u \colon \mathbb{R} \to \mathbb{R}$ is taken as

$$\mathscr{F}[u](\kappa) := \int_{-\infty}^{\infty} u(x) \exp(-i\kappa x)\, \mathrm{d}x,$$

where this exists. The Fourier sine transform of u is

$$\mathscr{F}_s[u](\kappa) := \sqrt{\frac{2}{\pi}} \int_0^{\infty} \sin(\kappa x) u(x)\, \mathrm{d}x. \tag{8}$$

Note that the relation $\mathscr{F}[u] = -i\mathscr{F}_s[u]$ holds when u is an odd function.

We define the dispersion relation to be the symbol of the linear operator L_c. We determine this through the calculation

$$\mathscr{F}[L_c \varepsilon](\kappa) = D(\kappa) \mathscr{F}[\varepsilon](\kappa),$$

where

$$D(\kappa) := -c^2\kappa^2 + 4\sin^2\left(\tfrac{1}{2}\kappa\right) \tag{9}$$

is the *dispersion relation*. It proves convenient to define the function

$$d(\kappa) := \left(\frac{\sin\left(\frac{1}{2}\kappa\right)}{\frac{1}{2}\kappa} \right)^2 \tag{10}$$

so that we can rewrite the dispersion relation as $D(\kappa) = (d(\kappa) - c^2)\kappa^2$. As a consequence κ is a zero of the dispersion relation if and only if $d(\kappa) = c^2$.

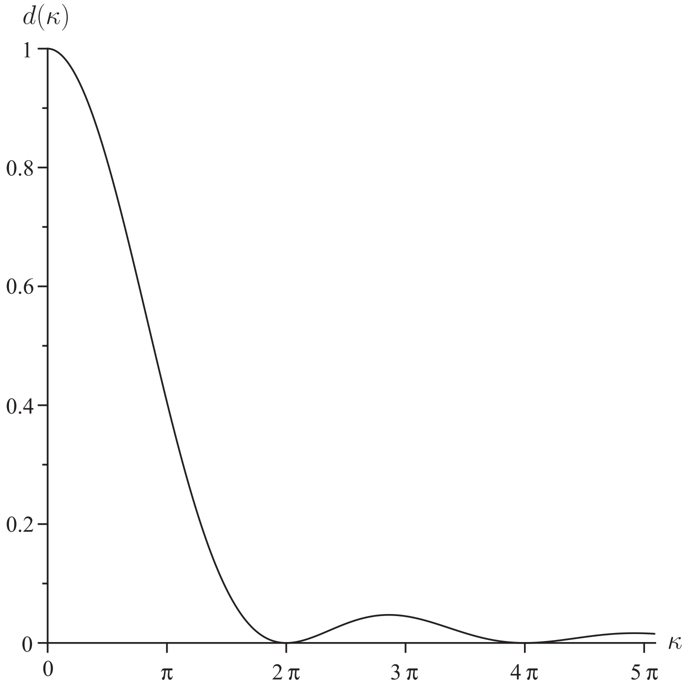

FIGURE 1. Graph of $d(\kappa)$ for $0 \le \kappa \le 5\pi$

In this paper we consider values of c such that the equation $d(\kappa) = c^2$ has precisely three roots. This situation has been studied numerically by Slepyan *et al.* in [11]. Instead of specifying the wave speed directly we prescribe a root of the dispersion relation. This in turn defines the wave speed and the other roots. Let $\hat{\kappa}$ be the value of κ corresponding to the unique maximum of d on $[2\pi, 4\pi]$. Specifically, for $0 < \rho < \frac{1}{2}$, let $\kappa_1 := \hat{\kappa} - \rho$. We interpret κ_1 as a root of the equation $d(\kappa) = c_\rho^2$ for some wave speed c_ρ. Denote the two other roots of this equation κ_0 and κ_2, such that $\kappa_0 < \kappa_1 < \kappa_2$. See Figure 2.

The nonexistence result of this paper can be stated as follows.

Theorem 3.1. *For wave speeds c_ρ^2 with $0 < \rho < \frac{1}{2}$, and V as in* (4)*, there is no travelling wave solving* (3) *that satisfies the single transition property* (SC) *and has bounded strain.*

One can numerically estimate that the range of wave speeds for which Theorem 3.1 holds is $[0.04420, 0.04719]$. Before giving an outline proof we make the following observation. A function $\varepsilon\colon \mathbb{R} \to \mathbb{R}$ satisfies (SC) if and only if

$$f(x) := \Delta_1 H(\varepsilon) = \begin{cases} 1 & \text{for } x \in (-1, 0), \\ -1 & \text{for } x \in (0, 1), \\ 0 & \text{else}. \end{cases} \tag{11}$$

Consequently by assuming the sign condition we may reduce the nonlinear right-hand side of (7) into a function depending just on x and so any solution of (7) satisfying the sign condition (SC) also satisfies the inhomogeneous equation

$$L_c \varepsilon(x) = -2f(x). \tag{12}$$

We note here that since f is piecewise constant and compactly supported it has a Fourier sine transform that can be calculated to be

$$\mathscr{F}_s[f](\kappa) = -\frac{1}{\sqrt{2\pi}} \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{\kappa}. \tag{13}$$

The proof outline is as follows. Assume for contradiction that there exists a solution (1) that satisfies (SC) for the range of wave speeds considered here. The

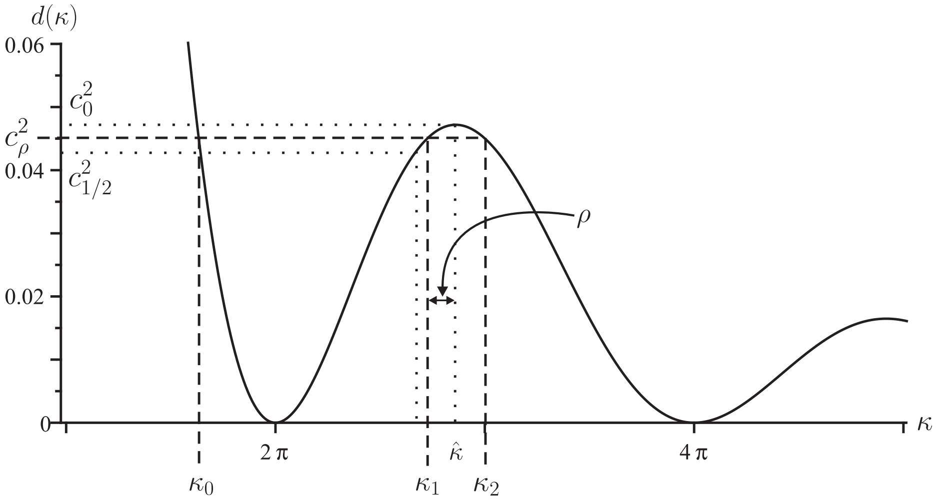

FIGURE 2. Key notation for this paper

first step is to show that equation (12) has a solution under these hypotheses. Secondly we then need to demonstrate that the solution we find violates (SC). In a final step, since the solution we find in the first step is not unique, we demonstrate that any other distributional solution to (12) also fails (SC).

4. PROFILE-CORRECTOR METHOD

The profile-corrector method in [8] works as follows. Define an explicit *profile function*, called $\varepsilon_{\mathrm{pr}}$, that is designed to collect all the singularities in

$$\frac{\mathscr{F}[f](\kappa)}{D(\kappa)}.$$

Then show that $\varepsilon_{\mathrm{pr}}$ satisfies

$$L_c \varepsilon_{\mathrm{pr}}(x) = -2f(x) + \Phi(x), \tag{14}$$

where $\Phi \in L^2(\mathbb{R})$. We then define the *corrector function*, denoted by $\varepsilon_{\mathrm{cor}}$, as the solution to

$$L_c\varepsilon_{\mathrm{cor}}(x) = \Phi(x). \tag{15}$$

Then $\varepsilon := \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ obviously solves (12). We may then demonstrate failure of the sign condition (SC) as follows. First we calculate some points of the profile function where the sign condition is violated. Then we show that the $L^\infty(\mathbb{R})$ norm of $\varepsilon_{\mathrm{cor}}$ is sufficiently small as to not change the sign of ε in the neighbourhood of the points found in the first step.

We define the profile function as follows. Suppose we have selected $\rho \in (0, \frac{1}{2})$ and obtain the wave speed c_ρ and the roots κ_i of $d(\kappa) = c_\rho^2$ for $i = 0, 1, 2$. Let α_i and β_i be real constants for $i = 0, 1, 2$ that we define as

$$\alpha_i := \frac{c_\rho^2\kappa_i^3}{c_\rho^2\kappa_i - \sin(\kappa_i)}, \tag{16}$$

and $\beta_i > 0$ defined to satisfy

$$\gamma_i^2 := \left(1 + \frac{\kappa_i^2}{\beta_i^2}\right)^{-1} := |\alpha_i|\,\frac{c_\rho^2(1-c_\rho^2)}{\kappa_i^2}. \tag{17}$$

We state some useful properties of the α_i and postpone the proof until the auxiliary statements section.

Corollary 1. *For every* $0 < \rho < \frac{1}{2}$ *it follows that* $\alpha_0, \alpha_2 > 0$ *and* $\alpha_1 < 0$.

Adapting the approach of [8] we define the profile as follows. First let us introduce an oscillating part as

$$\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}(x) := \operatorname{sign}(x)\left[\sum_{i=0}^{2}\alpha_i\left(\frac{2\sin^2\left(\frac{1}{2}\kappa_i x\right)}{\kappa_i^2} + \frac{1-\exp(-\beta_i|x|)}{\beta_i^2}\right)\right]. \tag{18}$$

The purpose of $\varepsilon_{\mathrm{pr}}^{\mathrm{osc}}$ is to capture potential oscillating tails of the solution and join them smoothly at the origin. Note that $\varepsilon_{\mathrm{pr}}^{\mathrm{osc}} \in C^2(\mathbb{R})$ for all values of κ_i and β_i, $i = 0, 1, 2$. We then define the jump part of the profile,

$$\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}(x) := \mathrm{sign}(x)\frac{1}{4}|x|^2. \tag{19}$$

The reason we include the jump part of the function in the profile is that when once takes its discrete Laplacian it compensates the jumps that occur in the right-hand side of (12). We are now in a position to define the profile function,

$$\varepsilon_{\mathrm{pr}}(x) := \varepsilon_{\mathrm{pr}}^{\mathrm{osc}}(x) - \frac{2}{c_\rho^2}\Delta_1[\varepsilon_{\mathrm{pr}}^{\mathrm{jump}}](x). \tag{20}$$

As outlined in the introduction to this section, given the profile function defined above we need to show that there exists a function satisfying the corresponding corrector equation.

Lemma 4.1. *The profile function defined in* (20) *gives rise to a* $\Phi \in L^2(\mathbb{R})$ *as defined in* (14)*. Furthermore, given* Φ*,* (15) *has a unique solution in* $L^2(\mathbb{R})$*.*

Proof. We begin by calculating the identity

$$\mathscr{F}_s[L_c\varepsilon_{\mathrm{pr}}](\kappa) = \sqrt{\frac{2}{\pi}}D(\kappa)\left(\sum_{i=0}^{2}\frac{\alpha_i}{\kappa(\kappa_i^2-\kappa^2)}\frac{\beta_i^2+\kappa_i^2}{\beta_i^2+\kappa^2} - \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{\kappa}\frac{1}{c_\rho^2\kappa^2}\right). \tag{21}$$

By (13), (14) and (21) it follows that

$$\begin{aligned}\mathscr{F}_s[\Phi](\kappa) &= \mathscr{F}_s[L_c\varepsilon_{\mathrm{pr}}](\kappa) + 2\mathscr{F}_s[f](\kappa)\\ &= \sqrt{\frac{2}{\pi}}\left\{D(\kappa)\left(\sum_{i=0}^{2}\frac{\alpha_i}{\kappa(\kappa_i^2-\kappa^2)}\frac{\beta_i^2+\kappa_i^2}{\beta_i^2+\kappa^2} - \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{c_\rho^2\kappa^3}\right) - \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{\kappa}\right\}. \qquad (22)\end{aligned}$$

Obviously the only candidates for singularities in the Fourier transform of Φ are $\kappa \in \{0, \kappa_0, \kappa_1, \kappa_2\}$. The singularities are all removable. From these observations we conclude that the Fourier transform of Φ is bounded. Using Parseval's identity we consequently find that $\Phi \in L^2(\mathbb{R})$. It remains to show that, given Φ, (15) has a unique solution in $L^2(\mathbb{R})$. We make the following definitions

$$P(\kappa) := \prod_{j=0}^{2} (\kappa_j^2 - \kappa^2) \text{ and } p_i(\kappa) = \frac{P(\kappa)}{(\kappa_i^2 - \kappa^2)} \text{ for } i = 0, 1, 2.$$

We also define the rescaled variables $\ell_i := \kappa/\kappa_i$. Taking the Fourier transform of (15) we find that

$$\begin{aligned}
\mathscr{F}_s[\varepsilon_{\text{cor}}](\kappa) &= \frac{\mathscr{F}_s[\Phi](\kappa)}{D(\kappa)} \\
&= \sqrt{\frac{2}{\pi}} \left\{ \left(\sum_{i=0}^{2} \frac{\alpha_i}{\kappa(\kappa_i^2 - \kappa^2)} \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{c_\rho^2 \kappa^3} \right) - \frac{4\sin^2\left(\frac{1}{2}\kappa\right)}{\kappa D(\kappa)} \right\} \\
&= \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{\kappa P(\kappa)} \left(\sum_{i=0}^{2} \alpha_i p_i(\kappa) \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{\left(4\sin^2\left(\frac{1}{2}\kappa\right)\right)^2}{c_\rho^2 \kappa^4} \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right) \right\} \\
&= \sqrt{\frac{2}{\pi}} \frac{1}{\kappa P(\kappa)} \left(\sum_{i=0}^{2} \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2(1 - \ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2\sin\left(\frac{1}{2}\kappa\right)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right). \qquad (23)
\end{aligned}$$

As before with the Fourier transform of Φ we see that the only candidates for singularities in (23) are $\kappa \in \{0, \kappa_0, \kappa_1, \kappa_2\}$. Taking the limit $\kappa \to \kappa_i$ for any $i = 0, 1, 2$ and applying L'Hôpitals rule, noting that the range of ρ ensures D has roots of single multiplicity, we find that

$$\lim_{\kappa \to \kappa_i} \left(\sum_{i=0}^{2} \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2(1 - \ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2\sin\left(\frac{1}{2}\kappa\right)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right) = p_i(\kappa_i) \left(\alpha_i - \frac{c_\rho^2 \kappa_i^3}{c_\rho^2 \kappa_i - \sin(\kappa_i)} \right), \qquad (24)$$

which vanishes by the definition of α_i. The function in (24) therefore has a continuous extension at κ_i and in particular the continuous extension has a root at κ_i. Hence $\mathscr{F}_s[\varepsilon_{\text{cor}}]$ is bounded for $\kappa \in \{\kappa_0, \kappa_1, \kappa_2\}$. To show that $\mathscr{F}_s[\varepsilon_{\text{cor}}]$ is bounded as $\kappa \to 0$ we need to apply L'Hôpitals rule twice to find that (23) becomes

$$\sum_{i=0}^{2} \frac{\alpha_i}{\kappa_i^2 \gamma_i^2} - \frac{1}{c_\rho^2(1-c_\rho^2)} = \sum_{i=0}^{2} \frac{\operatorname{sign}(\alpha_i)}{c_\rho^2(1-c_\rho^2)} - \frac{1}{c_\rho^2(1-c_\rho^2)} = 0,$$

again by the choice of β_i and the fact that $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$. We have shown that $\mathscr{F}_s[\varepsilon_{\text{cor}}]$ is bounded at all of the potential singularities and therefore bounded on $\mathbb{R}$. Parseval's identity then gives us the existence and uniqueness of $\varepsilon_{\text{cor}} \in L^2(\mathbb{R})$ satisfying (15). $\square$

The following lemma proves useful when estimating the $L^\infty(\mathbb{R})$ norm of ε_{cor} at arbitrarily large distances from the origin.

Lemma 4.2. *For all $\delta > 0$ the set $\{x : |\varepsilon_{cor}(x)| > \delta\}$ is compact.*

Proof. We have that $\mathscr{F}[\varepsilon'_{\text{cor}}](\kappa) = i\kappa\mathscr{F}[\varepsilon_{\text{cor}}](\kappa) = \kappa\mathscr{F}_s[\varepsilon_{\text{cor}}](\kappa)$ and therefore

$$\mathscr{F}[\varepsilon'_{\text{cor}}](\kappa) = \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{P(\kappa)} \left(\sum_{i=0}^{2} \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2(1-\ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2\sin\left(\frac{1}{2}\kappa\right)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right) \right\}.$$

We can see that the pole at $\kappa = 0$ is removeable and the remaining potential poles are handled by the choice of α_i $i = 0, 1, 2$, as before. Then $\mathscr{F}[\varepsilon'_{\text{cor}}]$ is bounded and therefore by the Plancherel theorem we have that $\varepsilon'_{\text{cor}} \in L^2(\mathbb{R})$. Therefore $\varepsilon_{\text{cor}} \in H^1(\mathbb{R})$ and the result follows by the Sobolev embedding theorem [5, Theorem 8.54]. $\square$

To maintain the flow of the main argument we just state the next two lemmata and remark that their proof can be found in the next section. The first result determines explicitly all solutions to the homogeneous version of (12).

Lemma 4.3. *Let $\varepsilon \in L^\infty(\mathbb{R})$. Then $L_c\varepsilon = 0$ if and only if*

$$\varepsilon \in K := \mathit{span}\left(\{1\} \cup \{\cos(\kappa_i x)\}_{i=0}^2 \cup \{\sin(\kappa_i x)\}_{i=0}^2 \right).$$

Since (12) is an inhomogeneous linear equation, the solution to (12) is only unique modulo K. From this observation it is clear that even if one shows that ε fails the sign condition (SC) then it may still satisfy it if we add a suitable combination of functions from K. Schwetlick and Zimmer show [9] that in addition to the point symmetric wave found in [8], there also exists a family of asymmetric heteroclinic travelling waves for the same range of wave speeds. This is achieved by adding suitable combinations of functions from K and showing that the sign condition (SC) is still satisfied. The next lemma demonstrates that every solution of (12) fails to satisfy the sign condition (SC).

Lemma 4.4. *For $0 < \rho < \frac{1}{2}$ and every $\eta \in K$ there exists a sequence $\{z_n\}_{n=1}^{\infty} \subset \mathbb{R}$ with $|z_n| \to \infty$ as $n \to \infty$ such that either $z_n > 1$ and $\varepsilon_{pr}(z_n) + \eta(z_n) < -\frac{1}{10}$ or $z_n < -1$ and $\varepsilon_{pr}(z_n) + \eta(z_n) > \frac{1}{10}$ for every $n \in \mathbb{N}$.*

We are now in a position to prove the main theorem.

Proof of Theorem 3.1. Fix $0 < \rho < \frac{1}{2}$ and suppose the solution ε to (7) satisfies the sign condition (SC). Then, decomposing $\varepsilon = \varepsilon_{\mathrm{pr}} - \varepsilon_{\mathrm{cor}}$ with $\varepsilon_{\mathrm{pr}}$ as in (20) gives rise to a corrector function $\varepsilon_{\mathrm{cor}}$ by Lemma 4.1. It follows that this is only unique modulo K and find that the general solution to (12) is $\varepsilon + \eta$, $\eta \in K$.

By Lemma 4.2 we have that $|\varepsilon_{\mathrm{cor}}(x)| \to 0$ as $|x| \to \infty$ so there is a $M \in \mathbb{R}$ such that if $|x| > M$ then $|\varepsilon_{\mathrm{cor}}(x)| < \frac{1}{20}$. By Lemma 4.4 there exists a sequence $\{z_n\}_{n=1}^{\infty} \subset \mathbb{R}$ with $|z_n| \to \infty$ as $n \to \infty$ such that either $z_n > 1$ and $\varepsilon_{\mathrm{pr}}(z_n) + \eta(z_n) < -\frac{1}{10}$ or $z_n < -1$ and $\varepsilon_{\mathrm{pr}}(z_n) + \eta(z_n) > \frac{1}{10}$ for each $n \in \mathbb{N}$. Choose N sufficiently large so that $|z_N| > M$. Then either

$$\varepsilon(z_N) < |\varepsilon_{\mathrm{cor}}(z_N)| - \tfrac{1}{10} < -\tfrac{1}{20} \quad \text{if } z_N > 1$$

or

$$\varepsilon(z_N) > -|\varepsilon_{\mathrm{cor}}(z_N)| + \tfrac{1}{10} > \tfrac{1}{20} \quad \text{if } z_N < 1.$$

Therefore for each solution of (12) we can find a point where the sign condition (SC) is not satisfied. This contradicts the assumption that the sign condition holds. □

5. Auxiliary Results

In this section we prove some auxiliary results necessary for the proof of the main theorem.

5.1. **Real Roots of the Dispersion Relation.**

In order to determine the failure of the sign condition (SC) it proves useful to examine the dispersion relation in greater detail. It was mentioned in Section 3 that by setting the parameter $0 < \rho < \frac{1}{2}$ and defining $\kappa_1 := \hat{\kappa} - \rho$ we obtain three roots κ_0, κ_1 and κ_2 of the dispersion relation. This section is dedicated to proving that this is indeed the case. We also determine uniform bounds on the values which the roots could attain and estimates for the corresponding range of wave speeds.

The following lemmata give a rigorous description of what can be seen in Figures 1 and 2. In Lemma 5.1 it is demonstrated that d is monotonic on intervals that contain the roots of the dispersion relation. The existence and uniqueness of $\hat{\kappa}$ is also shown, an important result as we perform the subsequent analysis relative to this quantity. Using this one can compute bounds on important quantities such as the wave speeds for the parameter range (Lemma 5.3) and the values of the additional roots (Lemmata 2 and 5.4). The bounds we compute are essential for determining the sign of the profile in Proposition 1. Furthermore, it is demonstrated that for the parameter range we have exactly three real roots (Lemma 5.2). Once the structure of the roots is rigorously developed we are then able to determine properties of functions evaluated at these roots (Corollaries 1 and 3).

Lemma 5.1. *The function d has a unique maximum, $\hat{\kappa}$, on $(2\pi, 4\pi)$ and d is strictly monotonic decreasing on $(0, 2\pi)$ and $(\hat{\kappa}, 4\pi)$. Furthermore, d is strictly monotonic increasing on $(2\pi, \hat{\kappa})$.*

Proof. Calculating d' one finds,

$$d'(\kappa) = \frac{8}{\kappa^3} \sin^2\left(\tfrac{1}{2}\kappa\right)\left(\tfrac{1}{2}\kappa \cot\left(\tfrac{1}{2}\kappa\right) - 1\right) =: \frac{8}{\kappa^3} \sin^2\left(\tfrac{1}{2}\kappa\right)\psi(\kappa). \tag{25}$$

So obviously the sign of $d'(\kappa)$ equals the sign of $\psi(\kappa)$ for $\kappa > 0$. The function ψ is well defined and continuous on $\mathbb{R}^+ \setminus \{2\pi n\}_{n=0}^{\infty}$. A calculation shows that

$$\psi'(\kappa) = -\frac{1}{2} \cdot \frac{\kappa - \sin(\kappa)}{1 - \cos(\kappa)} < 0 \quad \text{for} \quad \kappa \in \mathbb{R}^+ \setminus \{2\pi n\}_{n=0}^{\infty}. \tag{26}$$

It follows from (26) that ψ is strictly monotonically decreasing on each connected component of its domain. On $(0, 2\pi)$ since ψ is continuous, strictly monotonically decreasing and $\lim_{\kappa \searrow 0} \psi(\kappa) = 0$, $\lim_{\kappa \nearrow 2\pi} \psi(\kappa) = -\infty$ it follows that ψ is negative. Similarly on $(2\pi, 4\pi)$ since ψ is continuous, strictly monotonically decreasing and $\lim_{\kappa \searrow 2\pi} \psi(\kappa) = \infty$, $\lim_{\kappa \nearrow 4\pi} \psi(\kappa) = -\infty$ it follows that there exists a unique point $\hat{\kappa}$ such that $\psi(\hat{\kappa}) = 0$. Furthermore we have that ψ is positive on $(2\pi, \hat{\kappa})$ and negative on $(\hat{\kappa}, 4\pi)$. The monotonicity of d follows as a consequence of (25). □

We now provide a bound for $\hat{\kappa}$ in terms of two constants $\hat{\kappa}^-$ and $\hat{\kappa}^+$.

Corollary 2. *It holds that $\hat{\kappa}^- < \hat{\kappa} < \hat{\kappa}^+$ where $\hat{\kappa}^{\pm} := 8.9868 \pm 10^{-4}$.*

Proof. A calculation demonstrates that $d'\left(\hat{\kappa}^-\right) > 0$ and $d'\left(\hat{\kappa}^+\right) < 0$. So by the uniqueness of $\hat{\kappa}$ on $(2\pi, 4\pi)$ by Lemma 5.1 we have $\hat{\kappa}^- < \hat{\kappa} < \hat{\kappa}^+$. □

Lemma 5.2. *For* $0 < \rho < \frac{1}{2}$ *the equation* $d(\kappa) = c_\rho^2$ *has three solutions in* $(0, \infty)$ *that correspond to simple roots of the equation* $D(\kappa) = 0$.

Proof. Recall that for a fixed wave speed c^2 we have that κ is a root of $D(\kappa) = 0$ if and only if $d(\kappa) = c^2$. By Lemma 5.1 $d((0, 2\pi)) = (0, 1)$, $d((2\pi, \hat{\kappa})) = (0, c_0^2)$ and $d((\hat{\kappa}, 4\pi)) = (0, c_0^2)$, cf. Figures 1 and 2. Note also that d is injective when restricted to $(0, 2\pi)$, $(2\pi, \hat{\kappa})$ and $(\hat{\kappa}, 4\pi)$. Therefore given any $c^2 \in (0, c_0^2)$ it follows that the equation $d(\kappa) = c^2$ has at least three solutions $\kappa_0 \in (0, 2\pi)$, $\kappa_1 \in (2\pi, \hat{\kappa})$ and $\kappa_2 \in (\hat{\kappa}, 4\pi)$. By strict monotonicity on each of $(0, 2\pi)$, $(2\pi, \hat{\kappa})$ and $(\hat{\kappa}, 4\pi)$ it follows that the solutions obtained here correspond to simple roots of $D(\kappa) = 0$.

Recall that $c_\rho^2 := d(\hat{\kappa} - \rho)$. By Lemma 5.1 it follows that c_ρ^2 is strictly monotonically decreasing as a function in ρ. Therefore given any $0 < \rho < \frac{1}{2}$ it follows that $c_\rho^2 \in (c_{1/2}^2, c_0^2)$, cf. Figure 2. Therefore as $(c_{1/2}^2, c_0^2) \subset (0, c_0^2)$ we have three simple roots on $(0, 4\pi]$. We may include the points $\{2\pi, 4\pi\}$ since these just correspond to zeroes of d. It remains to demonstrate that they are the only solutions. Observe that for $\kappa \in (4\pi, \infty)$ it holds that

$$d(\kappa) < (2\pi)^{-2} < d(\hat{\kappa}^- - \tfrac{1}{2}) < c_{1/2}^2.$$

Therefore there cannot exist any solutions to $d(\kappa) = c_\rho^2$ for $0 < \rho < \frac{1}{2}$ on $(4\pi, \infty)$.

□

Lemma 5.3. *Let* $0 < \rho < \frac{1}{2}$. *Then* $c_-^2 < c_\rho^2 < c_+^2$, *where* $c_-^2 := 0.044189$ *and* $c_+^2 := 0.047193$.

Proof. Given any $0 < \rho < \frac{1}{2}$ it follows that $c_\rho^2 \in (c_{1/2}^2, c_0^2)$. By Corollary 2, $\hat{\kappa}^- < \hat{\kappa} < \hat{\kappa}^+$. Recall that $c_0^2 = d(\hat{\kappa})$; in order to bound c_0^2 we bound $d(\kappa)$ on $(\hat{\kappa}^-, \hat{\kappa}^+)$. As $(\hat{\kappa}^-, \hat{\kappa}^+) \subset (2\pi, 3\pi)$ it follows that $\sin\left(\frac{1}{2}\kappa\right)$ is strictly monotonic decreasing therefore $4\sin^2\left(\frac{1}{2}\kappa\right) < 4\sin^2\left(\frac{1}{2}\hat{\kappa}^+\right)$. A numerical comparison yields $d(\kappa) < 4\sin^2\left(\frac{1}{2}\hat{\kappa}^+\right)(\hat{\kappa}^-)^{-2} < c_+^2$ on $(\hat{\kappa}^-, \hat{\kappa}^+)$. In the proof of Lemma 5.2 it was seen that $d(\hat{\kappa}^- - \frac{1}{2}) < c_{1/2}^2$; calculating the lower bound one finds $c_-^2 < c_{1/2}^2$. $\square$

Lemma 5.4. *For* $0 < \rho < \frac{1}{2}$ *we have that* $\kappa_0 \in (5.10, 5.15)$ *and* $\kappa_2 \in (\hat{\kappa}, \hat{\kappa} + 0.52)$.

Proof. Given any $0 < \rho < \frac{1}{2}$ it follows that $c_\rho^2 \in (c_{1/2}^2, c_0^2)$. Using the fact from Lemma 5.1 that d is strictly monotonic decreasing on $(0, 2\pi)$ it holds that $d(5.15) < d(\kappa) < d(5.10)$ for all $\kappa \in (5.10, 5.15)$. A trivial calculation verifies that $d(5.15) < c_-^2 - 10^{-4}$ and $d(5.10) > c_+^2 + 10^{-4}$. Therefore given any $0 < \rho < \frac{1}{2}$ it follows from Lemma 5.3 that $c_\rho^2 \in (d(5.15), d(5.10))$ and therefore the unique root κ_0 as found in Lemma 5.2 is in $(5.10, 5.15)$.

Similarly, using the fact from Lemma 5.1 that d is strictly monotonic decreasing on $(\hat{\kappa}, 4\pi)$ it holds that $d(\hat{\kappa}^+ + 0.52) < d(\kappa) < c_0^2$. A numerical calculation using Corollary 2 shows that, $d(\hat{\kappa}^+ + 0.52) < c_-^2 - 10^{-6}$. Therefore given any $0 < \rho < \frac{1}{2}$ it follows that $c_\rho^2 \in d((\hat{\kappa}, \hat{\kappa} + 0.52))$ and therefore the unique root κ_2 as found in Lemma 5.2 is in $(\hat{\kappa}, \hat{\kappa} + 0.52)$. $\square$

With the properties of ψ and a bound on the locations of the roots of the dispersion relation one has sufficient information to prove Corollary 1.

Proof of Corollary 1. We may rearrange the form of α_i from (16) to obtain

$$\alpha_i = \kappa_i^2\left(\frac{1}{1 - \frac{1}{2}\kappa_i\cot(\frac{1}{2}\kappa_i)}\right) = -\frac{\kappa_i^2}{\psi(\kappa_i)}, \tag{27}$$

where ψ is defined in (25). In the proof of Lemma 5.1 it was demonstrated that $\psi < 0$ on $(0, 2\pi)$ and $(\hat{\kappa}, 4\pi)$. Since by Lemma 5.4 $\kappa_0 \in (0, 2\pi)$ and $\kappa_2 \in (\hat{\kappa}, 4\pi)$ we have $\alpha_0, \alpha_2 > 0$. Similarly $\psi > 0$ on $(2\pi, \hat{\kappa})$ by Lemma 5.4 $\kappa_1 \in (2\pi, \hat{\kappa})$ and we have $\alpha_1 < 0$. $\square$

Corollary 3. *As functions in ρ, α_1/κ_1^2 and α_2/κ_2^2 are strictly monotonic decreasing and increasing respectively.*

Proof. Rearrange (27) to obtain

$$\frac{\alpha_i}{\kappa_i^2} = -\frac{1}{\psi(\kappa_i)}.$$

The result then follows from the properties of ψ derived in Lemma (5.1). □

5.2. **Essentially Bounded Solutions of the Linearised Equation.** The purpose of this subsection is to prove Lemma 4.3. To do this we use tempered distributions. We first recall some basic properties.

Let $\mathscr{S}$ denote the space of complex valued rapidly decreasing test functions on $\mathbb{R}$, that is, functions υ which for all $m, n \in \mathbb{N}_0$ there exists $U_{m,n} \in \mathbb{R}$ such that

$$\left|\kappa^m \upsilon^{(n)}(\kappa)\right| \leq U_{m,n} \tag{28}$$

for all $\kappa \in \mathbb{R}$. We denote by $\mathscr{S}'$ the space of *tempered distributions*, that is, the space of linear sequentially continuous functionals acting on $\mathscr{S}$. Denote by $\langle u, \upsilon\rangle$ the action of $u \in \mathscr{S}'$ on $\upsilon \in \mathscr{S}$. Using tempered distributions one can extend the Fourier transform as a linear mapping $\mathscr{F} : \mathscr{S}' \to \mathscr{S}'$, defined as

$$\langle \mathscr{F}[f], \upsilon\rangle := \langle f, \mathscr{F}[\upsilon]\rangle,$$

which is bijective. A function ψ is a *multiplier* in the space $\mathscr{S}$ if it is in $C^\infty(\mathbb{R})$ and for each $n \in \mathbb{N}_0$ there exists $M_n \in \mathbb{N}_0$ such that

$$\sup_{\kappa\in\mathbb{R}} \left| \frac{\psi^{(n)}(\kappa)}{(1+|\kappa|^2)^{M_n}} \right| < \infty. \tag{29}$$

The space of tempered distributions is closed under multiplication by multipliers in the space $\mathscr{S}$ [13, Section 4.3]. We denote the Dirac delta distribution by δ.

The first lemma provides a decomposition of arbitrary testing functions in $\mathscr{S}$.

Lemma 5.5. *Let* $a_{\pm i} := \pm\kappa_{i-1}$ *for* $i = 1, 2, 3$ *and for convenience set* $a_0 := 0$. *Then* $\eta \in \mathscr{S}$ *has the following unique representation*

$$\eta(\kappa) = \sum_{i=-3}^{3} \eta(a_i)\lambda_i(\kappa) + \eta'(0)\kappa\lambda_0(\kappa) + \chi(\kappa) \tag{30}$$

where $\chi(a_i) = 0$ *for* $i = -3, \ldots, 3$ *and* $\chi'(0) = 0$. *Furthermore* $\lambda_i \in \mathscr{S}$ *for* $i = -3, \ldots, 3$, $\lambda_i(\kappa)$ *has zeroes of at least multiplicity 2 at each* a_j *with* $i \neq j$ *and* $\lambda_i(a_i) = 1$ *and* $\lambda_i^{(m)}(a_i) = 0$ *for* $i = -3, \ldots, 3$ *and* $m = 1, 2$.

Proof. The proof is, *mutatis mutandis*, the same as in [13, Section 7.10, Lemma 2] but given here for the readers convenience. It follows that χ is uniquely determined by the given η, a_i and λ_i. Furthermore $\chi \in \mathscr{S}$ since η and λ_i are. The fact that $\chi(a_i) = 0$ for $i = -3, \ldots, 3$ is determined by evaluating (30) and $\chi'(0) = 0$ follows by differentiating (30). □

It proves useful to know a growth estimate for all derivatives of $1/D(\kappa)$ for κ large enough.

Lemma 5.6. *For each* $n \in \mathbb{N}_0$ *and each* $0 < \rho < \frac{1}{2}$ *there exists a* $P_{n,\rho} \in \mathbb{R}$ *such that*

$$\left| \left(\frac{1}{D(\kappa)} \right)^{(n)} \right| < P_{n,\rho}$$

for all $\kappa \in \mathbb{R} \setminus [-Q_\rho, Q_\rho]$, *where* $Q_\rho := \max\{\kappa_2, 2/c^2\} + 1$.

Proof. Faà di Bruno's formula [6, Theorem 1.3.2] implies

$$\left| \left(\frac{1}{D(\kappa)} \right)^{(n)} \right| \leq \sum_{r=0}^{n} \frac{r!}{|D(\kappa)^{r+1}|} \sum_{j \in W(n,r)} \binom{n}{j_1, \ldots, j_{n-r+1}} \prod_{q=1}^{n-r+1} \left| \frac{D^{(q)}(\kappa)}{q!} \right|^{j_q} \tag{31}$$

for $\kappa \in \mathbb{R} \setminus [-\kappa_2, \kappa_2]$, where

$$W(n,r) := \left\{ j \in \mathbb{N}_0^{n-r+1} : \sum_{i=1}^{n-r+1} j_i = r \text{ and } \sum_{i=1}^{n-r+1} i j_i = n \right\}.$$

Since

$$\begin{aligned} \left| \left(4\sin^2(\tfrac{1}{2}\kappa)\right)^{(n)} \right| &\le 4 \cdot \sum_{\tau=0}^{n} \binom{n}{\tau} \left| \left(\sin(\tfrac{1}{2}\kappa)\right)^{(\tau)} \left(\sin(\tfrac{1}{2}\kappa)\right)^{(n-\tau)} \right| \\ &\le \frac{4}{2^n} \cdot \sum_{\tau=0}^{n} \binom{n}{\tau} = 4 \end{aligned} \tag{32}$$

for all $n \in \mathbb{N}$ and clearly $D^{(n)}(\kappa) = \left(4\sin^2(\tfrac{1}{2}\kappa)\right)^{(n)}$ when $n > 2$, it follows that $\left|D^{(n)}(\kappa)\right| \le 4$ when $n > 2$ for all $\kappa \in \mathbb{R}$. Trivially $|D''(\kappa)| \le 2c^2 + 4$ on $\mathbb{R}$. Define constants

$$C_{n,j,r} := \binom{n}{j_1, \dots, j_{n-r+1}} \prod_{q=2}^{n-r+1} \left(\frac{\|D^{(q)}\|_\infty}{q!} \right)^{j_q};$$

it then follows that

$$\sum_{j \in W(n,r)} \binom{n}{j_1, \dots, j_{n-r+1}} \prod_{q=1}^{n-r+1} \left| \frac{D^{(q)}(\kappa)}{q!} \right|^{j_q} \le \sum_{j \in W(n,r)} C_{n,j,r} \left|D'(\kappa)\right|^{j_1}. \tag{33}$$

The definition of $W(n,r)$ implies that $0 \le j_1 \le r$, therefore the bound in (33) is a polynomial of at most degree r. It is easy to verify that

$$|D(\kappa)| \ge c^2\kappa^2 - 4 \text{ and } |D'(\kappa)| \le 2c^2 |\kappa| + 4 \tag{34}$$

for $\kappa \in \mathbb{R} \setminus \left([-\kappa_2, \kappa_2] \cup [-2/c^2, 2/c^2]\right)$. Hence combining (31), (33) and (34), we conclude

$$\left| \left(\frac{1}{D(\kappa)} \right)^{(n)} \right| \le \sum_{r=0}^{n} \sum_{j \in W(n,r)} r!\, C_{n,j,r} \frac{\left(|\kappa| + \frac{2}{c^2}\right)^{j_1}}{\left(\kappa^2 - \frac{2}{c^2}\right)^{r+1}} \tag{35}$$

for $\kappa \in \mathbb{R} \setminus \left([-\kappa_2, \kappa_2] \cup [-2/c^2, 2/c^2]\right)$. Since the summands in (35) are rational functions whose numerator is of a lower degree then the denominator, we may uniformly bound each summand by $A_{j,r}$ on $\mathbb{R}\setminus[-Q_\rho, Q_\rho]$. The choice of Q_ρ ensures that κ is sufficiently far away from the poles of (35). By setting

$$P_{n,\rho} := \sum_{p=0}^{n} \sum_{j\in W(n,r)} r!\, C_{n,j,r} A_{j,r}$$

it follows that the result holds for $\kappa \in \mathbb{R}\setminus[-Q_\rho, Q_\rho]$. □

We now prove a further technical result enabling us to prove Lemma 4.3. Note that $D(\kappa)$ is even and therefore if κ_i is a root then so is $-\kappa_i$.

Lemma 5.7. *The function D as defined in* (9) *is a multiplier in $\mathscr{S}$. Furthermore, for $0 < \rho < \frac{1}{2}$ and $\phi \in \mathscr{S}'$ it follows that $D\phi = 0$ if and only if*

$$\phi(\kappa) \in \mathit{span}\left(\{\delta(\kappa), \delta'(\kappa)\} \cup \{\delta(\kappa-\kappa_i), \delta(\kappa+\kappa_i)\}_{i=0}^{2}\right).$$

Proof. Obviously $D \in C^\infty(\mathbb{R})$. Observe that (29) holds for D and $n \geq 2$ by setting $M_n := 0$ as was demonstrated in (32). It is clear that (29) holds for $n < 2$ when setting $M_n := 1$. Therefore the dispersion relation D is in $\mathscr{S}$ and the product $D\phi$ is well defined for all $\phi \in \mathscr{S}'$.

The next step is to demonstrate that for $\chi \in \mathscr{S}$ we can write $\chi(\kappa) = D(\kappa)\upsilon(\kappa)$ for all $\kappa \in \mathbb{R}$ with $\upsilon \in \mathscr{S}$ if and only if $\chi(a_i) = 0$ for $i = -3, \ldots, 3$ and $\chi'(0) = 0$, where the a_i are defined in Lemma 5.5. Necessity in this case is clear. Conversely, suppose that $\chi(a_i) = 0$ for $\chi(a_i) = 0$ for $i = -3, \ldots, 3$ and $\chi'(0) = 0$ for some $\chi \in \mathscr{S}$. Set $\upsilon(\kappa) := \chi(\kappa)/D(\kappa)$ and note that υ is smooth away from the zeros of D. Applying Taylor's theorem with integral remainder around the 0 one has

$$\frac{\chi(\kappa)}{D(\kappa)} = \frac{1}{D(\kappa)} \int_0^\kappa (\kappa - t)\chi''(t)\ \mathrm{d}t \tag{36}$$

in a punctured neighbourhood U_0 of 0 which contains no other root of D. The change of variable $t \mapsto \kappa s$ simplifies (36) to

$$\begin{aligned} \frac{1}{D(\kappa)} \int_0^\kappa (\kappa - t)\chi''(t)\, \mathrm{d}t &= \frac{\kappa^2}{D(\kappa)} \int_0^1 (1-s)\chi''(\kappa s)\, \mathrm{d}s \\ &= \frac{1}{f(\kappa)} \int_0^1 (1-s)\chi''(\kappa s)\, \mathrm{d}s. \end{aligned} \tag{37}$$

where f is smooth and nonzero in a neighbourhood V_0 of 0. It is then clear that υ on $U_0 \cap V_0$ has a continuous extension to 0 for all of its derivatives since we can differentiate under the integral in (37). A similar argument shows that υ has a smooth extension at all the zeros of D, therefore $\upsilon \in C^\infty(\mathbb{R})$. To determine the decay of υ, fix $m, n \in \mathbb{N}_0$. Then

$$\begin{aligned} \left|\kappa^m \upsilon^{(n)}(\kappa)\right| &\leq \sum_{r=0}^n \binom{n}{r} \left|\kappa^m \chi^{(r)}(\kappa) \left(D(\kappa)^{-1}\right)^{(n-r)}\right| \\ &\leq \sum_{r=0}^n \binom{n}{r} C_{m,r} P_{n-r,\rho} =: T_{m,n} \end{aligned}$$

on $\mathbb{R} \setminus [-Q_\rho, Q_\rho]$ due to $\chi \in \mathscr{S}$ and Lemma 5.6. By continuity there exists $U_{m,n}$ such that (28) holds on $[-Q_\rho, Q_\rho]$. Therefore each derivative of υ vanishes faster than any power of κ and hence $\upsilon \in \mathscr{S}$.

We are now able to determine the conclusion of the lemma. It is clear that sufficiency holds. Conversely, let $\upsilon \in \mathscr{S}$ be arbitrary. For the dispersion relation $D \in \mathscr{S}$ it holds that

$$\langle D\phi, \upsilon\rangle = \langle \phi, D\upsilon\rangle = 0. \tag{38}$$

Now applying Lemma 5.5 to any $\eta \in \mathscr{S}$ we may write

$$\langle \phi, \eta\rangle = \sum_{i=-3}^{3} \eta(a_i)\langle \phi, \lambda_i(\kappa)\rangle + \eta'(0)\langle \phi, \kappa\lambda_0(\kappa)\rangle + \langle \phi, \chi\rangle$$

for λ_i, a_i and χ as described in Lemma 5.5. Now since $\chi(a_i) = 0$ for $i = -3, \ldots, 3$ and $\chi'(0) = 0$ we use the first part of the proof to write $\chi = Dv$ for $v \in \mathscr{S}$, then by (38) it follows that $\langle \phi, \chi \rangle = 0$. Now defining, $\tilde{a}_i := \langle \phi, \lambda_i \rangle$ for $i = -3, \ldots, 3$ and $\tilde{b} = \langle \phi, \kappa\lambda_i \rangle$ we see that

$$\langle \phi, \eta \rangle = \sum_{i=-3}^{3} \tilde{a}_i \eta(a_i) + \tilde{b}\eta'(0)$$

which implies $\phi(\kappa) \in \operatorname{span}\left(\{\delta(\kappa), \delta'(\kappa)\} \cup \{\delta(\kappa - \kappa_i), \delta(\kappa + \kappa_i)\}_{i=0}^{2} \right)$. ☐

There is now enough information to complete the proof of Lemma 4.3.

Proof of Lemma 4.3. Taking the Fourier transform of the equation for $\varepsilon \in \mathscr{S}'$ we obtain

$$D(\kappa)\mathscr{F}[\varepsilon] = 0.$$

Since $\varepsilon \in \mathscr{S}'$ it follows that $\mathscr{F}[\varepsilon] \in \mathscr{S}'$. It follows by Lemma 5.7 that ε solves $L_c\varepsilon = 0$ in $\mathscr{S}'$ if and only if

$$\mathscr{F}[\varepsilon](\kappa) = \sum_{i=-3}^{3} \tilde{a}_i \delta(\kappa - a_i) + \tilde{b}\delta'(\kappa). \tag{39}$$

It is clear by inversion of the Fourier transform that (39) holds if and only if $\varepsilon \in K \cup \operatorname{span}\{x\}$. Consequently ε solves $L_c\varepsilon = 0$ in $L^\infty(\mathbb{R})$ if and only if $\varepsilon \in K$. ☐

5.3. **Sign Failure of the Profile.** The purpose of this section is to prove Lemma 4.4. Let $0 < \rho < \frac{1}{2}$ and write $K = K_{\text{odd}} + K_{\text{even}}$, where

$$K_{\text{odd}} := \operatorname{span}\left(\{1\} \cup \{\cos(\kappa_i x)\}_{i=0}^{2} \right) \text{ and } K_{\text{even}} := \operatorname{span}\left(\{\sin(\kappa_i x)\}_{i=0}^{2} \right).$$

Furthermore, let $\eta \in K_{\text{odd}}$ be given as, for some $\omega_i \in \mathbb{R}$,

$$\eta(x) = \sum_{i=0}^{2} \omega_i \sin(\kappa_i x). \tag{40}$$

Set

$$R_i := \left(\left(\frac{\alpha_i}{\kappa_i^2}\right)^2 + \omega_i^2\right)^{\frac{1}{2}} \text{ and } \theta_i := \arctan\left(-\frac{\omega_i\kappa_i^2}{\alpha_i}\right) \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}],$$

for notational convenience. Furthermore we defined the averages and differences of κ_i and θ_i $(i = 1, 2)$ as

$$\kappa_\sigma := \frac{\kappa_2 + \kappa_1}{2}, \quad \kappa_\delta := \frac{\kappa_2 - \kappa_1}{2}, \quad \theta_\sigma := \frac{\theta_2 + \theta_1}{2} \quad \text{and} \quad \theta_\delta := \frac{\theta_2 - \theta_1}{2}. \tag{41}$$

Then the following proposition holds.

Proposition 1. *There exists a sequence of points* $\{z_n\}_{n\in\mathbb{N}} \subset (1, \infty)$ *such that* $\varepsilon_{pr}(z_n) + \eta(z_n) < -\frac{1}{10}$ *with* η *as in* (40)*. Furthermore* $z_n \to \infty$ *as* $n \to \infty$*.*

Proof. When $x > 1$ by (20),

$$\begin{aligned}
\varepsilon_{\mathrm{pr}}(x) + \eta(x) &= \sum_{i=0}^{2} \frac{2\alpha_i}{\kappa_i^2}\sin^2\left(\tfrac{1}{2}\kappa_i x\right) + \sum_{i=0}^{2}\frac{\alpha_i}{\beta_i^2}\left(1 - e^{-\beta_i x}\right) - \frac{1}{c_\rho^2} + \eta(x) \\
&\le \sum_{i=0}^{2}\frac{\alpha_i}{\kappa_i^2}\left(1 - \cos(\kappa_i x)\right) + \sum_{i=0}^{2}\frac{\alpha_i}{\beta_i^2} - \frac{1}{c_\rho^2} + \eta(x) \\
&= \sum_{i=0}^{2}\left(\frac{\alpha_i}{\kappa_i^2} + \frac{\alpha_i}{\beta_i^2}\right) - \frac{1}{c_\rho^2} + \sum_{i=0}^{2}\omega_i \sin(\kappa_i x) - \frac{\alpha_i}{\kappa_i^2}\cos(\kappa_i x). \qquad (42)
\end{aligned}$$

An elementary calculation shows that

$$\omega_i \sin(\kappa_i x) - \frac{\alpha_i}{\kappa_i^2}\cos(\kappa_i x) = R_i \cos(\kappa_i x - \theta_i). \tag{43}$$

Substituting (17) and (43) into (42), it follows that

$$\varepsilon_{\mathrm{pr}}(x) + \eta(x) \le \sum_{i=0}^{2}\left(\frac{\alpha_i}{|\alpha_i|\, c_\rho^2(1 - c_\rho^2)}\right) - \frac{1}{c_\rho^2} + \sum_{i=0}^{2} R_i \cos(\kappa_i x - \theta_i),$$

and by Corollary 1, $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$ therefore

$$\varepsilon_{\mathrm{pr}}(x) + \eta(x) \le \frac{1}{1 - c_\rho^2} + \sum_{i=0}^{2} R_i \cos(\kappa_i x - \theta_i). \tag{44}$$

After some further trigonometric manipulation and using the definitions in (41), (44) becomes

$$\begin{aligned}\varepsilon_{\mathrm{pr}}(x)+\eta(x)\leq{}&\frac{1}{1-c_\rho^2}+R_0\cos(\kappa_0 x-\theta_0)\\&+(R_1+R_2)\cos(\kappa_\sigma x-\theta_\sigma)\cos(\kappa_\delta x-\theta_\delta)\\&+(R_1-R_2)\sin(\kappa_\sigma x-\theta_\sigma)\sin(\kappa_\delta x-\theta_\delta).\end{aligned}\tag{45}$$

Suppose for now that there exists a sequence of points $\{z_n\}_{n\in\mathbb{N}}$ where the following holds: $R_0\cos(\kappa_0 z_n-\theta_0)\leq 0$, $\cos(\kappa_\sigma z_n-\theta_\sigma)=1$, and the point z_n is within a distance of $4\pi/\kappa_\sigma$ of a minimum point of $\cos(\kappa_\delta x-\theta_\delta)$. Suppose also that $z_n\to\infty$ as $n\to\infty$. Evaluate (45) at z_n we find that

$$\varepsilon_{\mathrm{pr}}(z_n)+\eta(z_n)\leq\frac{1}{1-c_\rho^2}+(R_1+R_2)\cos(\kappa_\delta z_n-\theta_\delta).\tag{46}$$

The term containing the product of sines vanishes due to the choice of z_m. Using a second order Taylor expansion of $\cos(\kappa_\delta z_n-\theta_\delta)$ around x_n and the fact that $|x_n-z_n|\leq 4\pi/\kappa_\sigma$, we find that

$$\begin{aligned}\varepsilon_{\mathrm{pr}}(z_n)+\eta(z_n)&\leq\frac{1}{1-c_\rho^2}-(R_1+R_2)\left(1-\tfrac{1}{2}(x_n-z_n)^2\right)\\&\leq\frac{1}{1-c_\rho^2}-(R_1+R_2)\left(1-8\pi^2\frac{\kappa_\delta^2}{\kappa_\sigma^2}\right).\end{aligned}\tag{47}$$

Hence we have the failure of the sign condition for z_n with $n\in\mathbb{N}$ if

$$\frac{1}{1-c_\rho^2}-(R_1+R_2)\left(1-8\pi^2\frac{\kappa_\delta^2}{\kappa_\sigma^2}\right)\leq-\frac{1}{10}.$$

Or equivalently,

$$\left(1-8\pi^2\frac{\kappa_\delta^2}{\kappa_\sigma^2}\right)^{-1}\left(\frac{1}{1-c_\rho^2}+\frac{1}{10}\right)\leq R_1+R_2,\tag{48}$$

(note that

$$8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2} < 8\pi^2 \frac{(0.5+0.52)^2}{(2\hat{\kappa}^+ - 0.5)^2} \ll 1$$

by Lemma 5.4). Clearly

$$\left|\frac{\alpha_1}{\kappa_1^2}\right| + \left|\frac{\alpha_2}{\kappa_2^2}\right| \le R_1 + R_2, \tag{49}$$

and a calculation shows that

(50)

$$\left(1 - 8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2}\right)^{-1} \left(\frac{1}{1-c_\rho^2} + \frac{1}{10}\right) \le \left(1 - 8\pi^2 \frac{(0.5+0.52)^2}{(2\hat{\kappa}^+ - 0.5)^2}\right)^{-1} \left(\frac{1}{1-c_{1/2}^2} + \frac{1}{10}\right).$$

Since α_i/κ_i^2 is monotone by Corollary 3, using the explicit bounds in Lemma 5.3 one can bound (49) below and (50) above to verify by numerical comparison that (48) holds.

It remains to show that the sequence $\{z_n\}_{n\in\mathbb{N}}$ exists. Let

$$x_n := \frac{\pi}{\kappa_\delta}(2n+1) + \frac{\theta_\delta}{\kappa_\delta} \text{ and } z_n := \frac{2\pi}{\kappa_\sigma} n + \frac{\theta_\sigma}{\kappa_\sigma}, \text{ for } n \in \mathbb{N}.$$

It is clear that $\cos(\kappa_\delta x_n - \theta_\delta) = -1$ and $\cos(\kappa_\sigma z_n - \theta_\sigma) = 1$ for every n. Now fixing $n \in \mathbb{N}$ it can be seen that since $\cos(\kappa_\sigma x - \theta_\sigma)$ is $2\pi/\kappa_\sigma$-periodic that there exists $m \in \mathbb{N}$ such that $0 \le x_n - z_m < 2\pi/\kappa_\sigma$. See Figure 3 for a diagrammatic explanation of the notation; the solid and dashed intervals at the bottom indicates the intervals where $R_0\cos(\kappa_0 x - \theta_0)$ has a fixed sign and the dashed curve is $(R_1+R_2)\cos(\kappa_\delta x - \theta_\delta)$. Furthermore, it is obvious that $0 \le z_{m+1} - x_n < 2\pi/\kappa_\sigma$ and $2\pi/\kappa_\sigma \le z_{m+2} - x_n < 4\pi/\kappa_\sigma$. It remains to show that there exists an $x \in \{z_m, z_{m+1}, z_{m+2}\}$ such that $R_0\cos(\kappa_0 x - \theta_0) \le 0$.

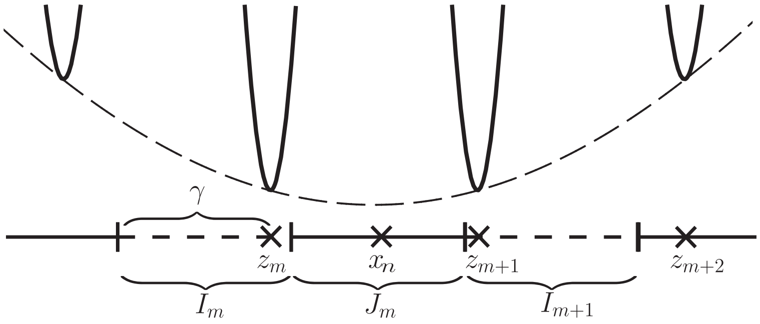

FIGURE 3. The notation used in the proof of Proposition 1

If $R_0\cos(\kappa_0 z_m - \theta_0) \le 0$ then no further work is required. Otherwise one concludes that there exists $p \in \mathbb{N}$ such that

$$z_m = \frac{1}{\kappa_0}\left(\frac{\pi}{2} + \theta_0\right) + \frac{\pi(2p+1)}{\kappa_0} + \gamma,$$

for $\gamma \in (0, \pi/\kappa_0)$. This holds since we can write $(0,\infty) = (\cup_{q\in\mathbb{N}_0} I_q) \cup (\cup_{q\in\mathbb{N}_0} J_q) \cup I$, where

$$I := \left(0, \frac{\pi}{2\kappa_0} + \frac{\theta_0}{\kappa_0}\right), \qquad I_q := \frac{\pi(2q+1)}{\kappa_0} + \frac{\pi}{2\kappa_0} + \frac{\theta_0}{\kappa_0} + \left(0, \frac{\pi}{\kappa_0}\right)$$

and

$$J_q := \frac{2\pi q}{\kappa_0} + \frac{\pi}{2\kappa_0} + \frac{\theta_0}{\kappa_0} + \left[0, \frac{\pi}{\kappa_0}\right].$$

A simple calculation demonstrates that $\cos(x) > 0$ on I_q and $\cos(x) \le 0$ on J_q. Since, by definition,

$$\begin{aligned} z_{m+1} &= z_m + \frac{2\pi}{\kappa_\sigma} \\ &= \frac{1}{\kappa_0}\left(\frac{\pi}{2} + \theta_0\right) + \frac{2\pi(p+1)}{\kappa_0} + \gamma + \frac{2\pi}{\kappa_\sigma} - \frac{\pi}{\kappa_0}, \end{aligned}$$

it follows that $R_0\cos(\kappa_0 z_{m+1} - \theta_0) \le 0$, or equivalently $z_{m+1} \in J_{p+1}$, if

$$0 \le \gamma + \frac{2\pi}{\kappa_\sigma} - \frac{\pi}{\kappa_0} \le \frac{\pi}{\kappa_0}. \tag{51}$$

Since we have explicit bounds for γ, κ_0 and κ_σ from Lemma 5.4 a calculation shows that the lower bound in (51) holds by default. The upper bound is not necessarily satisfied and therefore we can only be sure that $R_0 \cos(\kappa_0 z_{m+1} - \theta_0) \leq 0$ if $\gamma \leq 2\pi/\kappa_0 - 2\pi/\kappa_\sigma$. If we know $\gamma \leq 2\pi/\kappa_0 - 2\pi/\kappa_\sigma$ then we have found the required point, otherwise $2\pi/\kappa_0 - 2\pi/\kappa_\sigma < \gamma < \pi/\kappa_0$, the upper bound arising from the definition of γ. By definition,

$$\begin{aligned} z_{m+2} &= z_m + \frac{4\pi}{\kappa_\sigma} \\ &= \frac{1}{\kappa_0}\left(\frac{\pi}{2} + \theta_0\right) + \frac{2\pi(p+2)}{\kappa_0} + \gamma + \frac{4\pi}{\kappa_\sigma} - \frac{3\pi}{\kappa_0}. \end{aligned}$$

Proceeding as before, we have that it follows that $R_0 \cos(\kappa_0 z_{m+2} - \theta_0) \leq 0$, equivalently $z_{m+2} \in J_{p+2}$, if

$$0 \leq \gamma + \frac{4\pi}{\kappa_\sigma} - \frac{3\pi}{\kappa_0} \leq \frac{\pi}{\kappa_0}. \tag{52}$$

which is equivalent to

$$\frac{3\pi}{\kappa_0} - \frac{4\pi}{\kappa_\sigma} < \gamma < \frac{4\pi}{\kappa_0} - \frac{4\pi}{\kappa_\sigma}. \tag{53}$$

Using Lemma 5.4 and the assumption that $2\pi/\kappa_0 - 2\pi/\kappa_\sigma < \gamma < \pi/\kappa_0$ one can show that (53) holds. What we have demonstrated is that there is at least one point in $\{z_m, z_{m+1}, z_{m+2}\}$ such that $R_0 \cos(\kappa_0 z_{m+i} - \theta_0) \leq 0$. Denote this point as z_n. Furthermore, it is clear that $z_n \to \infty$ as $n \to \infty$ since $x_n \to \infty$ as $n \to \infty$. $\square$

We are now in a position to prove Lemma 4.4. The idea is simple, we know that the profile is odd and that by adding any odd kernel function we have a bi-infinite sequence of points, symmetric with respect to the origin, such that the sign condition (SC) fails. All we now have to do is account for adding an arbitrary function from K, in particular we need to account for when a function from K possesses a component from K_{even}.

Proof of Lemma 4.4. Let $\eta \in K$ and write $\eta = \eta_{\text{odd}} + \eta_{\text{even}}$ where $\eta_{\text{odd}} \in K_{\text{odd}}$ and $\eta_{\text{even}} \in K_{\text{even}}$. By Proposition 1 there exists a sequence of points $\{z_n\}_{n\in\mathbb{N}} \subset (1, \infty)$ such that $\varepsilon_{\text{pr}}(z_n) + \eta_{\text{odd}}(z_n) < -\frac{1}{10}$. Furthermore $z_n \to \infty$ as $n \to \infty$. By the point symmetry of $\varepsilon_{\text{pr}} + \eta_{\text{odd}}$ it follows that $\varepsilon_{\text{pr}}(-z_n) + \eta_{\text{odd}}(-z_n) > \frac{1}{10}$. Now consider $\varepsilon_{\text{pr}} + \eta$ and suppose that when we evaluate this at z_n we have that $\varepsilon_{\text{pr}}(z_n) + \eta(z_n) > 0$, then $\eta_{\text{even}}(z_n) > \frac{1}{10}$ and therefore $\varepsilon_{\text{pr}}(-z_n) + \eta(-z_n) > \frac{1}{5}$. Similarly if $\varepsilon_{\text{pr}}(-z_n) + \eta(-z_n) < 0$, then $\varepsilon_{\text{pr}}(z_n) + \eta(z_n) < -\frac{1}{5}$. This demonstrates that for each n either z_n or $-z_n$ fails a sign condition we select the sequence of points that fails the sign condition and call this $\{z_n\}_{n\in\mathbb{N}}$. □

6. Discussion

Here we have demonstrated that at wave speeds much less than the speed of sound, there are no travelling wave solutions that have bounded strain making a single transition between harmonic potential wells. In particular, we have shown that the solutions obtained in [8, 9] do not exist for the chosen significantly lower wave speeds. This confirms that for this model, the conjecture by Peyrard and Kruskal in [7] holds true and falls in line with the experimental observations of Förster and Scheil [4].

The main feature of the proof is that when the wave speed is low enough one can have two roots that become arbitrarily close together; then the contributions from the kernel function resonate, causing the failure of the sign condition. By studying the profile function numerically for wave speeds corresponding to more than three roots we observe that this behaviour persists. One can even show that

Lemmata 4.1, 4.2 and 4.3 hold when $D(\kappa)$ has an arbitrary number of roots, with obvious modifications. The key difficulty to determining a rigorous proof for lower wave speeds is showing the equivalent of Lemma 4.4, due to the lack of information regarding the commensurability of the roots of the dispersion relation. Specifically, should one be able to prove that the set of positive roots to the dispersion relation is linearly independent over the integers then one can prove an analogue of 4.4 using Kronecker's Theorem for simultaneous Diophantine approximation [1, Sections 7.4 and 7.5].

It may be possible that a certain combination of kernel functions, once added to a generalised version of the corresponding profile function, cancel the resonances generated and enable the existence of a single interface travelling wave solution. We expect, however, for wave speeds close to those corresponding to a double zero of the dispersion relation that this is not the case, as we have seen here. Should one be able to prove this then one would find that there exists a sequence of intervals converging to 0 such that the same type of nonexistence result we obtain holds.

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